



# ANS Winter Meeting & Expo

## 2018      Joining Forces to Advance Nuclear



# Computational Optimization of TEX Critical Experiment Design

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Catherine Percher, and David Heinrichs

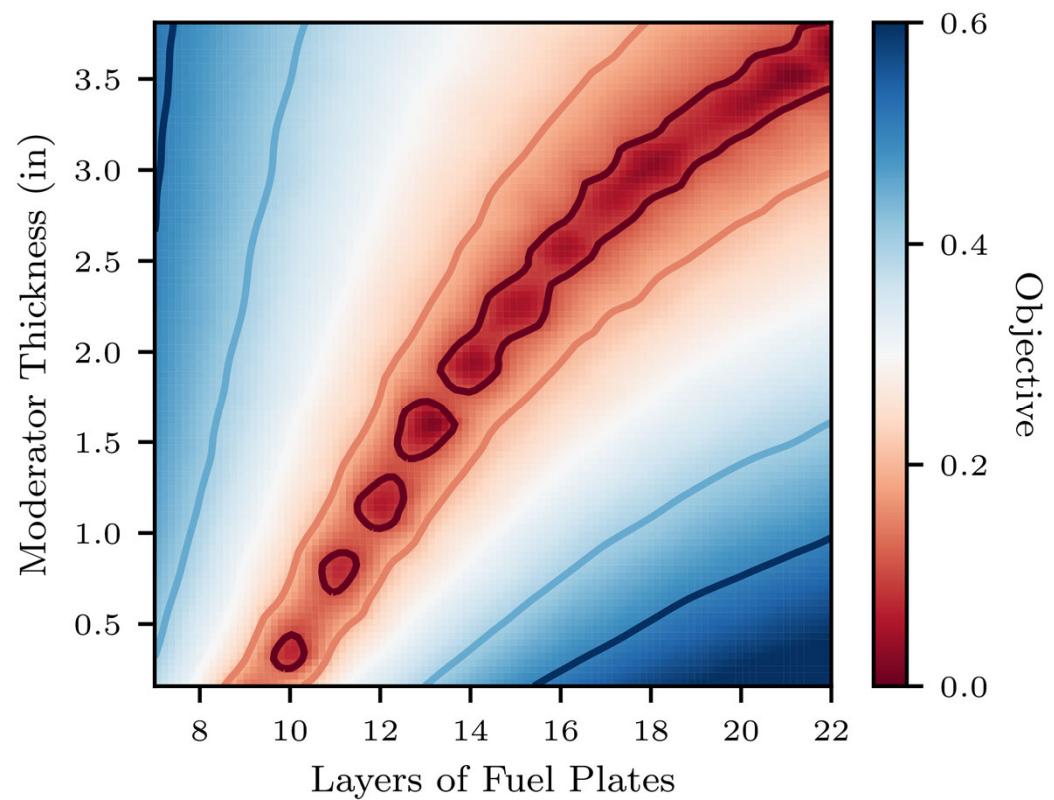
Lawrence Livermore National Laboratory



LLNL-PRES-761298

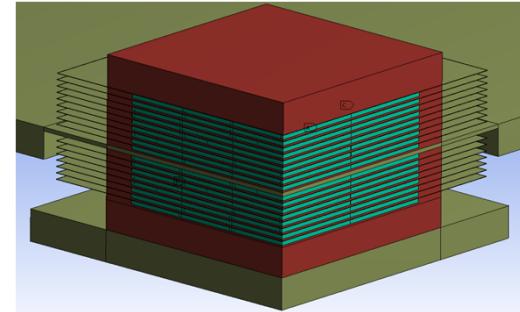
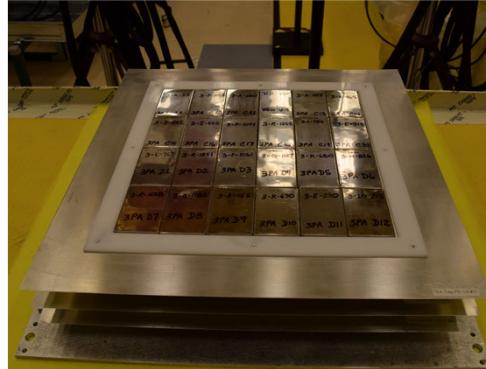
# Outline

- Thermal/Epithermal eXperiments
- $^{239}\text{Pu}/\text{Alumina}$  &  $^{233}\text{U}/\text{Polyethylene}$  TEX
- Optimus for Experiment Design
- Critical Configuration Results

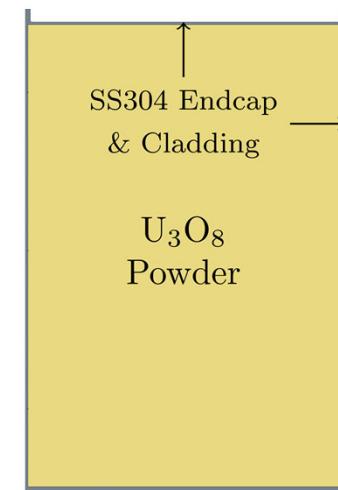
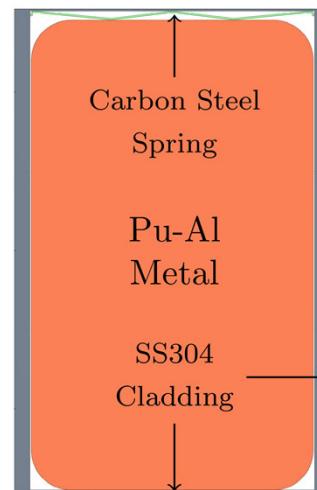
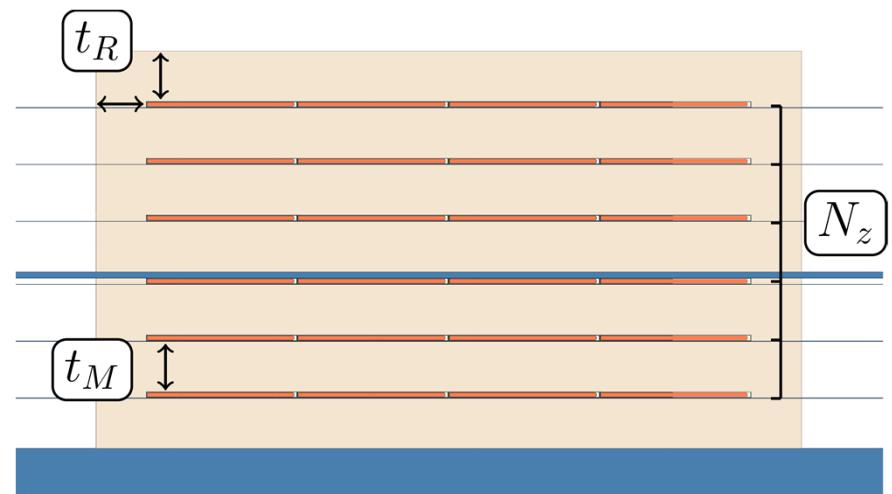
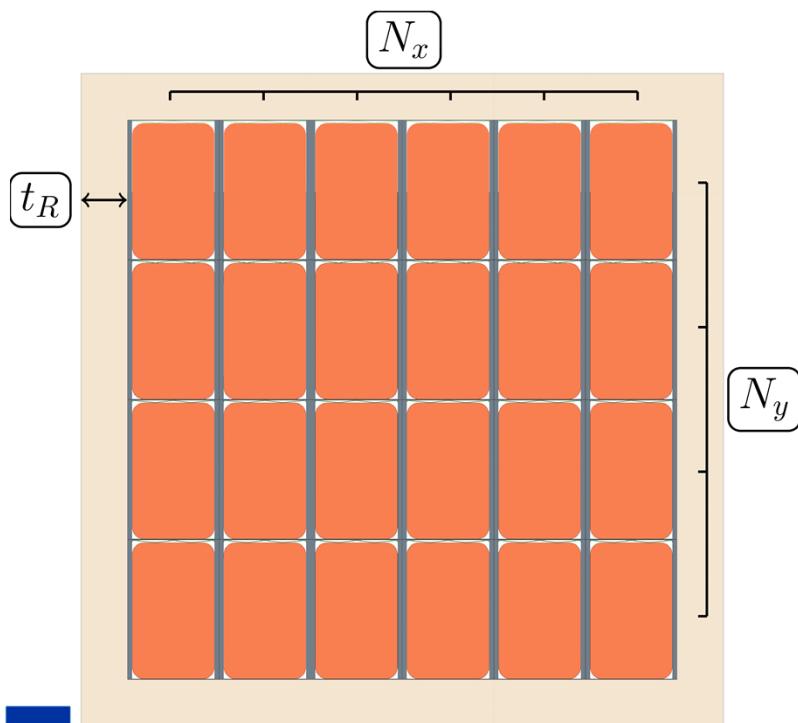


# Thermal/Epithermal eXperiments (TEX)

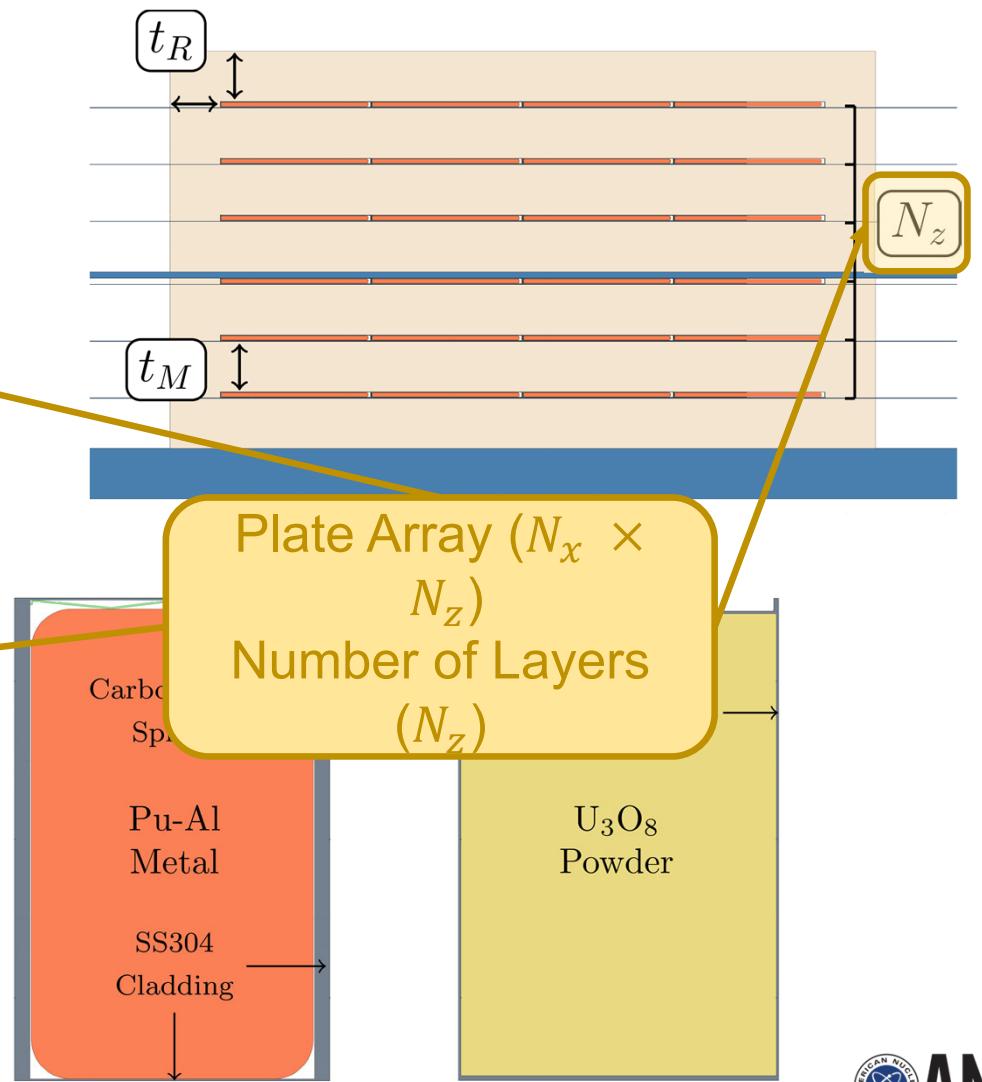
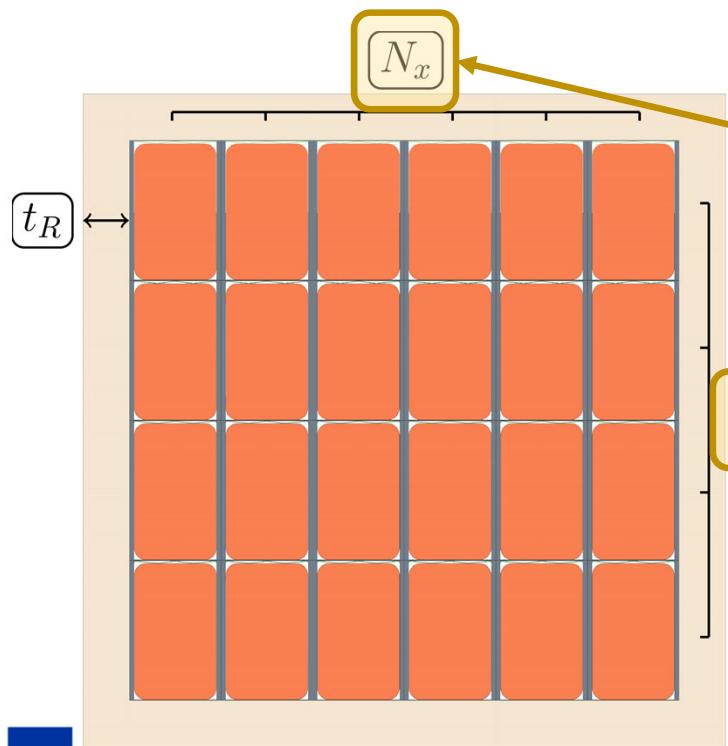
- Design and execute new critical experiments to address high priority nuclear data needs with an emphasis on the intermediate energy range
  - $0.625 \text{ eV} < E < 100 \text{ keV}$
- IER-184 TEX preliminary design using  $^{239}\text{Pu}$  and Polyethylene
- IER-329 using  $^{233}\text{U}$  and Polyethylene



