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Automated Design of HED Experiments on the Z Machine: a Metrics-Based Approach

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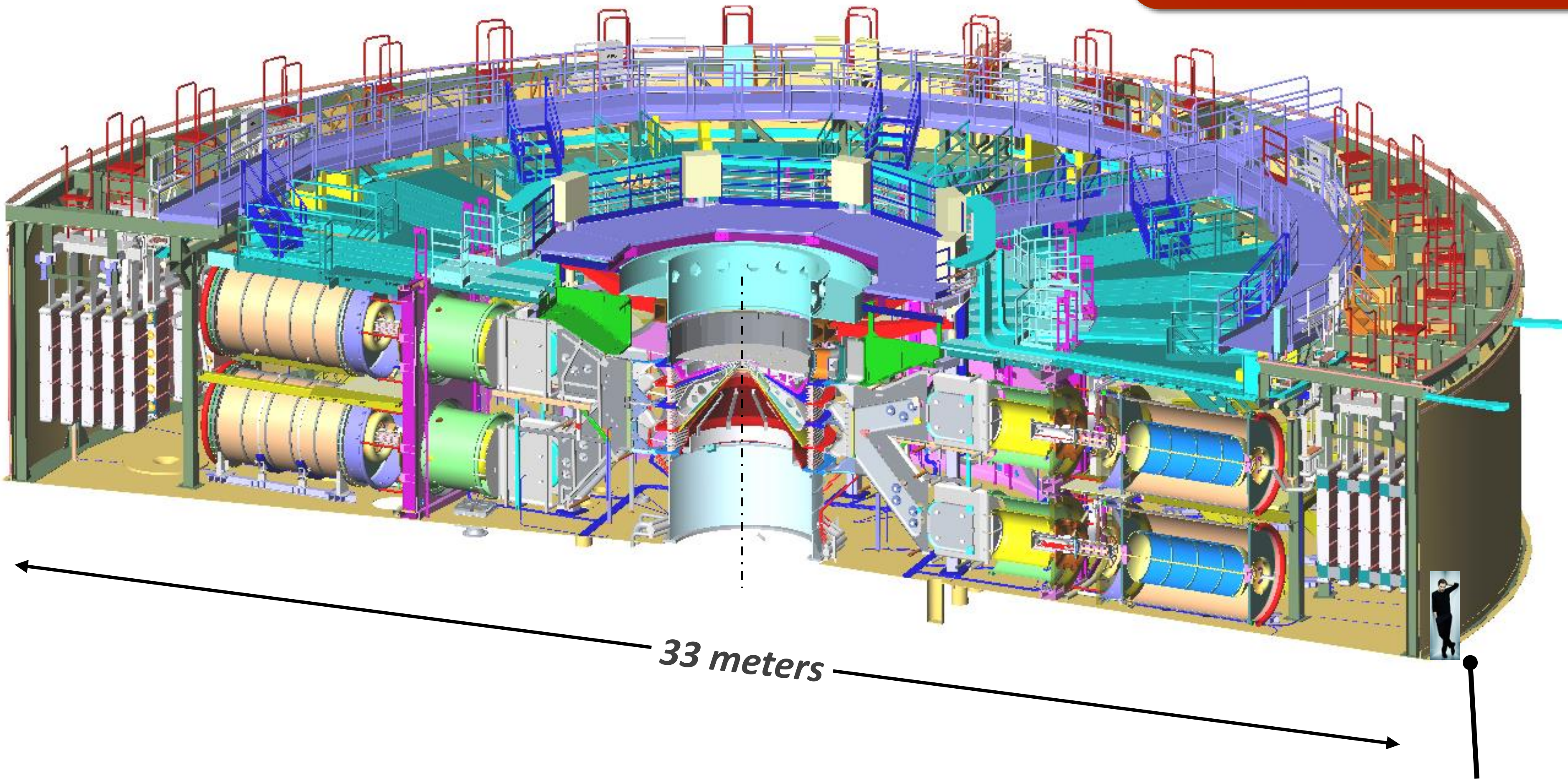
Z Machine at Sandia