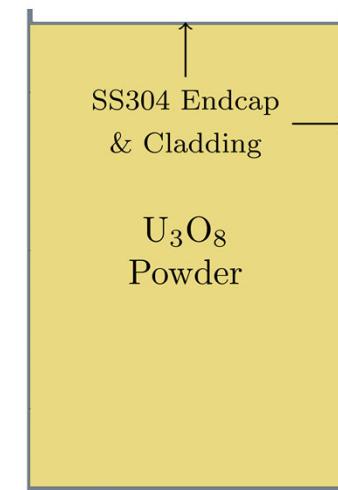
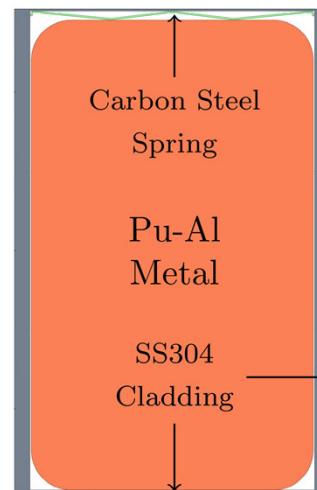
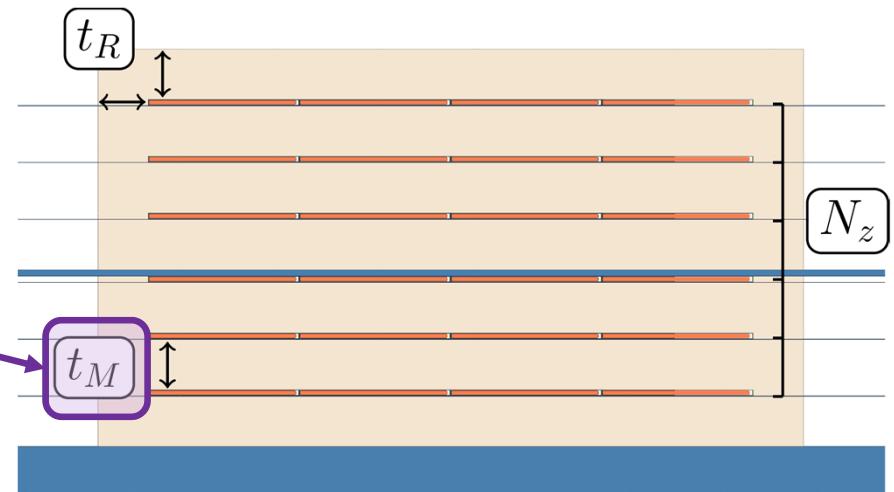
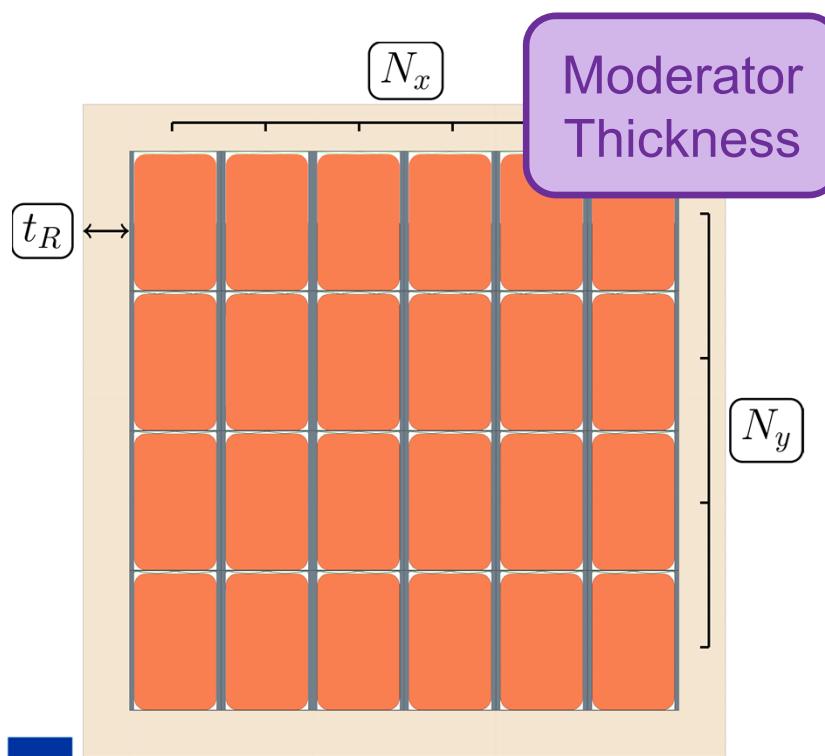
# TEX Configuration & Model



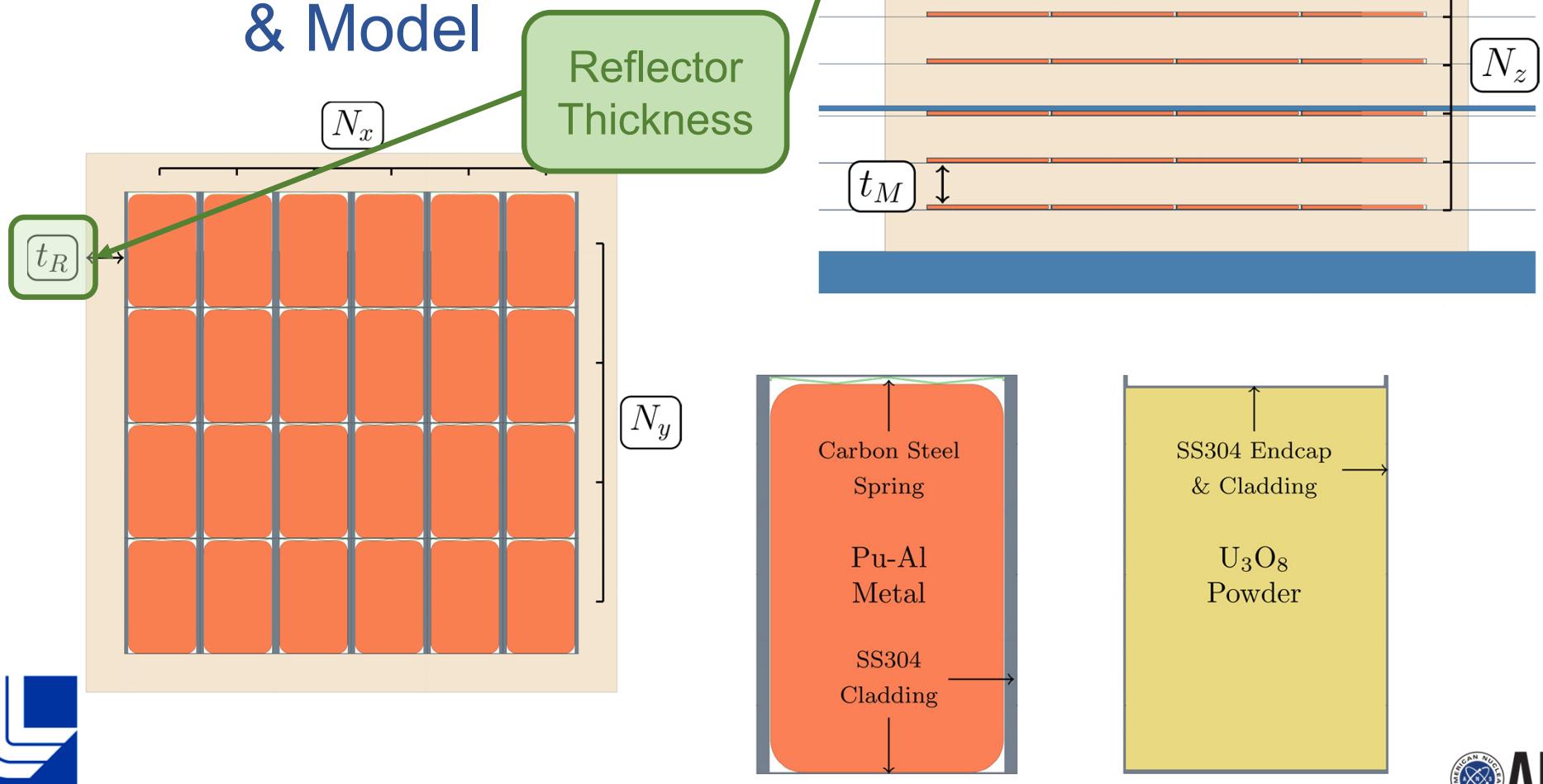
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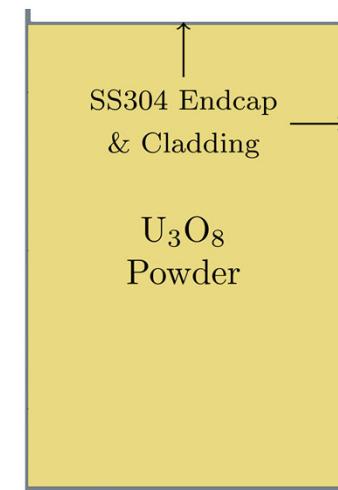
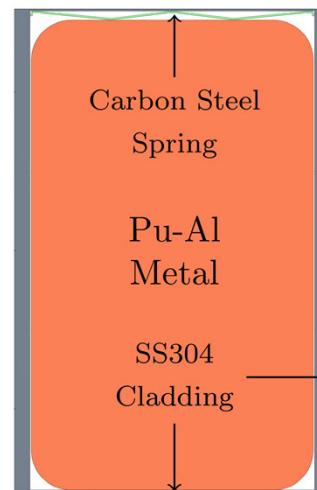
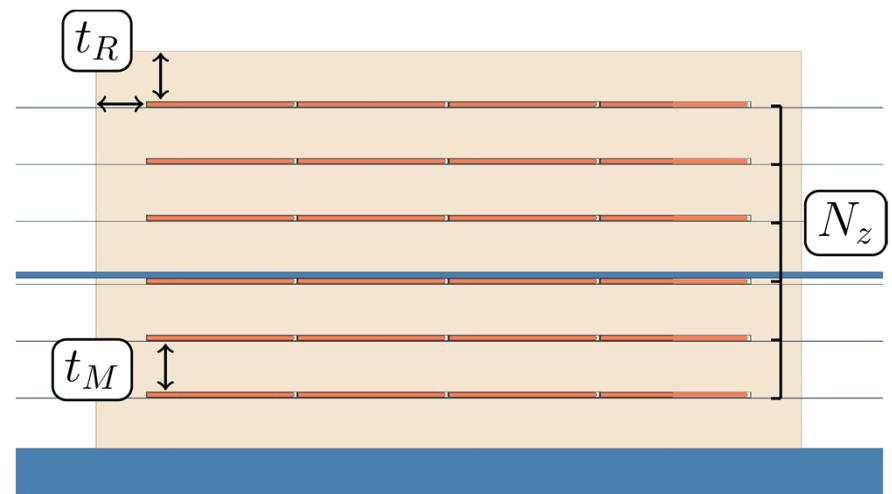
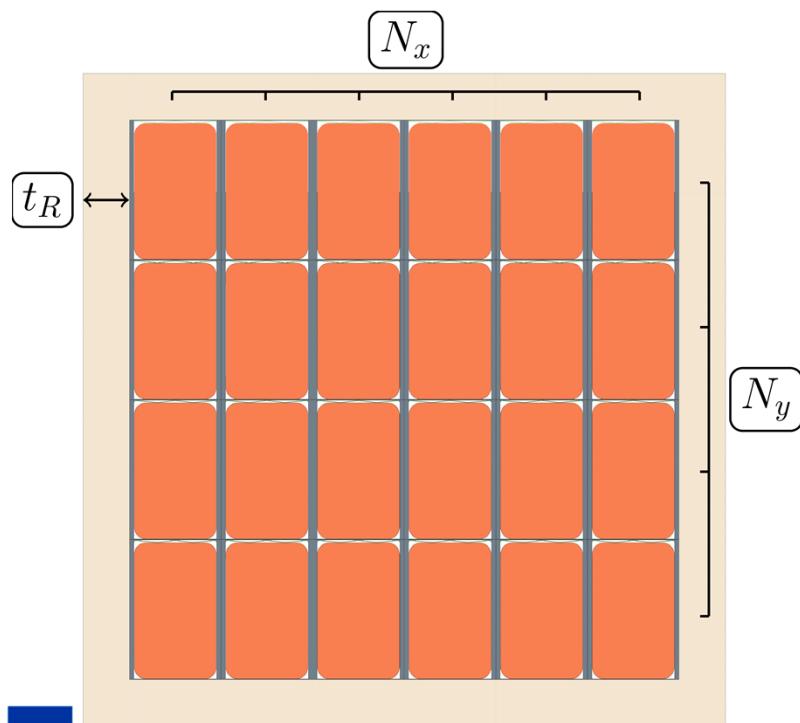
# TEX Configuration & Model



# TEX Configuration & Model



# TEX Configuration & Model



# Fuel Plates from Zero Power Physics Reactor (ZPPR)

## **$^{239}\text{Pu}$ (PANN) ZPPR Plates**

- Plutonium Aluminum No Nickel (PANN) plates
- Stainless steel (SS304) packets
- 105g of fuel per plate
  - 99g of Pu (95 wt%  $^{239}\text{Pu}$ )
- Density of 15.1 g/cm<sup>3</sup>

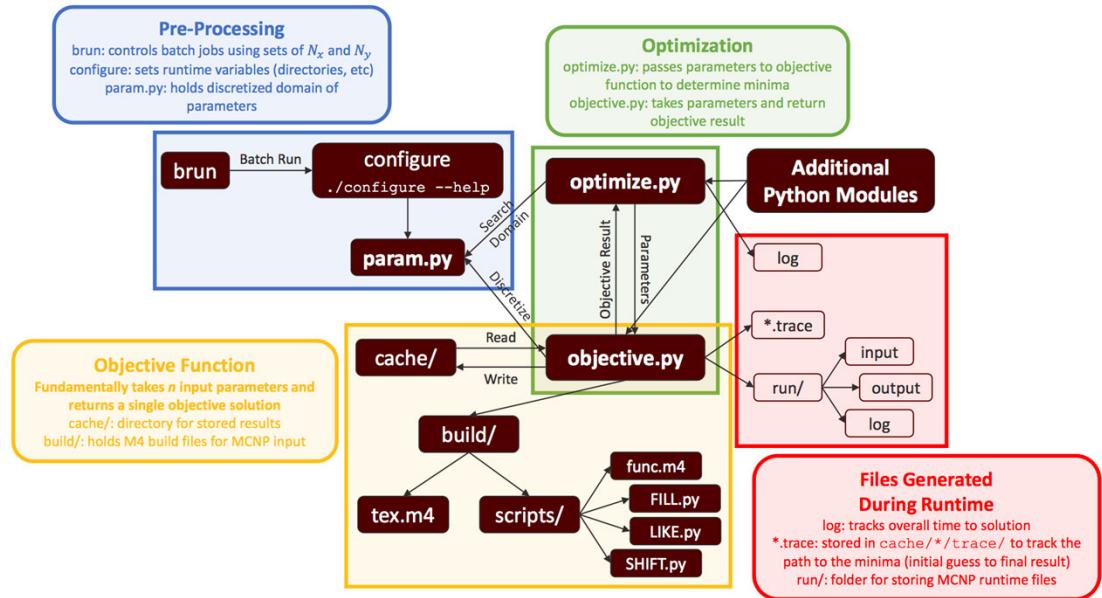
## **$^{233}\text{U}$ ZPPR Plates**

- Uranium oxide power
- Stainless steel (SS304) packets
- 33g of fuel per plate
  - 28g of  $^{233}\text{U}$
- Density of 1.62 g/cm<sup>3</sup>



# Optimus

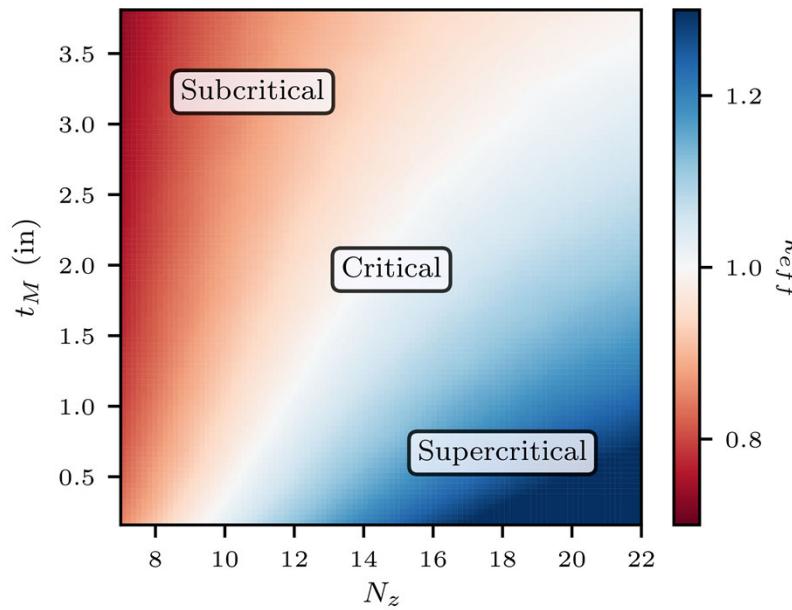
- Optimization and machine learning software package tailored specifically for designing critical experiments
- Developed by the Nuclear Criticality Safety Division at Lawrence Livermore and written in Python
- Being extended to support general criticality safety analysis



# Objective Function

- Create local minima where the configuration is critical

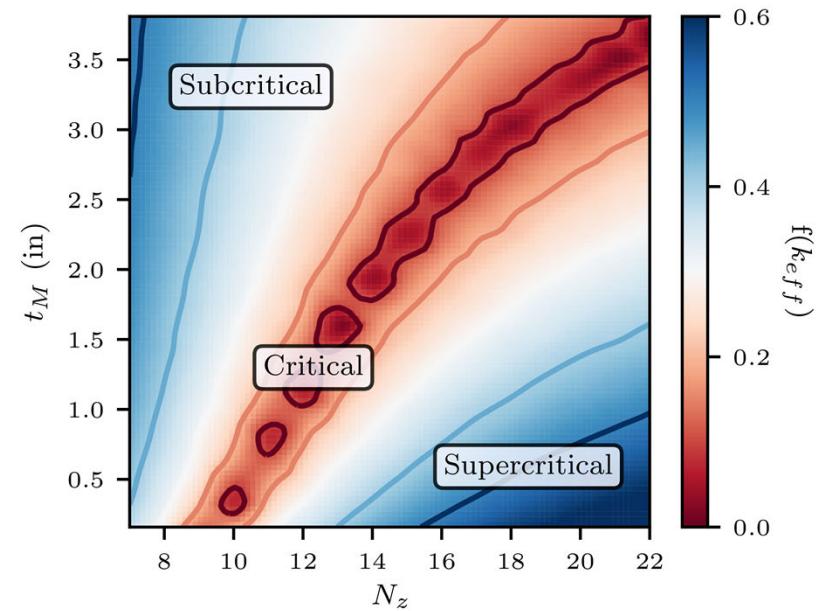
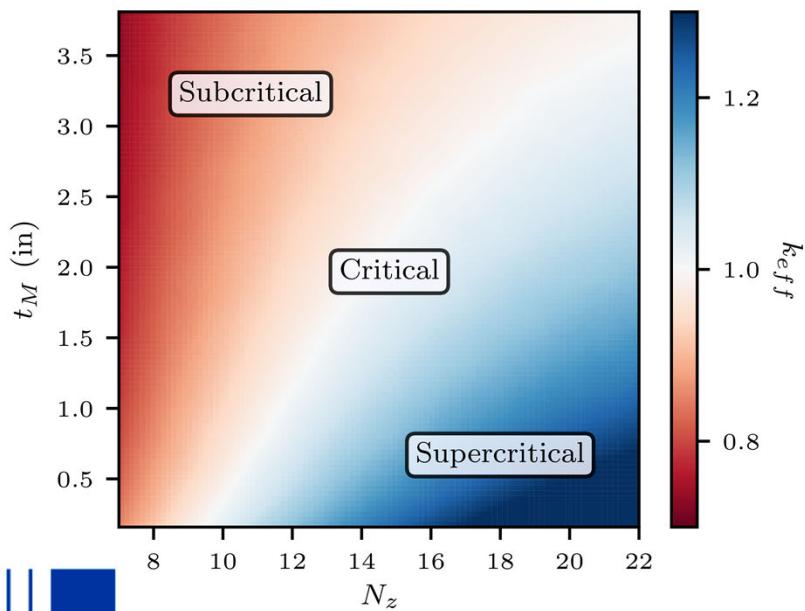
$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$



# Objective Function

- Create local minima where the configuration is critical

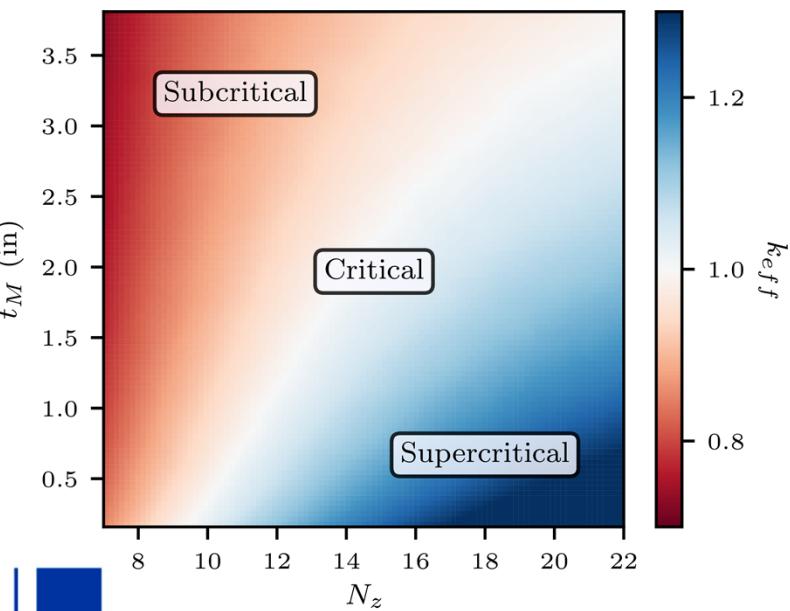
$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$



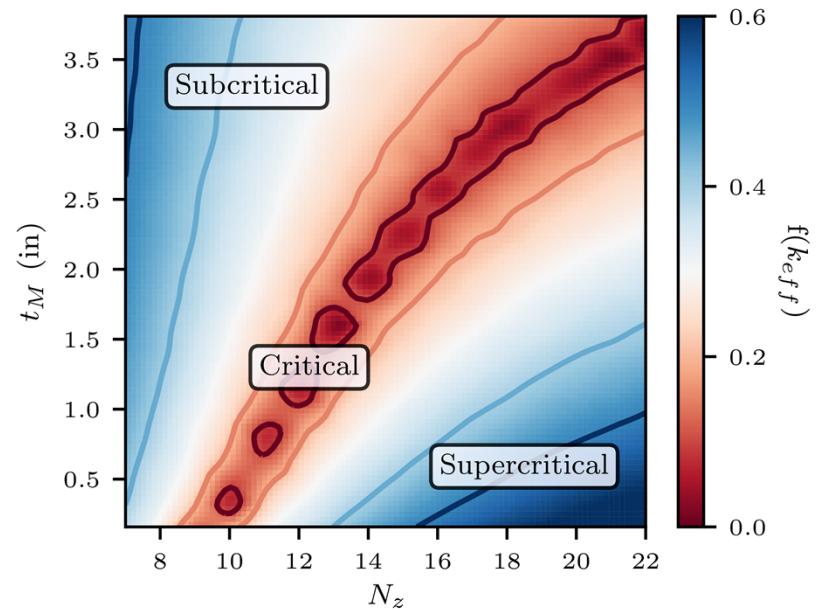
# Objective Function

- Create local minima where the configuration is critical

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Multiplication factor of the configuration based on the input parameters

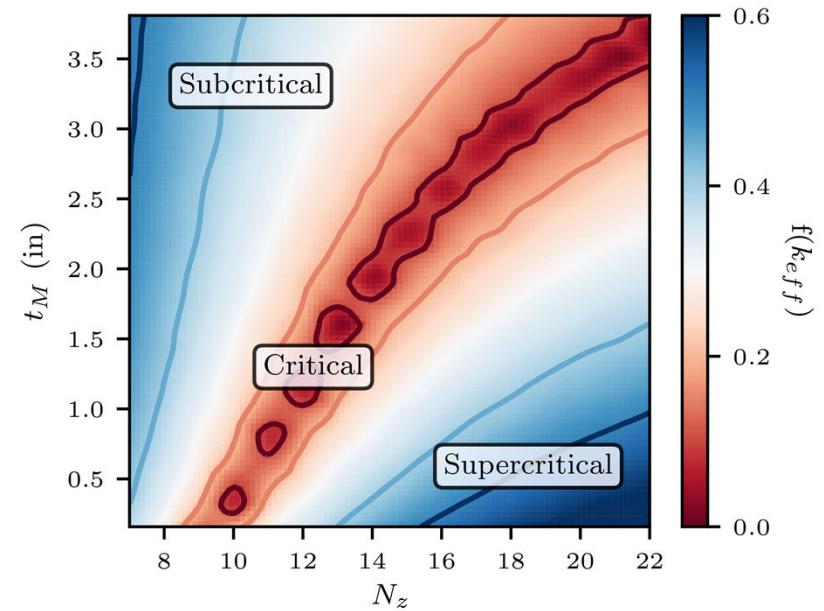
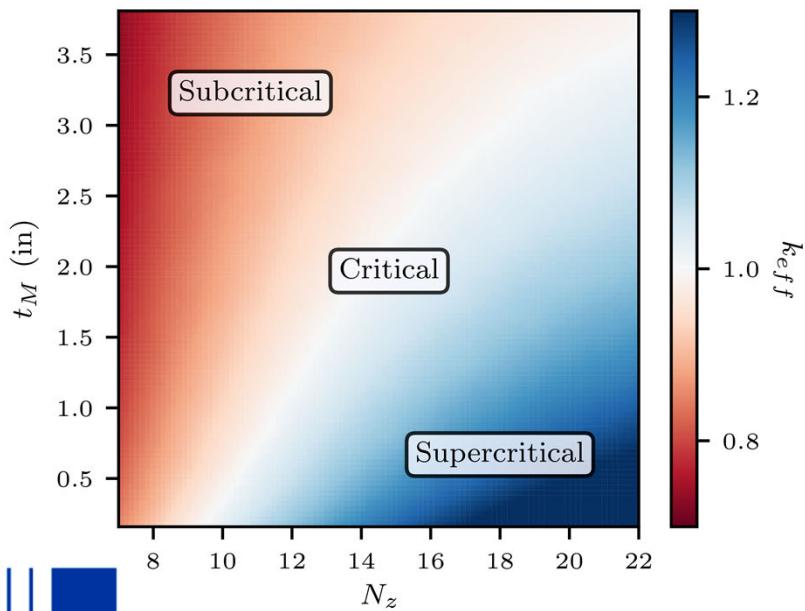