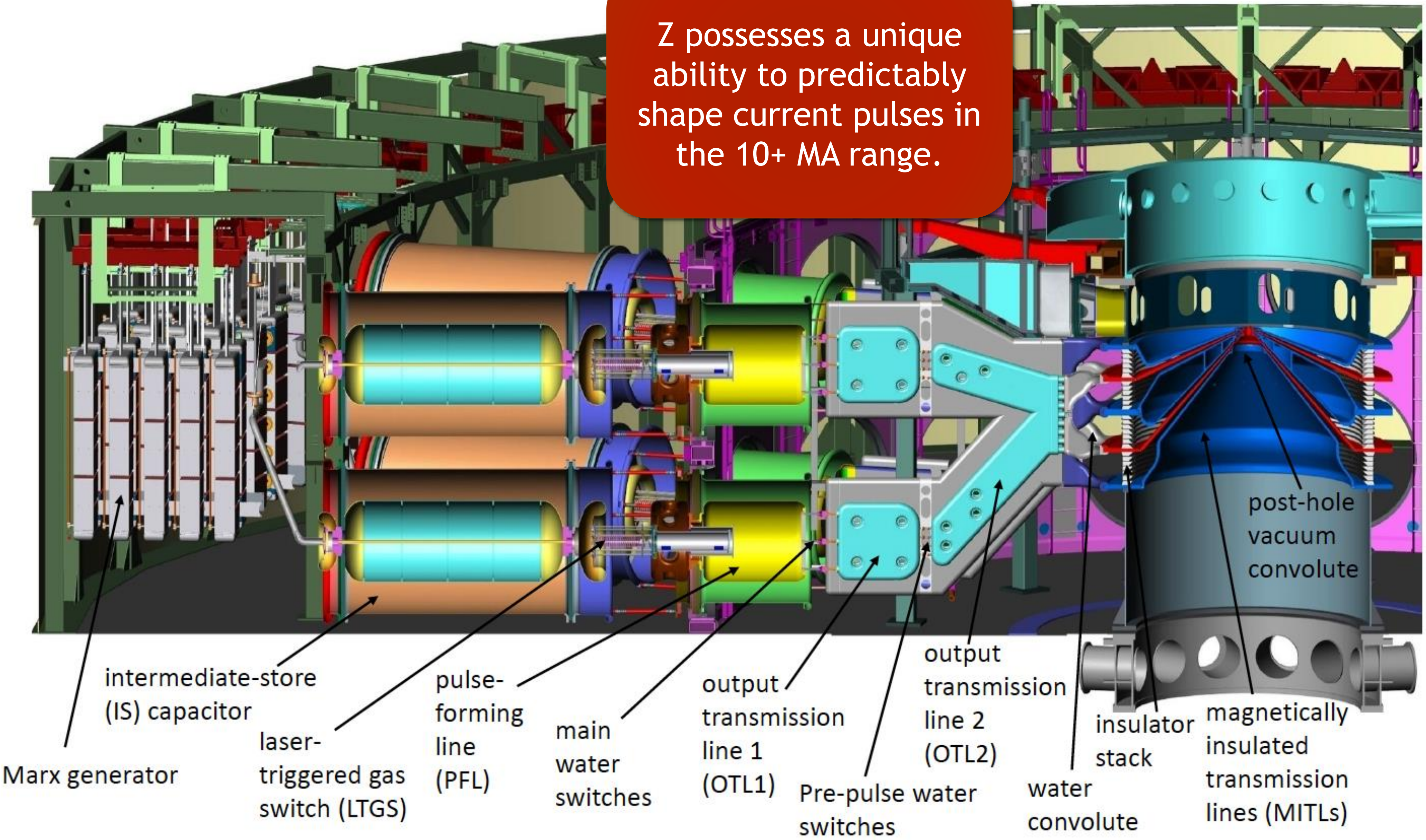
The Z Machine compresses energy spatially and temporally