# Objective Function

- Create local minima where the configuration is critical

$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$

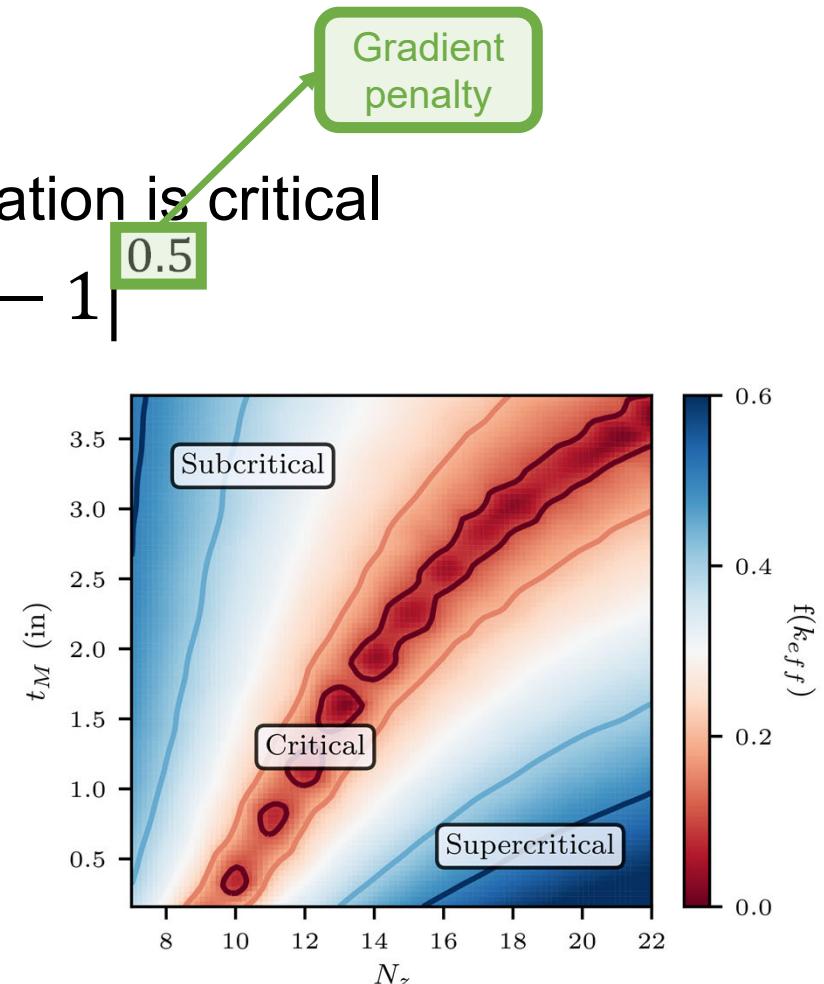
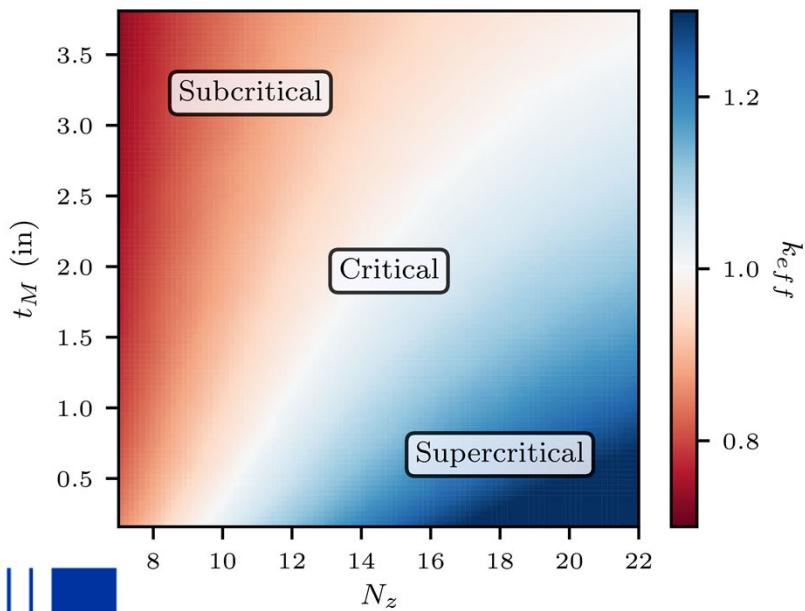
Desired multiplication factor



# Objective Function

- Create local minima where the configuration is critical

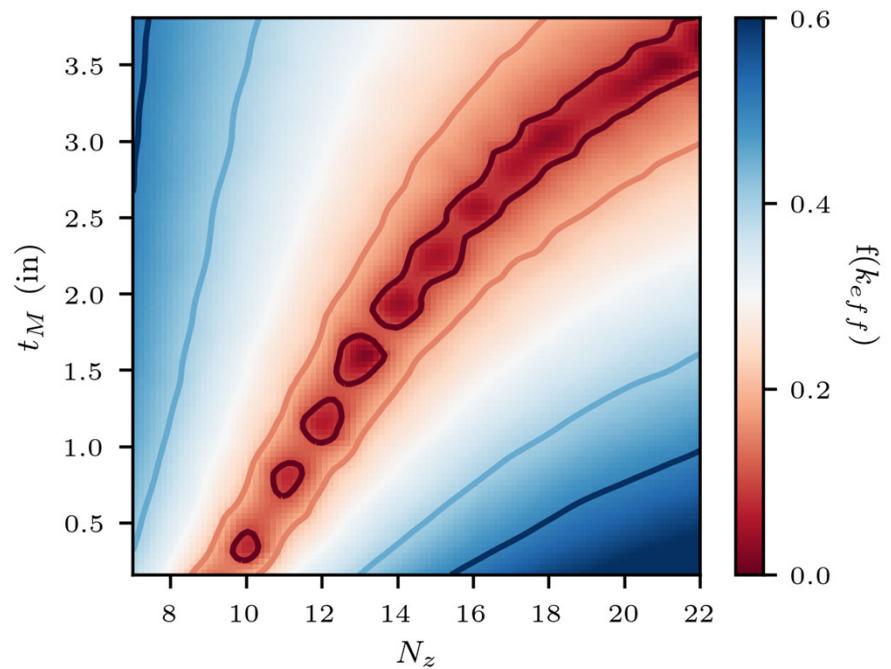
$$f(k_{eff}) = |k_{eff} - 1|$$



# Optimizing the Objective Function

$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$

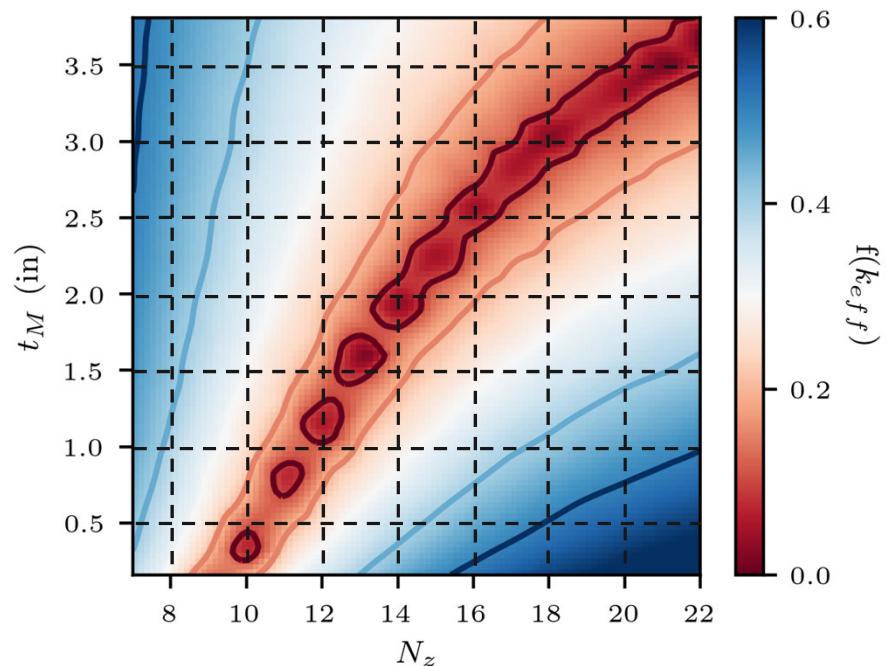
- Discretize the domain
- Apply an optimization method to determine the local minima (critical configurations)
  - Gradient descent
  - Linear search
- Powell's Method



# Optimizing the Objective Function

$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$

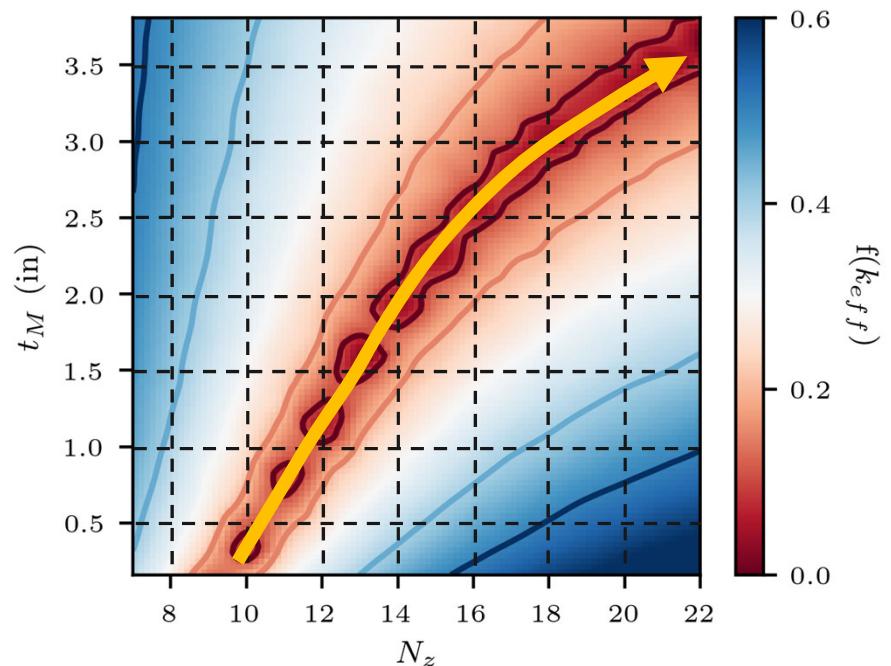
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# Optimizing the Objective Function

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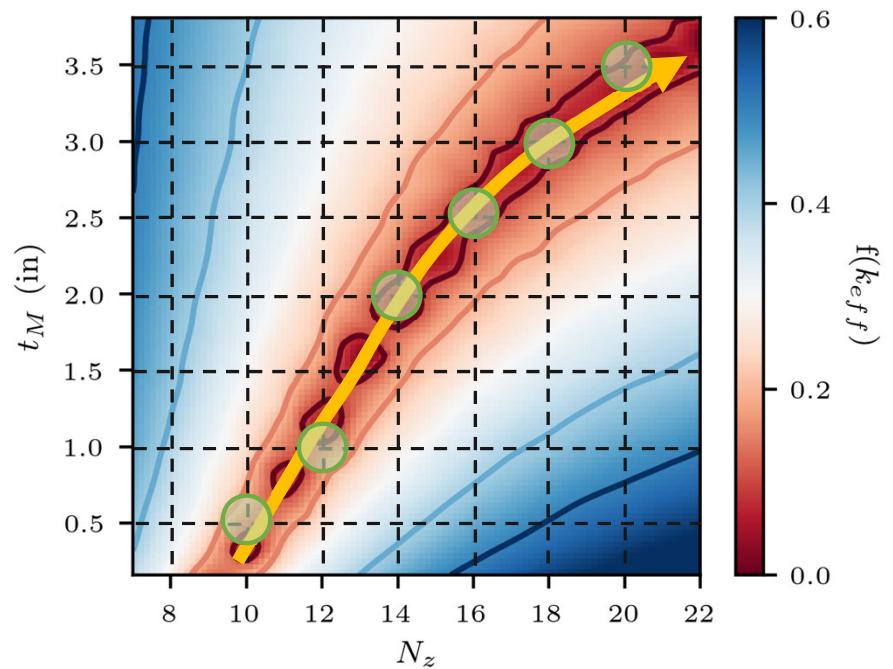
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# Optimizing the Objective Function

$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$

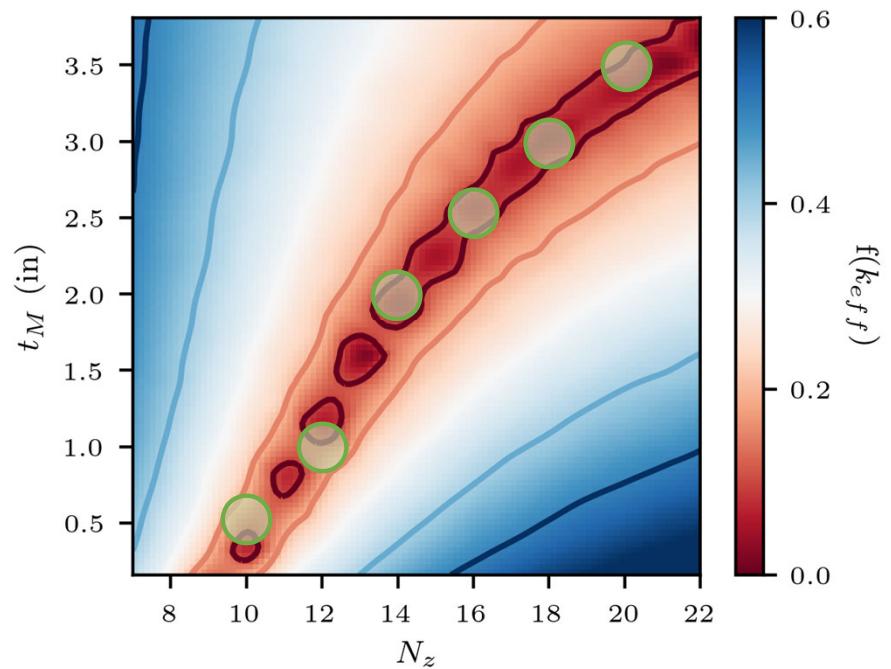
- Discretize the domain
- Apply an optimization method to *determine the local minima* (critical configurations)
  - Gradient descent
  - Linear search
- Powell's Method



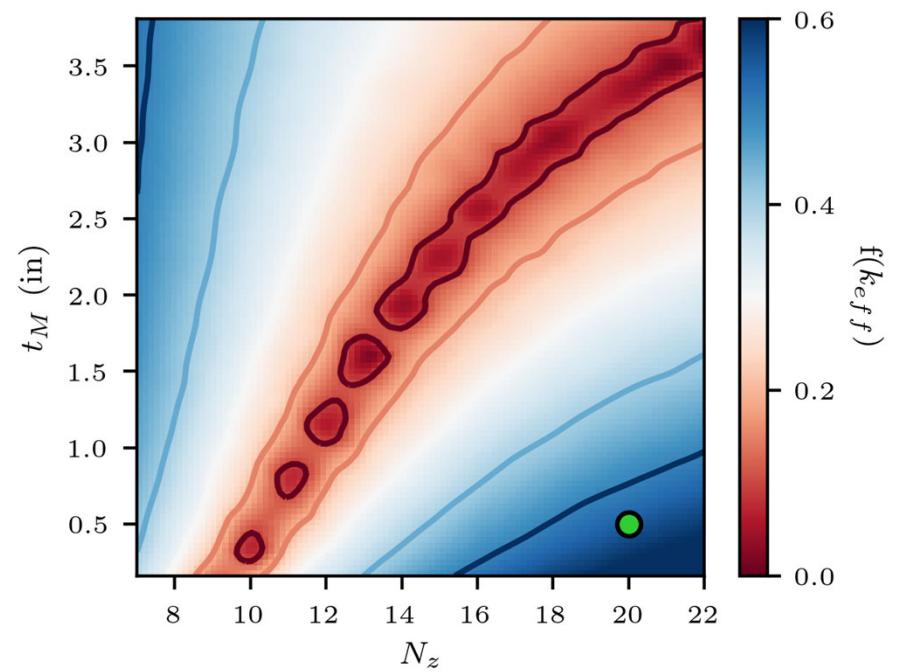
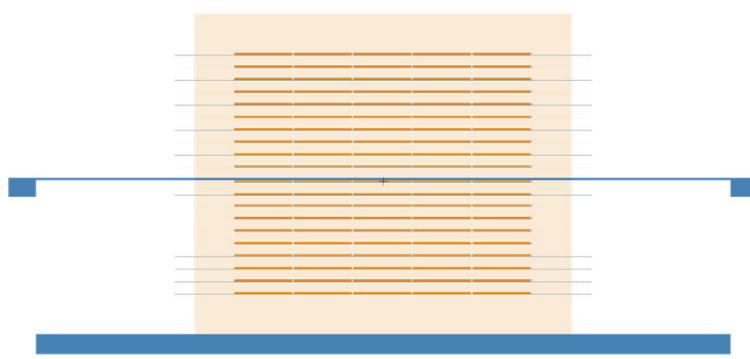
# Optimizing the Objective Function

$$f(k_{eff}) = |k_{eff} - 1|^{0.5}$$

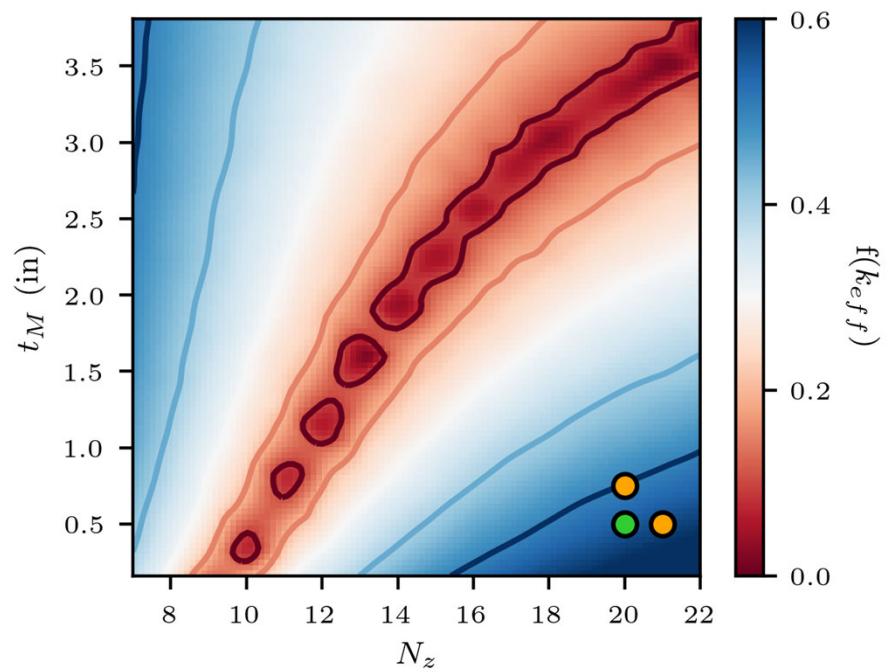
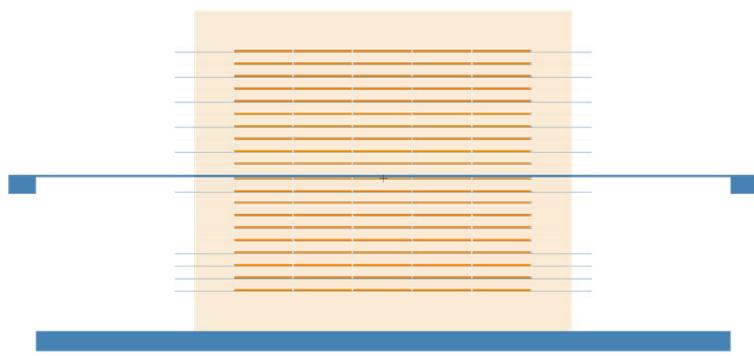
- Discretize the domain
- Apply an optimization method to determine the local minima (critical configurations)
  - Gradient descent
  - Linear search
- *Powell's Method*



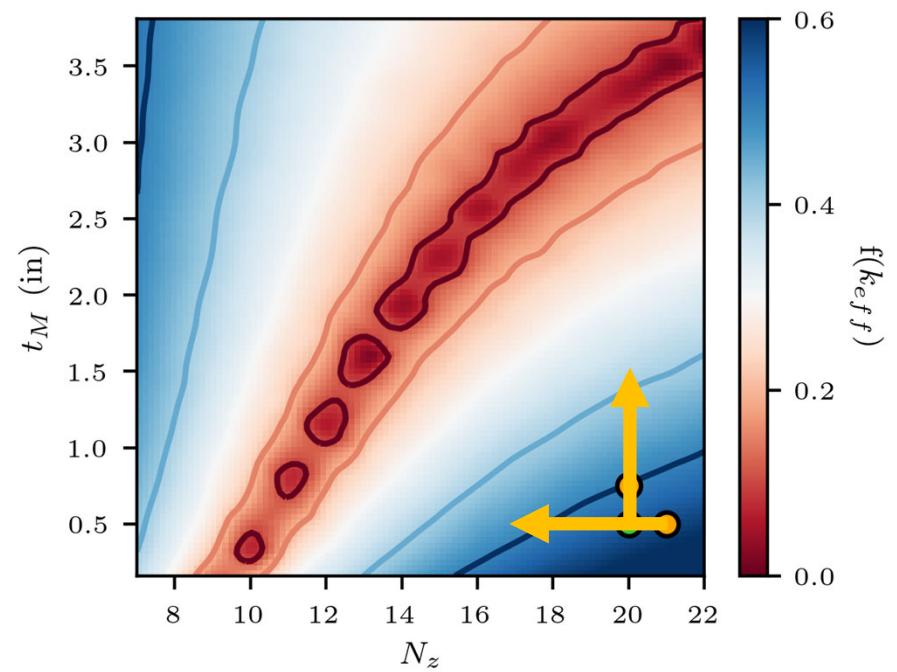
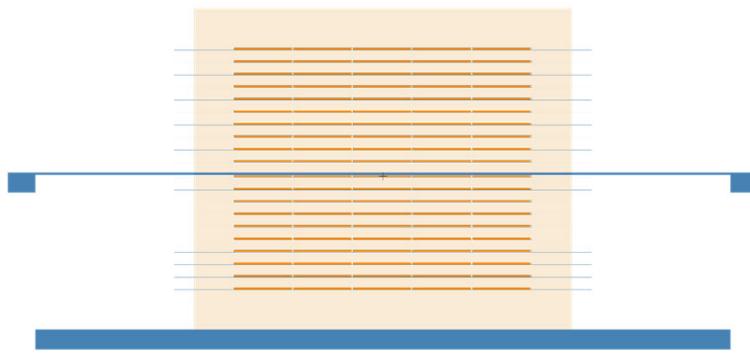
# Randomly selected starting point Supercritical Configuration ( $k > 1$ )



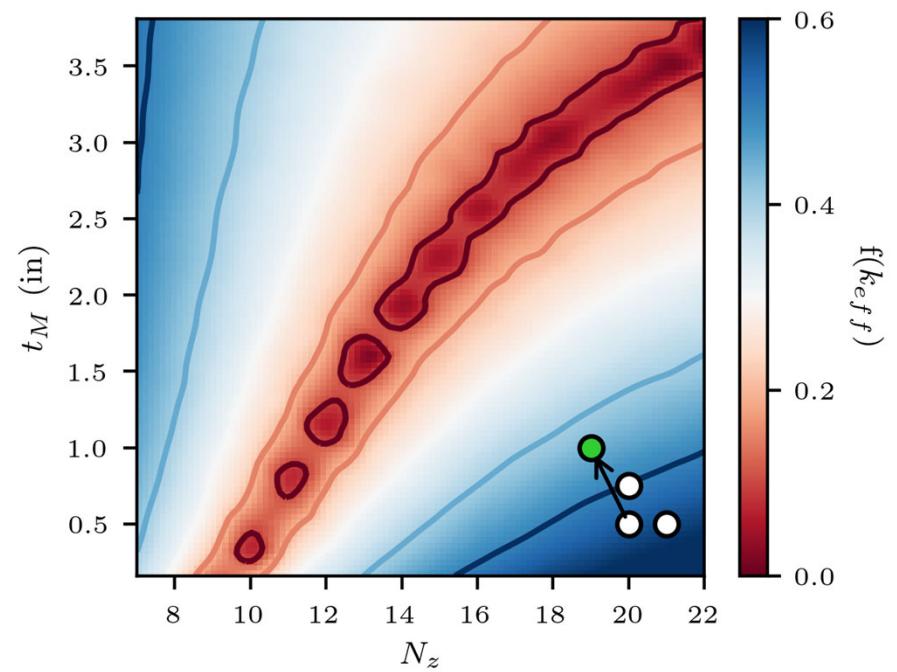
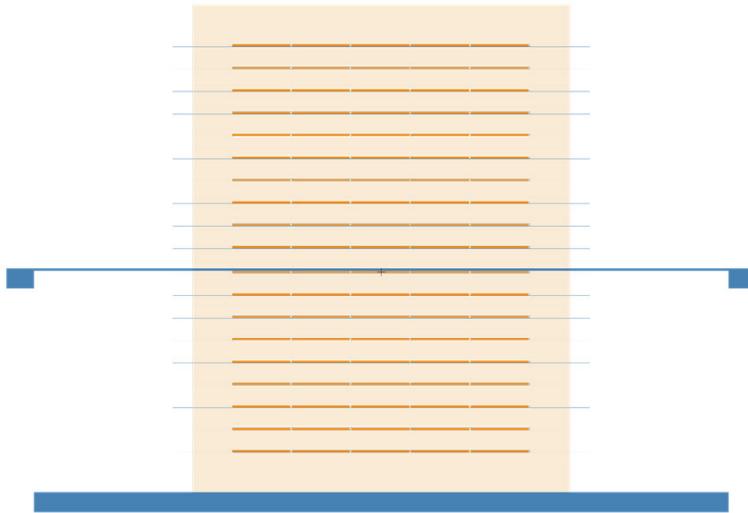
# Evaluate the gradients



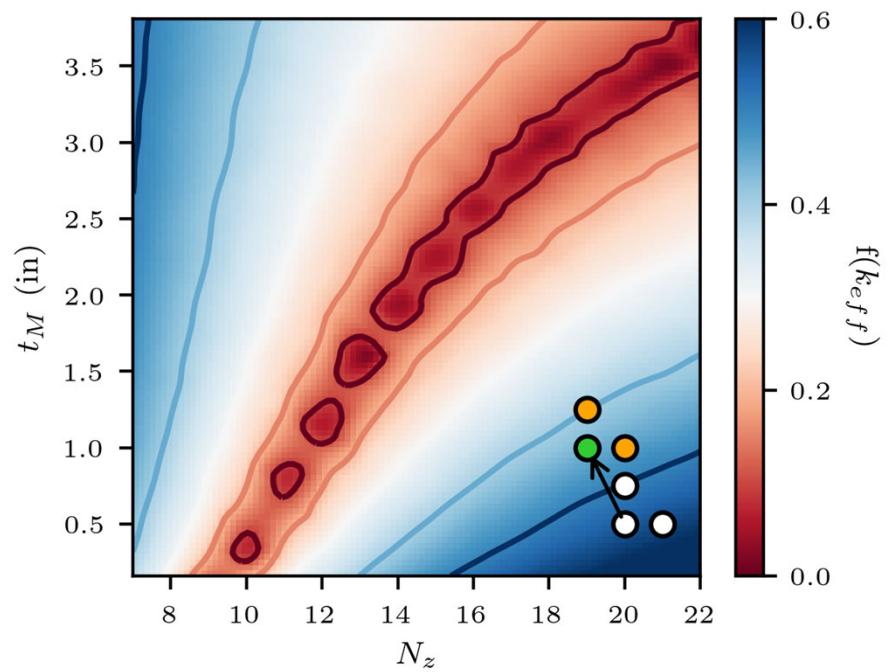
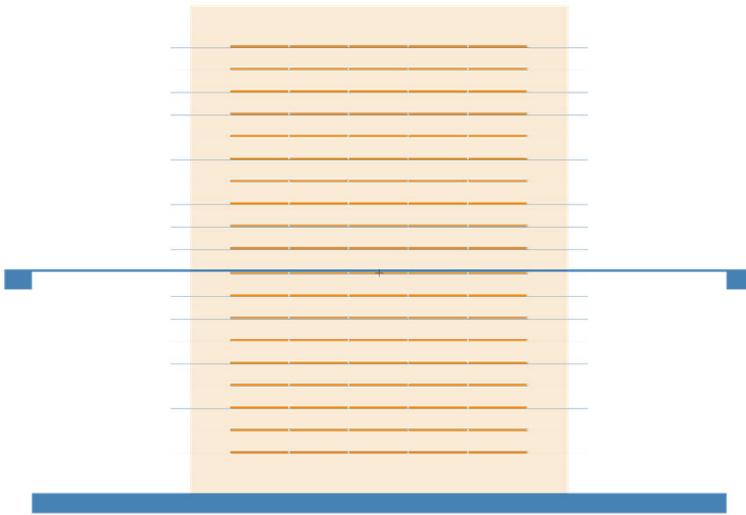
Evaluate the gradients  
Point towards less fuel and more moderation