Cumberbatch
for scale

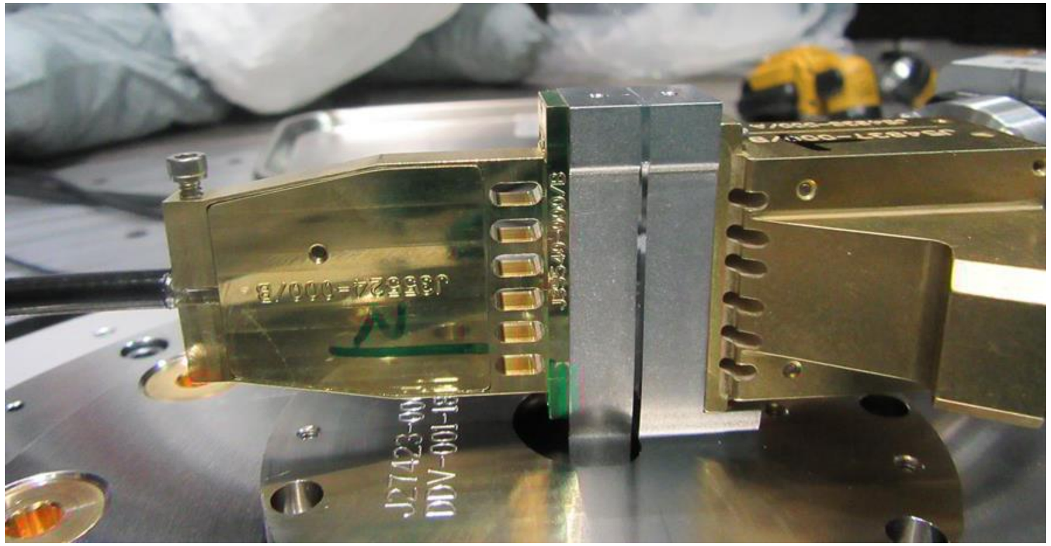
Pulse Forming Capabilities

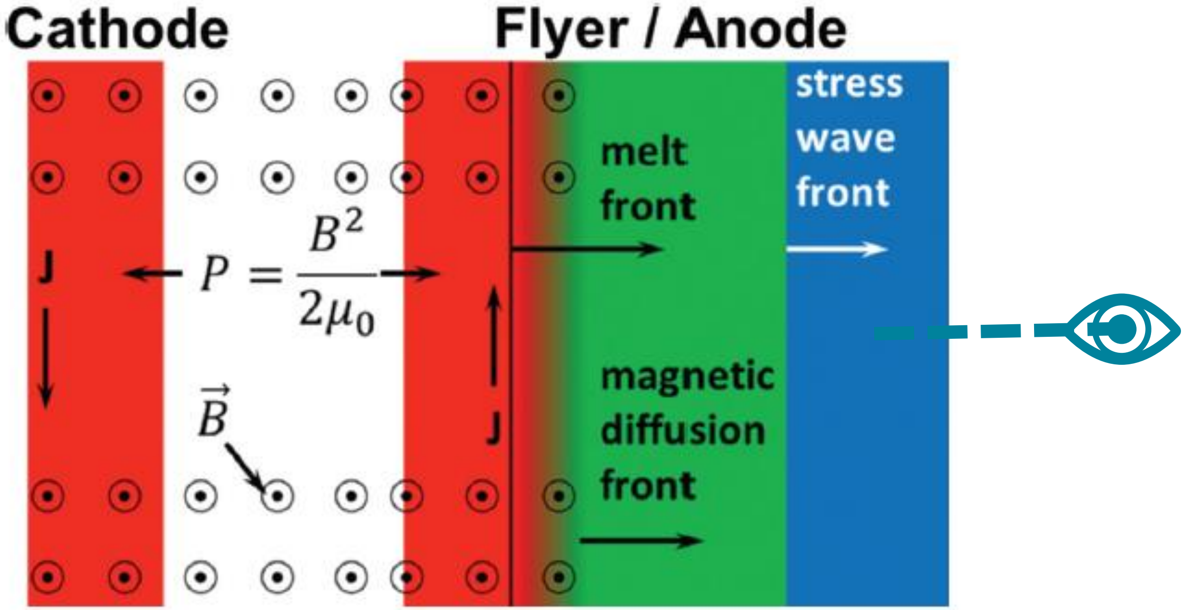
Z possesses a unique ability to predictably shape current pulses in the 10+ MA range.



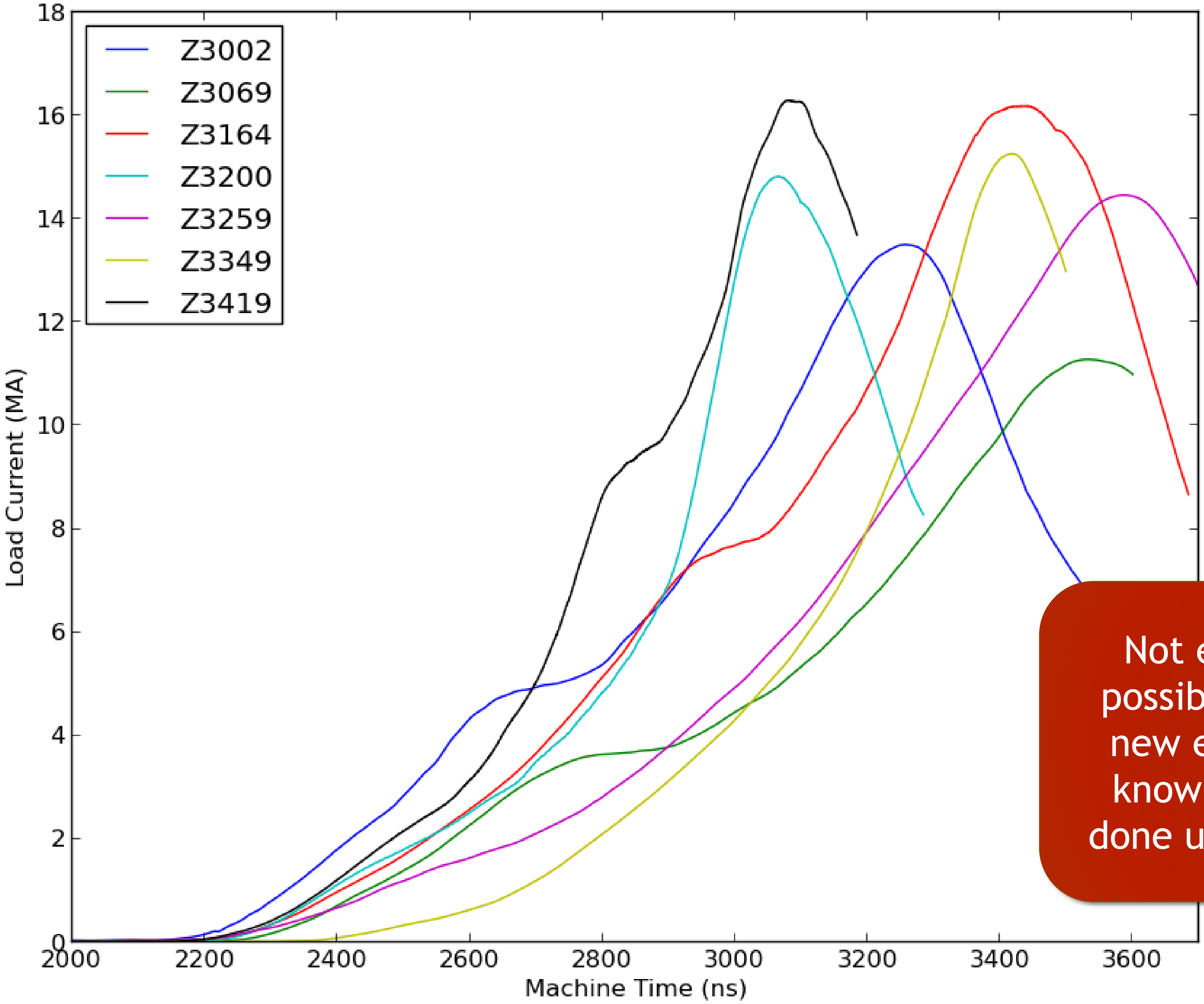
Compression to HED states using magnetic fields

- Z Machine can deliver a carefully shaped current pulse to a magnetically symmetric load that allows for compression to HED conditions.
- This current induces magnetic fields which propel the sample to high compression ratios.
- Shock-ramp: a controlled shock is produced (to melt the sample) and then the sample is ramp compressed to a higher pressure state.





Example pulse shapes -- much is possible!



Not every pulse shape is possible. When designing a new experiment we don't know if something can be done until the design exists.

Defining an experiment

NOW

- Labor intensive manual shot design with no inherent uncertainty quantification, numerical optimization, or probability sampling.
- Single bespoke design created.

Near Future

- Metrics defined and weighed for experiment success
  - Shockless compression
  - Peak sample input pressure
  - Smooth velocity gradient (surrogate for jitter)
  - Magnitude and uniformity of initial shock
  - Ability to differentiate between different material models (maximize difference in velocity response between models)
- Uncertainty and probability sampling possible.

Large parameter space just from Z

Variable	Number on Z	Parameter Space
Basis time shift	36	-250 to 600 ns (5 ns increments)
Basis pulse shape	36	7 options
Marx charge	1	55-85 Volts, 5 Volt increments
Marx triggering delay	9	Boolean
Marx triggering delay time	1	0 to 500 ns (5 ns increments)

Parameter space consists of more than 80 discrete variables that are manually adjusted with expert insight.

This does not include any parameters modified at the target (sample thickness, etc.)

Code Workflow

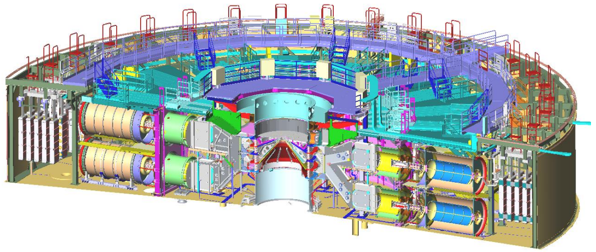
Dakota-MAD
- Calculate present response based on metric weights and aspirational targets
- Choose new input parameters or quit

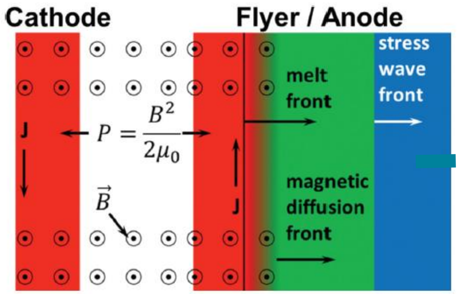
Z Circuit Model
- Produce current vs time waveform

1D MHD
- Drive panel/sample configuration
- Generate metric-relevant data

Python Wrapper
- Calculate resulting metrics
- Feed data to Dakota-MAD

```
shockthresh 80.
steptime 2.
minpeak 200.
allowableshocks 1
shockacceleration 1000.
targetshock 120.
targetdrift 2.
targetpeakp 1100.
smoothscale 1.e3
windowshockvelocity 2300.
```