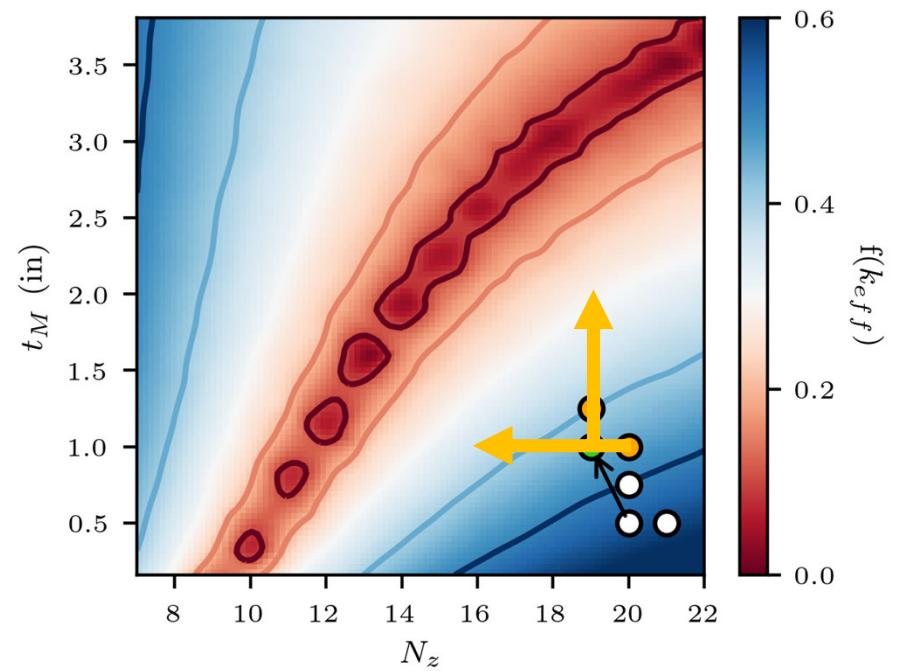
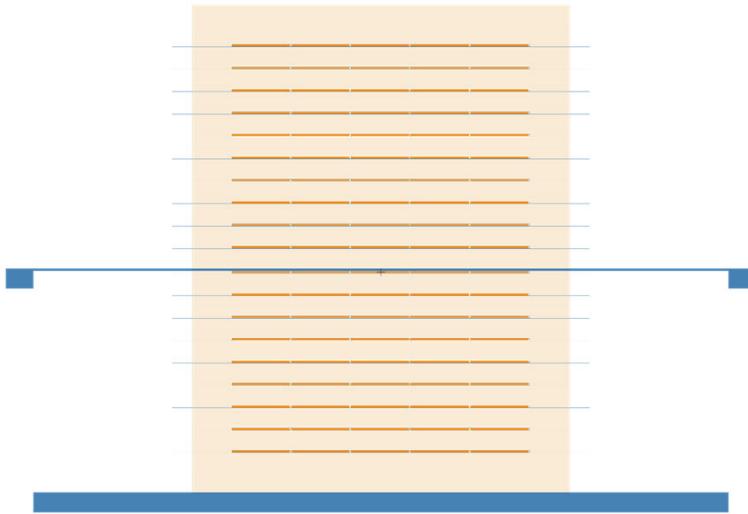
# Create a new configuration Again, supercritical ( $k > 1$ )



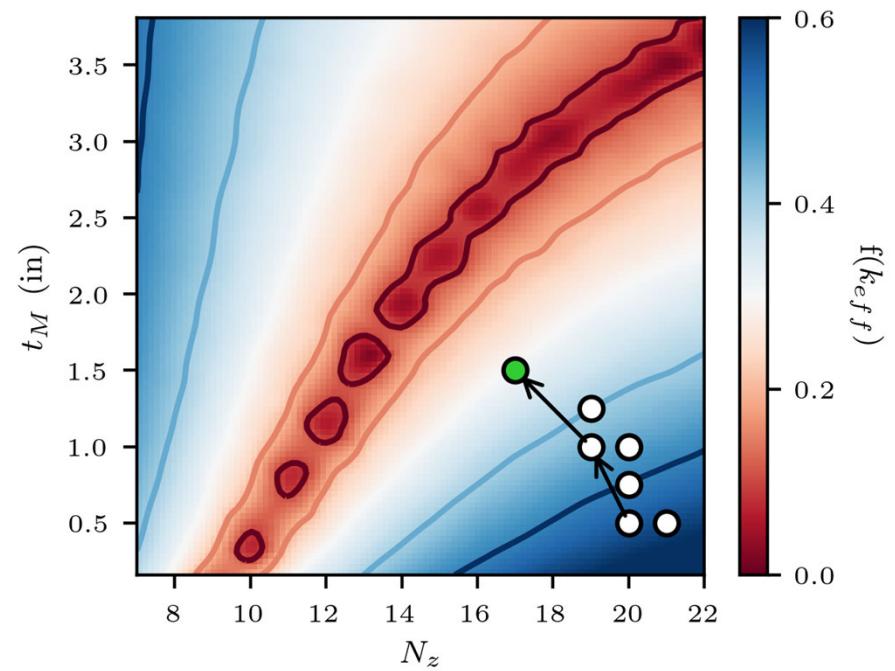
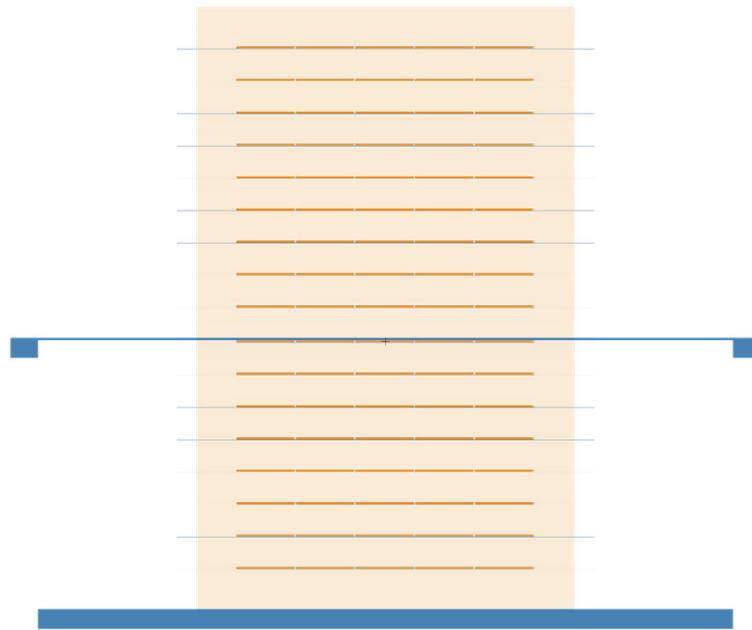
# Evaluate the gradients



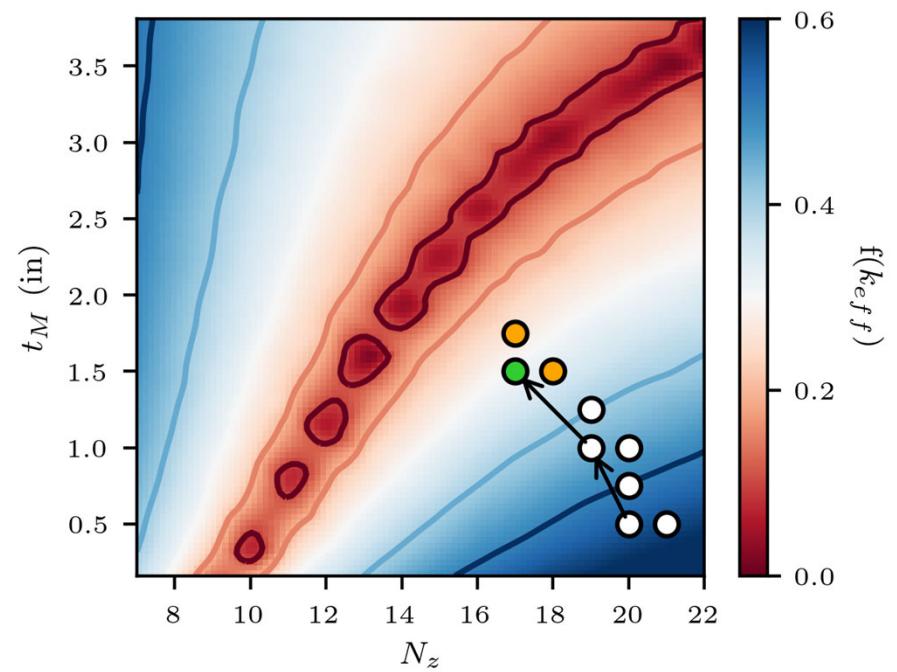
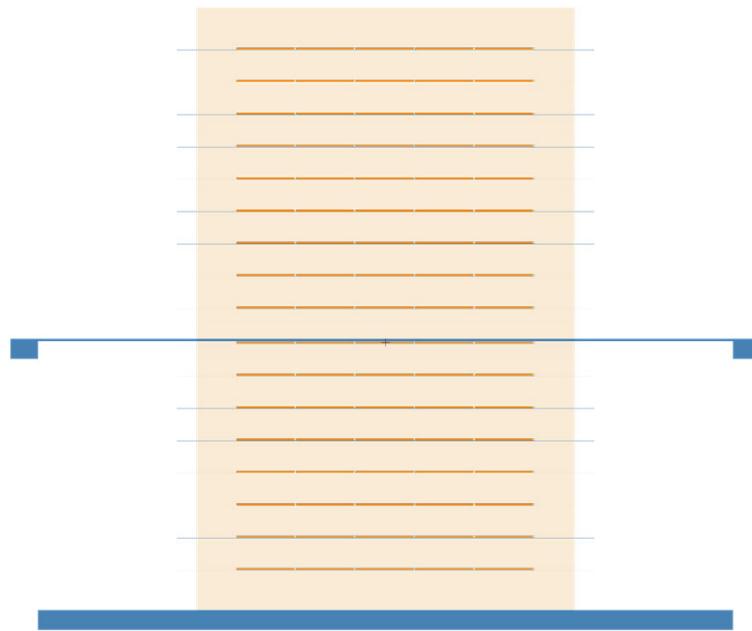
# Evaluate the gradients Again, point towards less fuel and more moderation



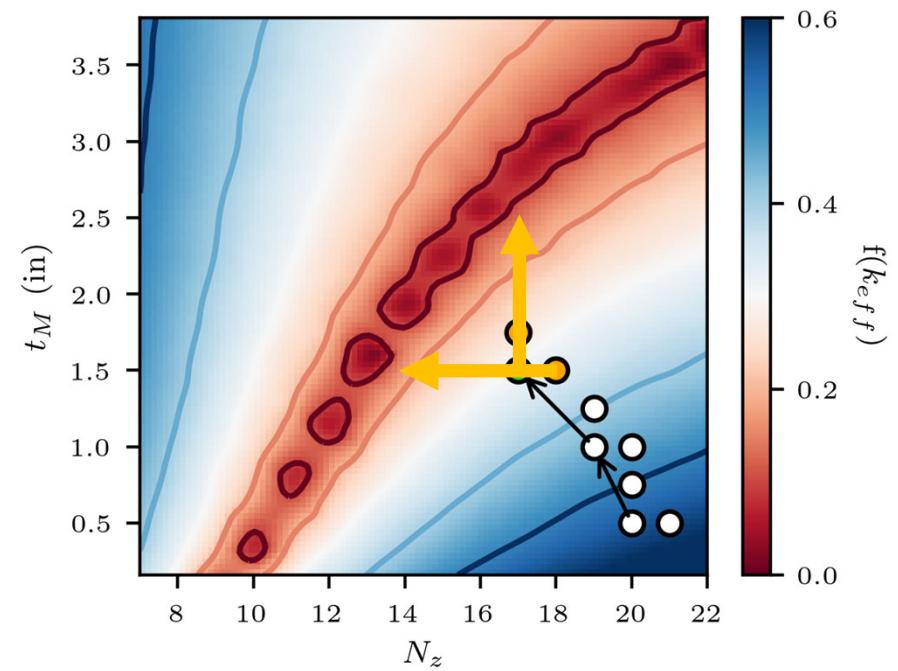
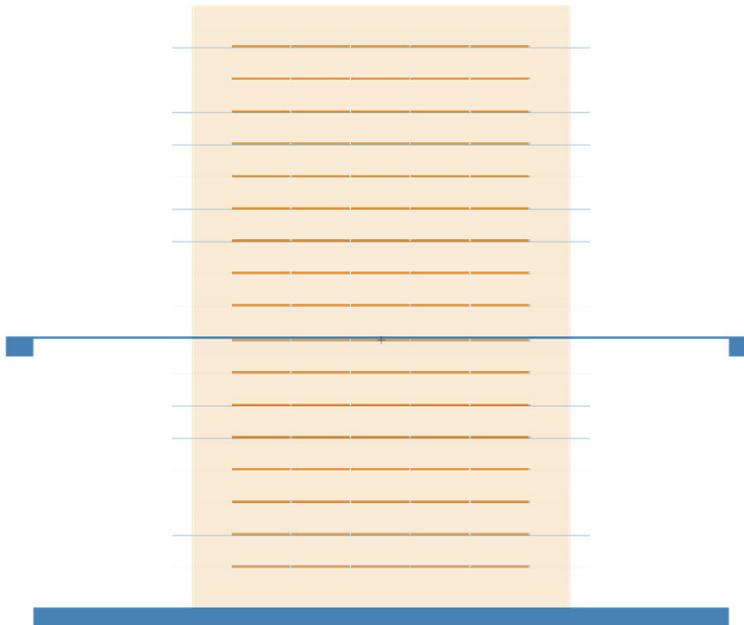
# Create a new configuration