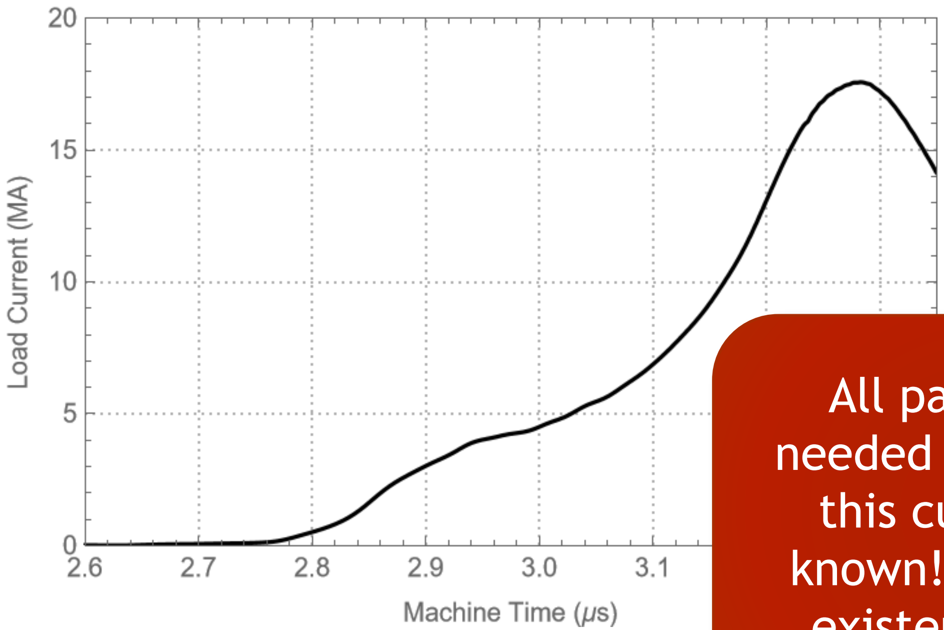



```
0.000000000000e+00 1.221220000000e+02
1.000000000000e+00 4.788000000000e+00
2.000000000000e+00 9.774890000000e+02
3.000000000000e+00 5.031986737500e+03
4.000000000000e+00 6.409878858834e-09
```

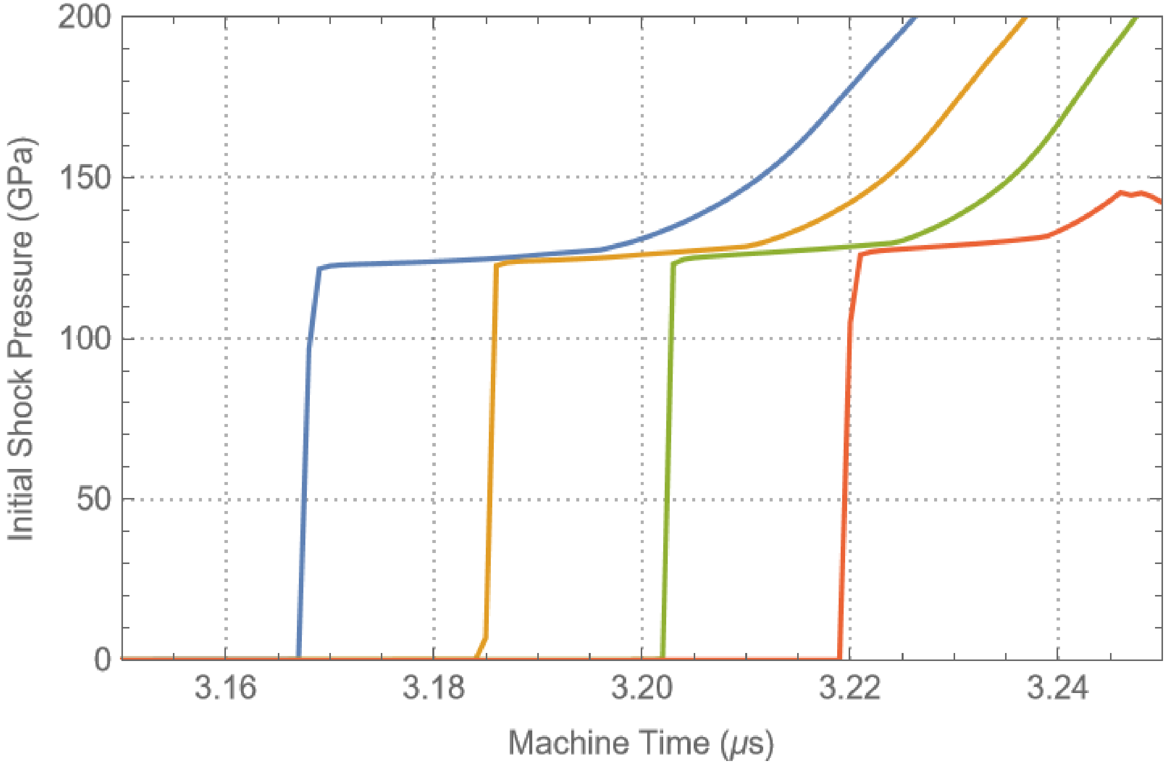
Sandia optimization code **Dakota** used with a mesh adaptive search algorithm to drive scripted workflow.
Rather than *one* bespoke design, *thousands* are generated and the “best” is identified automatically.

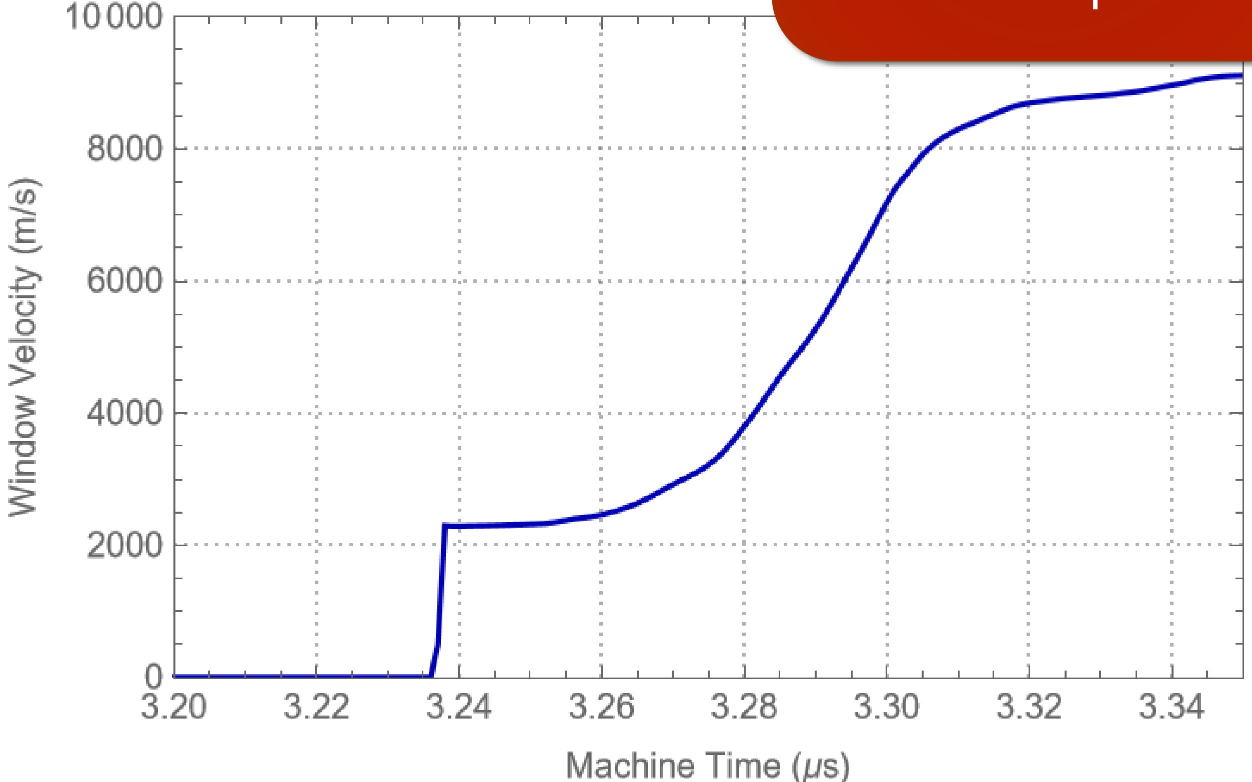
Initial test response

- Shock-ramp experiment, 5 metrics needed
  - Initial shock strength (0.10) **122/120 GPa**
  - Initial shock drift (0.10) **4.79/2.00 GPa**
  - Peak sample input pressure (0.74) **977/1100 GPa**
  - Velocity “smoothness” (0.01) *norm to O(1)*
  - Shock strength in window material (0.05) *bathtub*