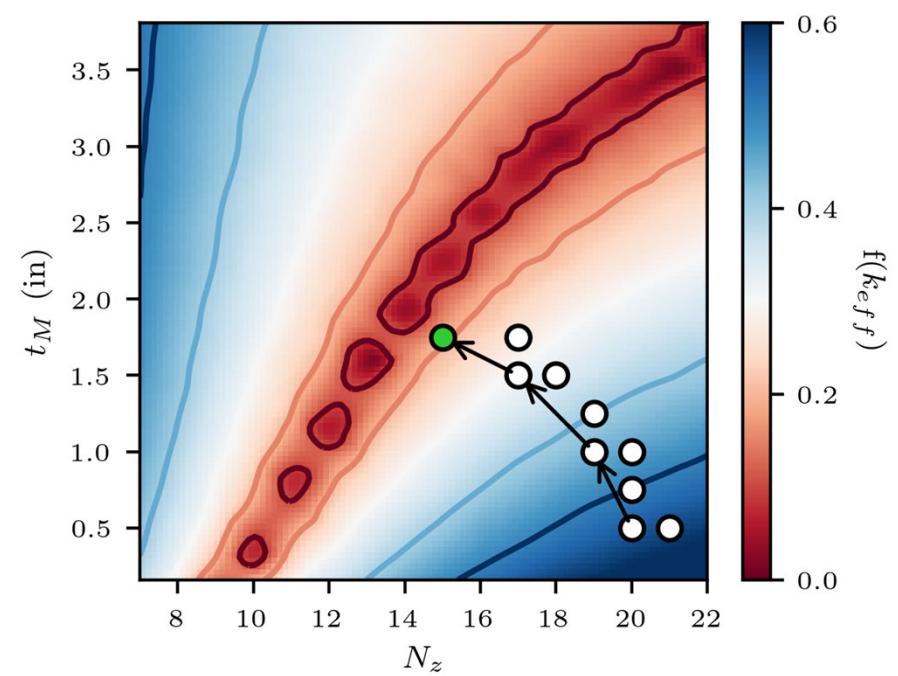
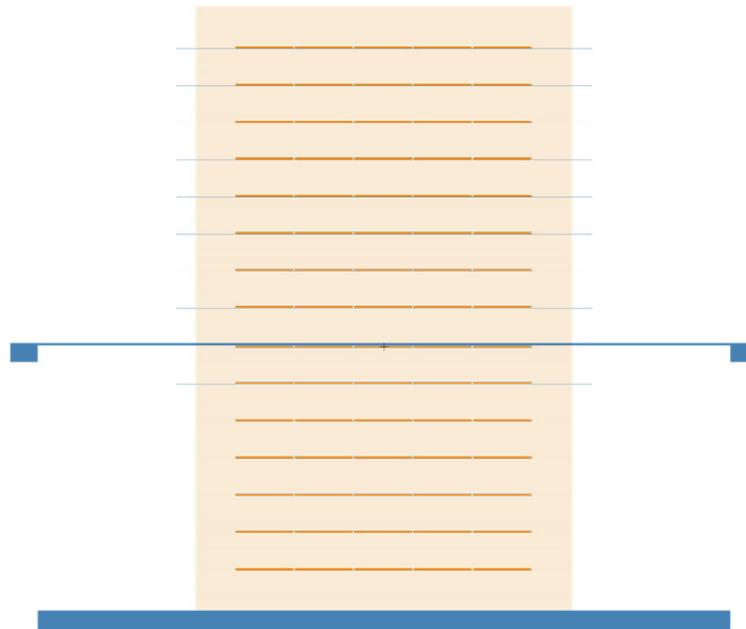
# Evaluate the gradients



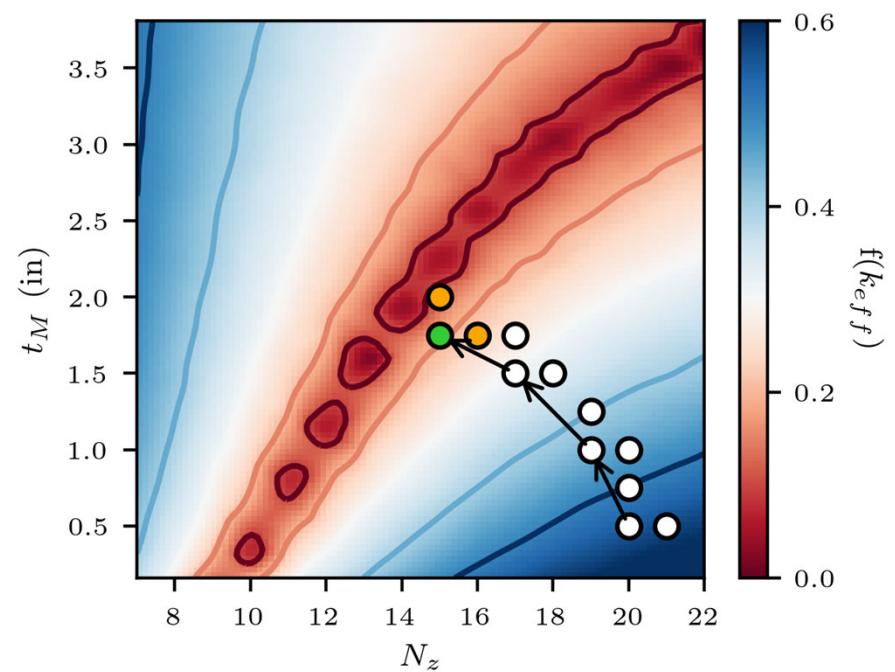
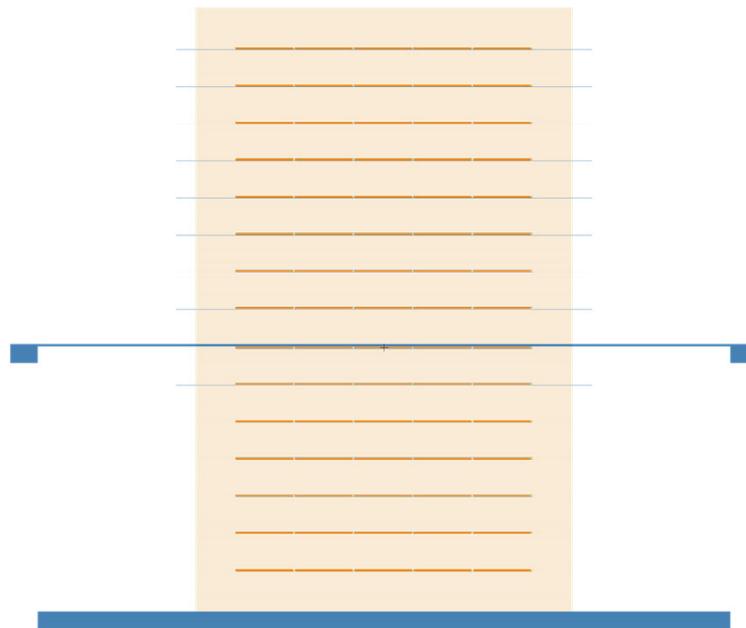
# Evaluate the gradients Still, point towards less fuel and more moderation



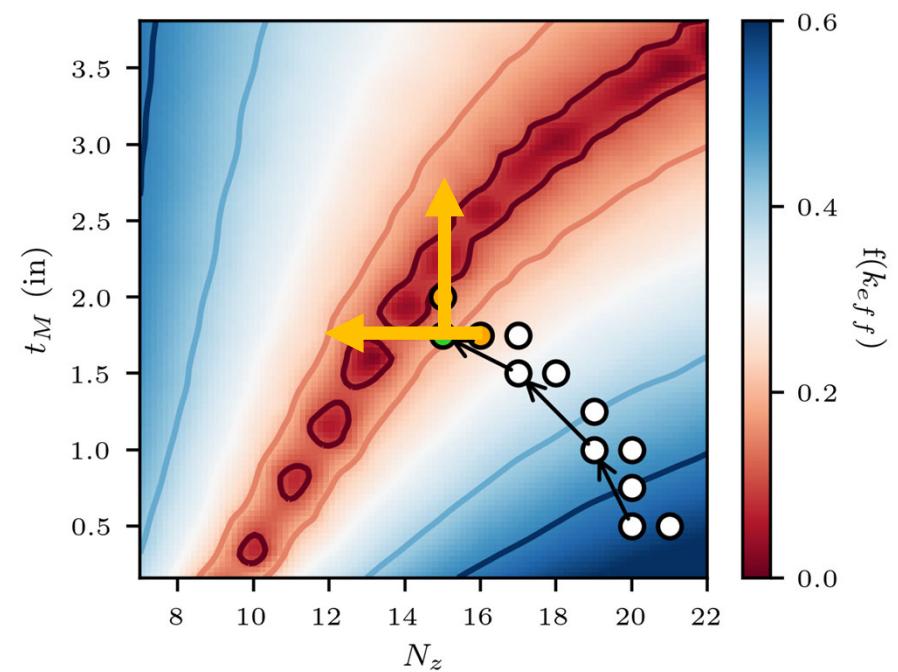
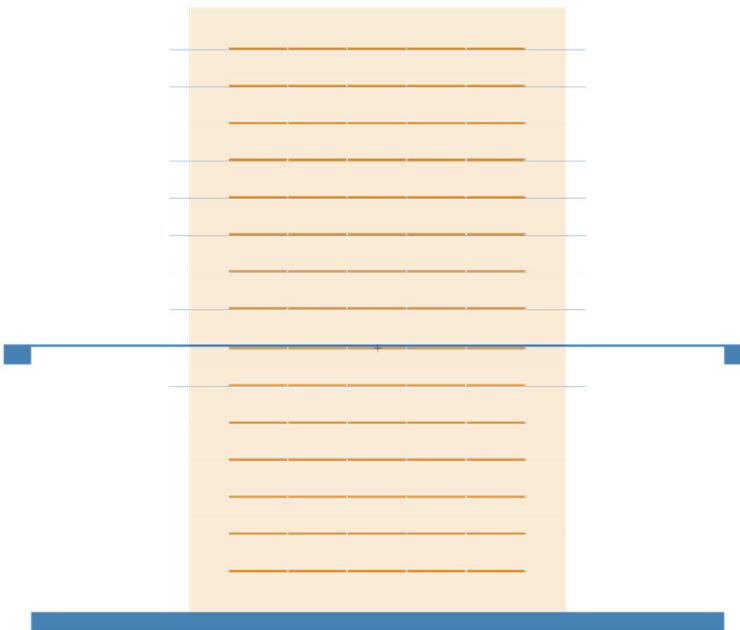
# Create a new configuration



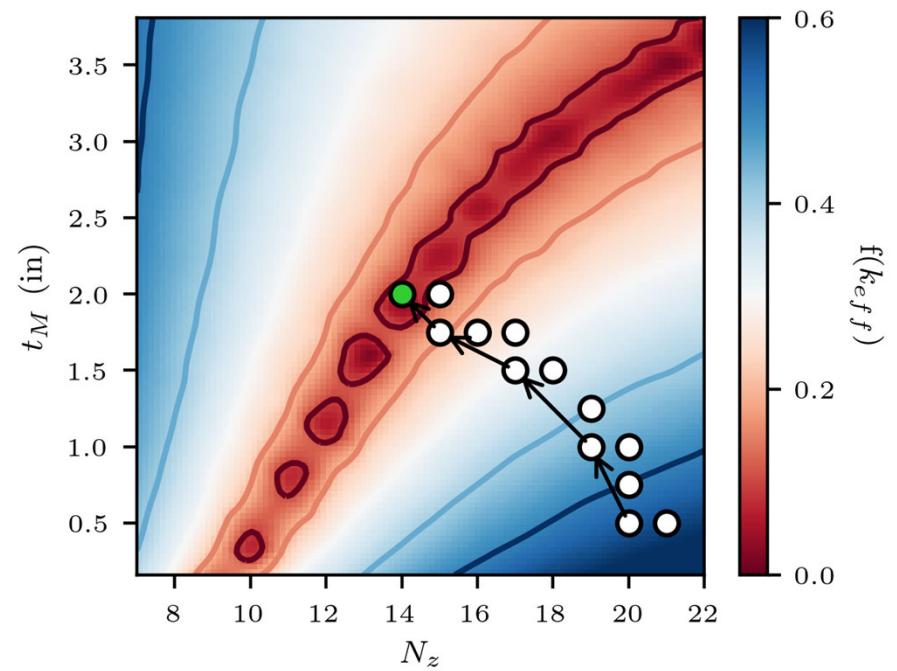
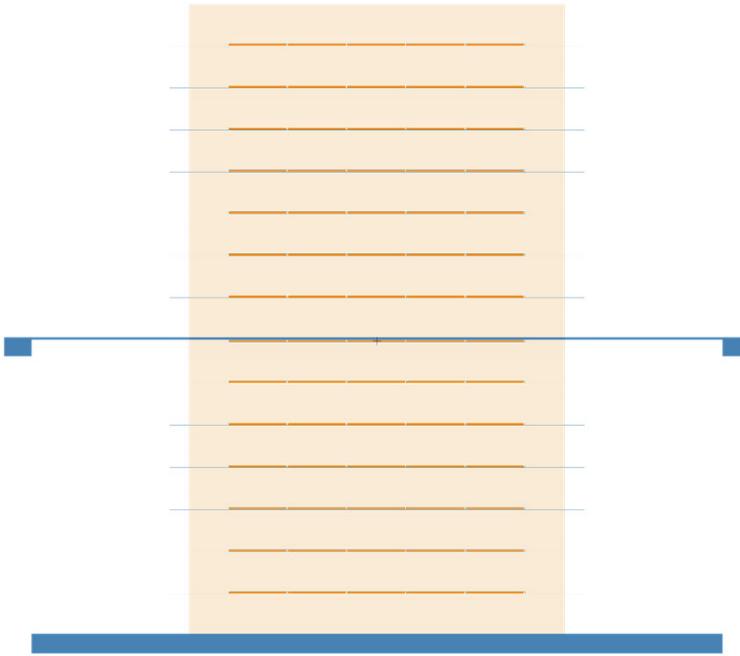
# Evaluate the gradients