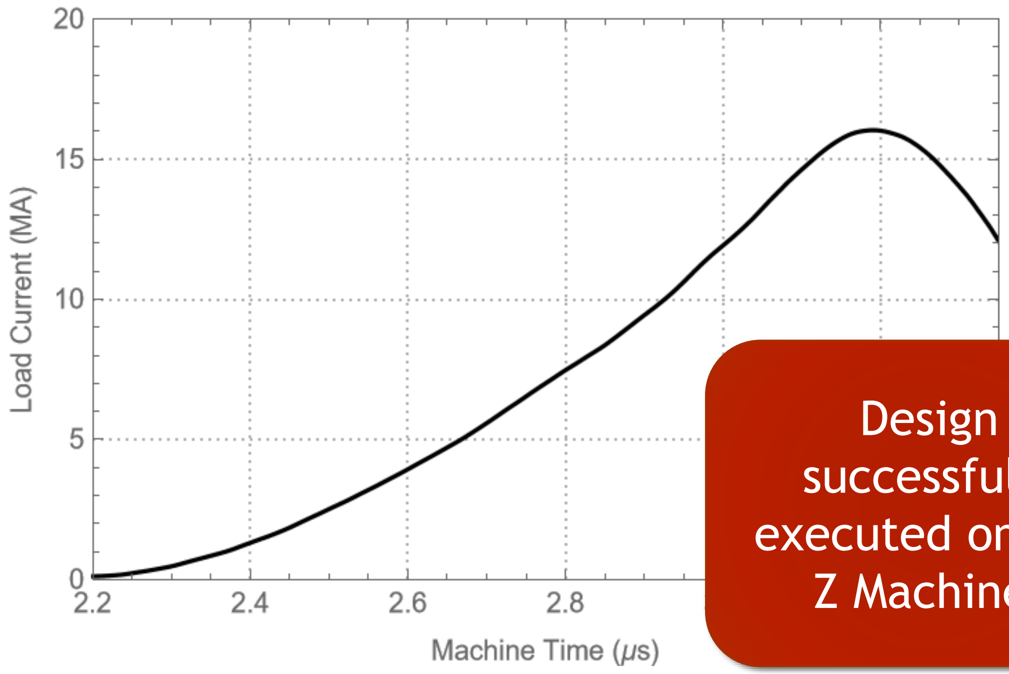
All parameters needed to generate this current are known! Eliminates existence proof!



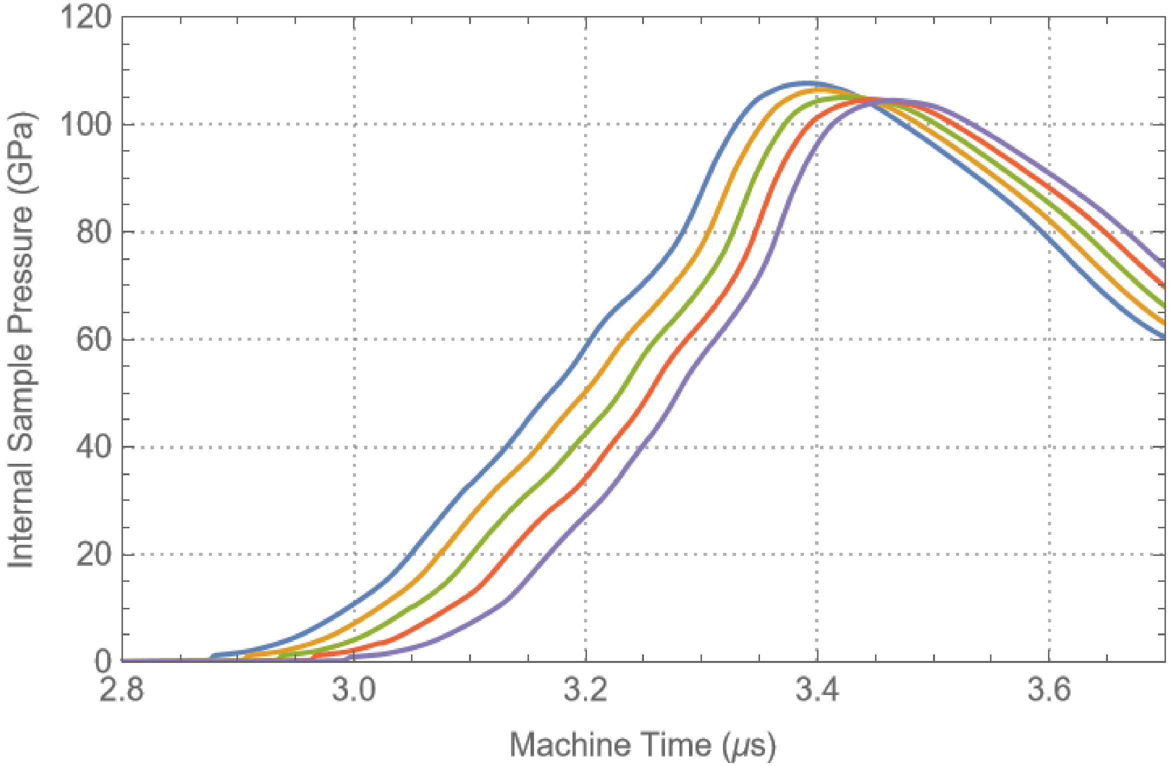


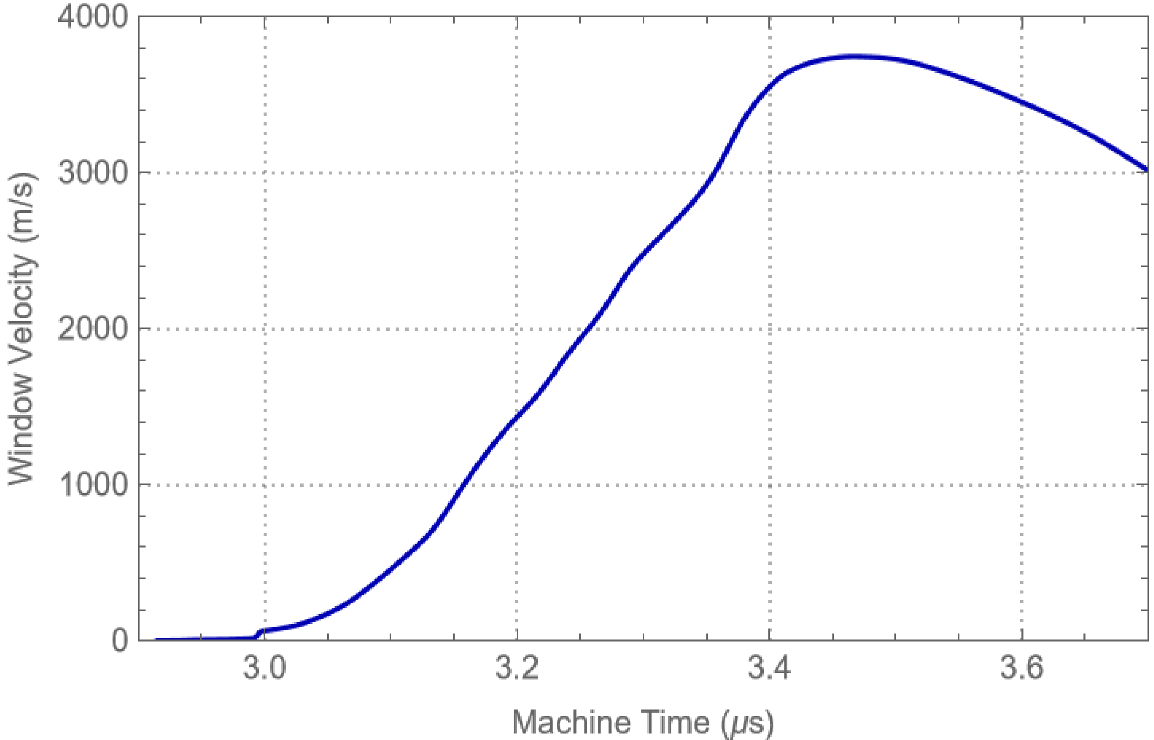
First experiment design by algorithm

- Ramp experiment, only 2 metrics needed
  - Peak sample input pressure (0.5) **91/180 GPa**
    - Target peak pressure set unobtainably high for this material to push optimizer to maximize pressure
  - Velocity "smoothness" (0.5) *norm to O(1)*
    - Note velocity & pressure "smoothness", since EOS was uncertain this minimizes the chances of forming a shock



Design successfully executed on the Z Machine!





"Advanced" metrics under consideration

- **Design an experiment to discriminate between two competing models**
  - For each design iteration, run 2+ MHD simulations, one for each model (EOS, Strength, etc.)
  - Calculate a new metric that will maximize the difference in velocity response for each model (perhaps a specific loading path triggers measurable differences between the models)
- **Sample dimensions can be optimized to aid other metrics**
  - Thickness and even panel width can be optimized to reach the highest possible peak pressure with minimal risk of inadvertent shock formation
  - Without the optimizer this is essentially designing multiple experiments at the same time
- **Pulse shaping "best practices"**
  - Research in ongoing to develop a list of "best practices" for pulse shaping that minimizes damage to the Z Machine; once imposed those metrics can be coded into the algorithm
  - Some of these metrics are not human intuitive and require additional software models to assess; those models can be run inline with the optimizer

Conclusion and Future Work

- This framework represents an exciting new capability for metric-based experimental optimization for HEDP applications.
- The initial implementation is cumbersome to initiate but robust and flexible.
- The optimization method (mesh adaptive search) can be replaced in the scripted framework with little effort. There is interest in exploring Bayesian options.
- This tool is being applied to experiments that are problematic do design due to the ease of unintentional shock creation.

Reach out:

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Abstract

We present a numerical optimization framework for automated design of high energy density (HED) materials science experiments on the Z Machine at Sandia National Laboratories. High energy density dynamic compression experiments in the 100s of GPa regime can only be performed on a limited number of experimental facilities, often requiring bespoke designs tailored to the individual objectives of the experiment. Through rigorous definition of traditional experimental objectives (peak pressure, shockless compression paths, etc.) we have developed a metric-based optimization method that computationally designs the experiment end-to-end, starting with the driver (Z Machine) input conditions. The system also allows for the incorporation of metrics less intuitively obvious to a human designer that can increase experimental objective success within known shot-to-shot driver variability. Initial results using this method will be presented, along with a discussion of advanced metrics under investigation, including the ability to optimize the difference between the observable response of various material models to design experiments to discriminate between theories.