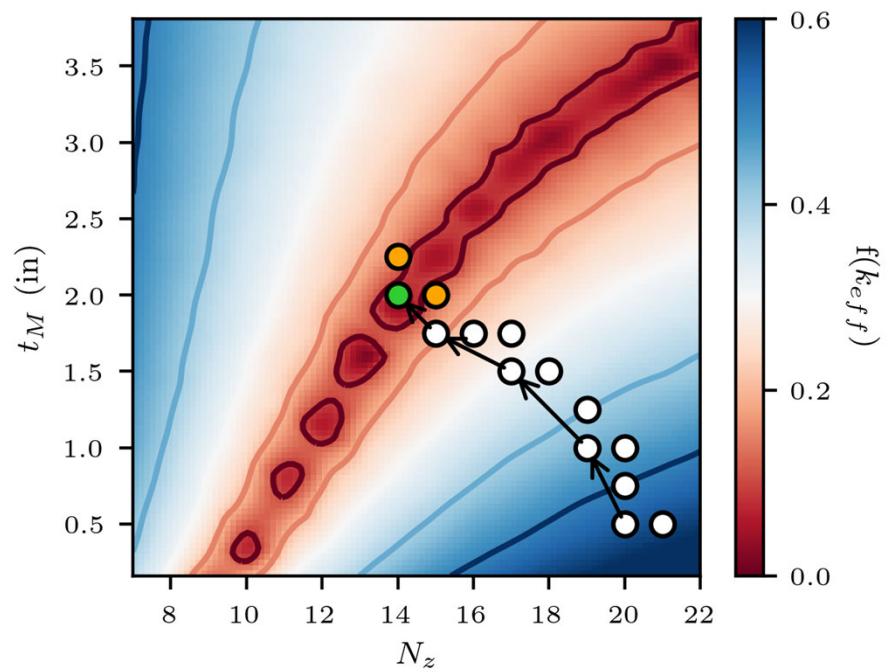
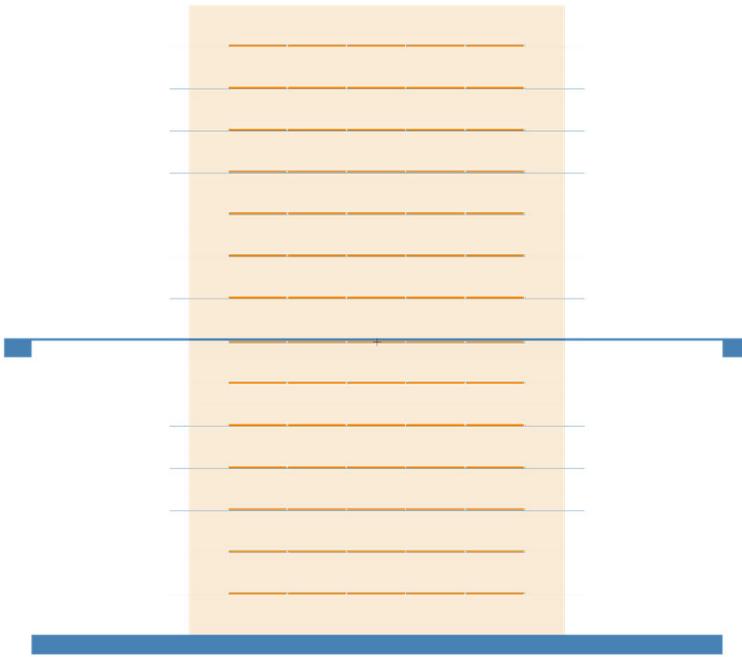
# Evaluate the gradients Less fuel and more moderation



Create a new configuration  
This one is roughly critical ( $k \sim 1$ )

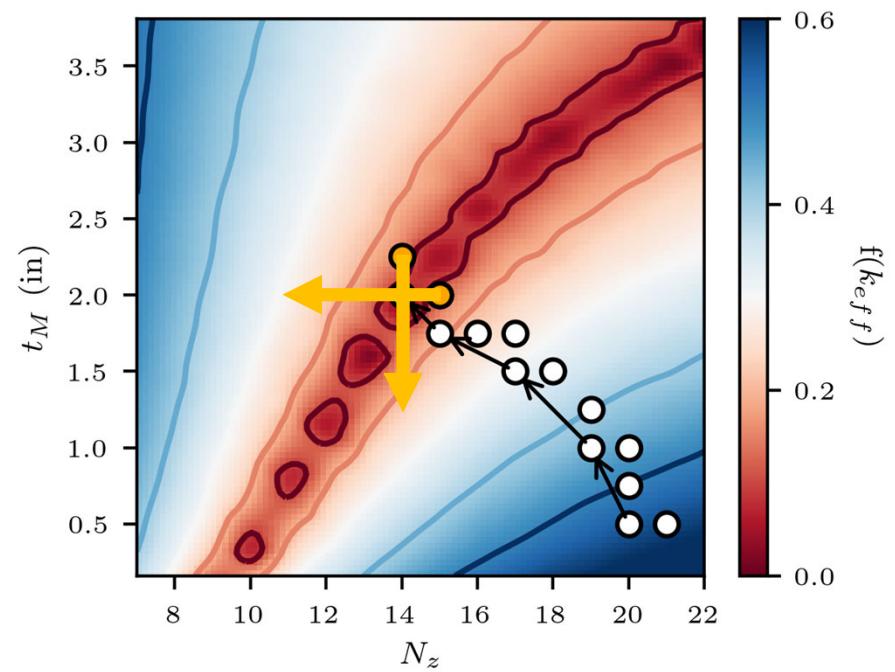
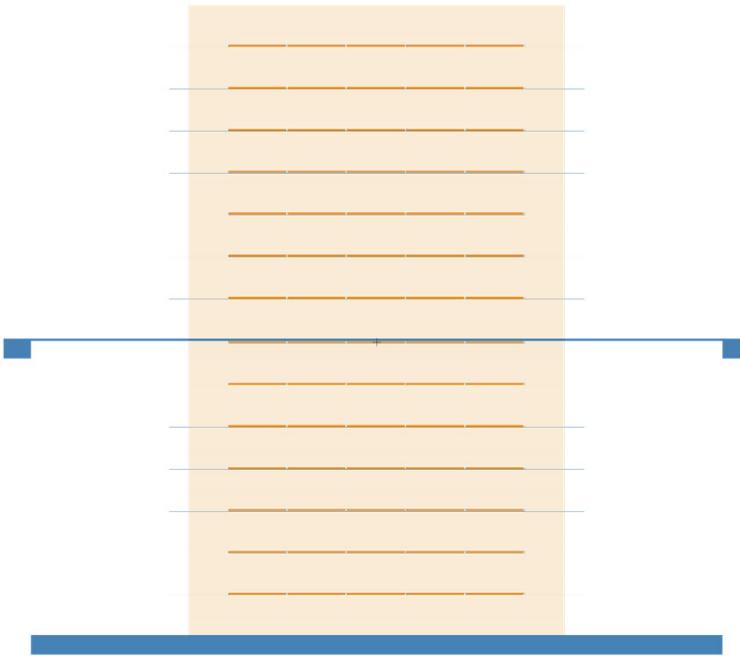


# Evaluate the gradients

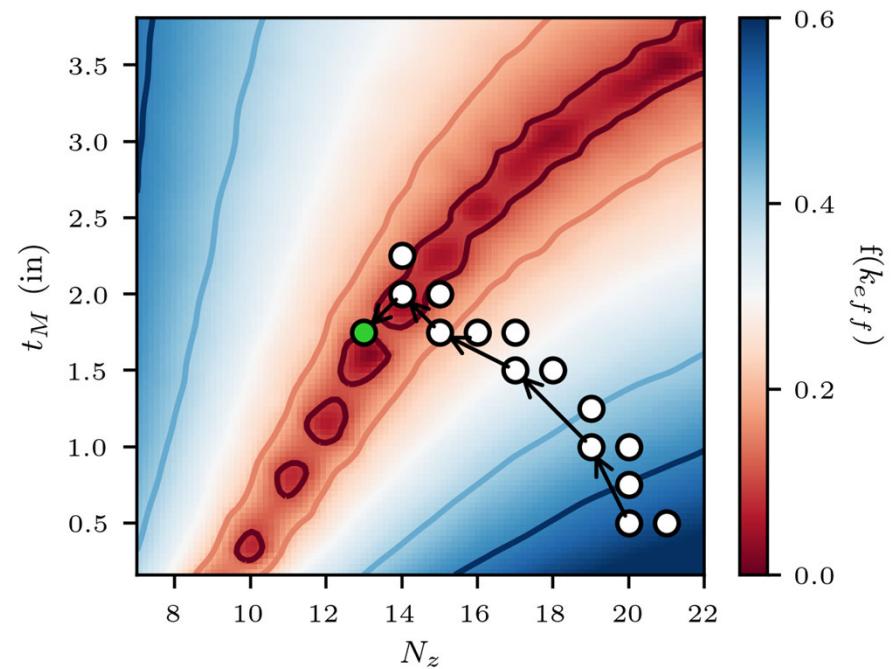
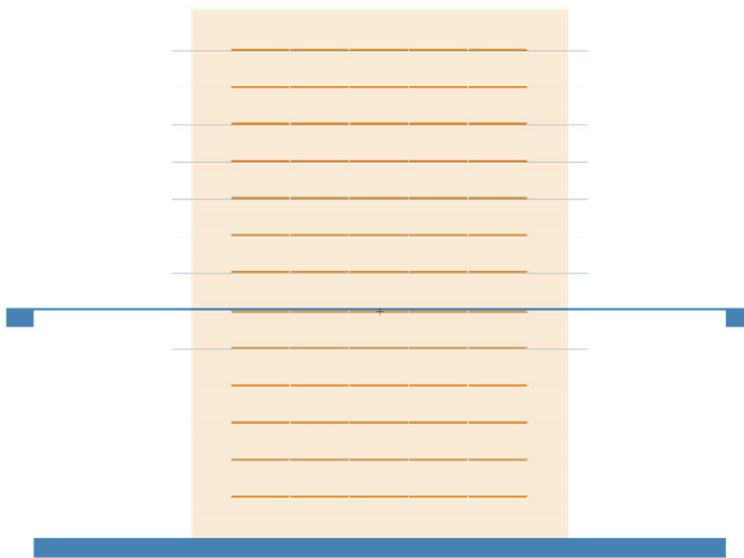


# Evaluate the gradients

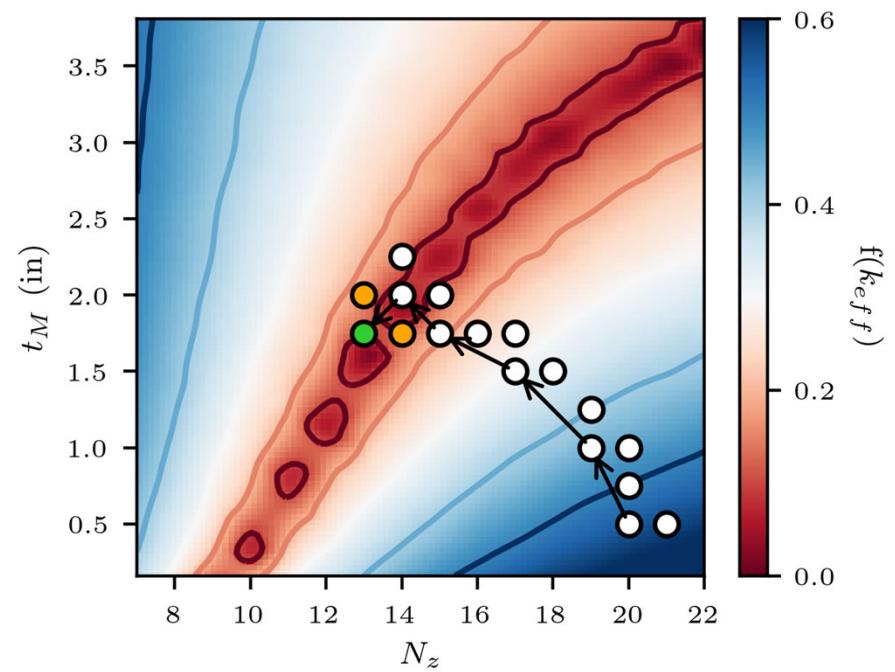
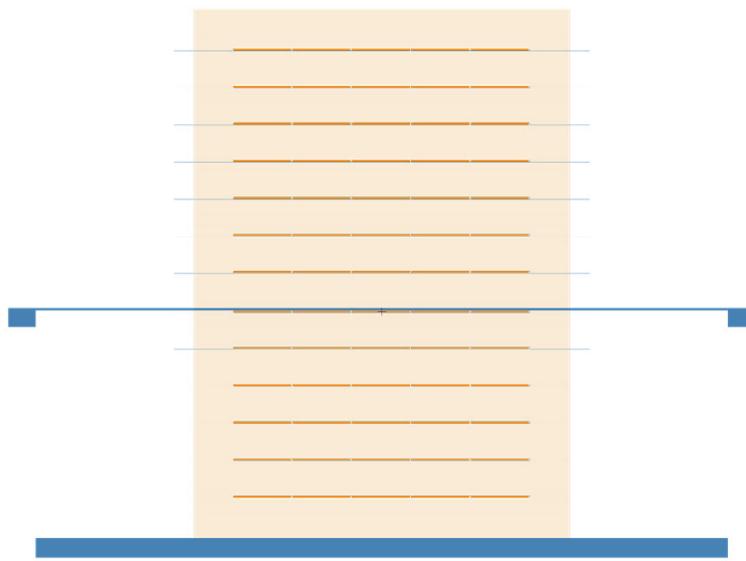
Now, points towards less fuel and *less moderation*



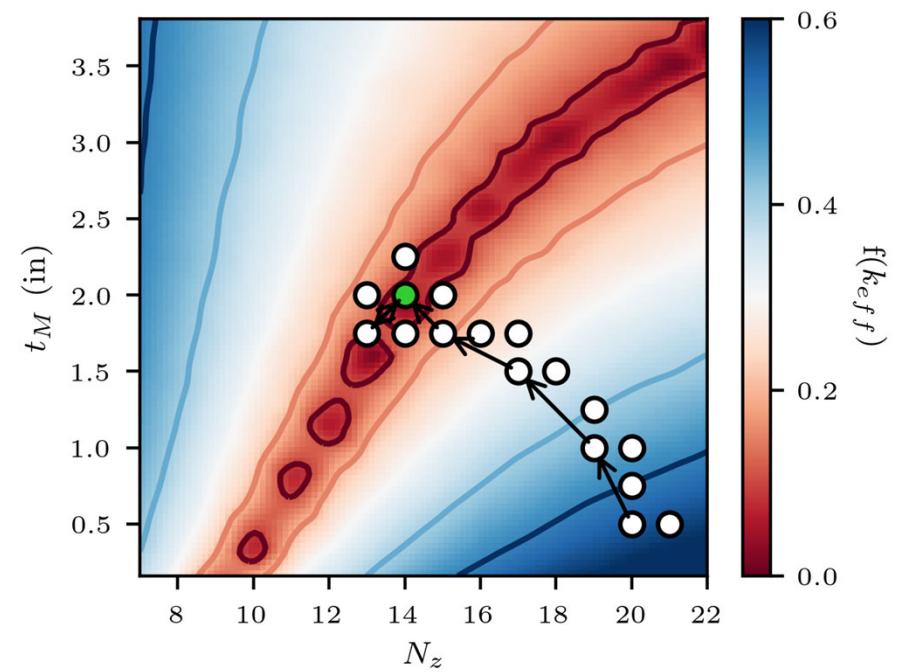
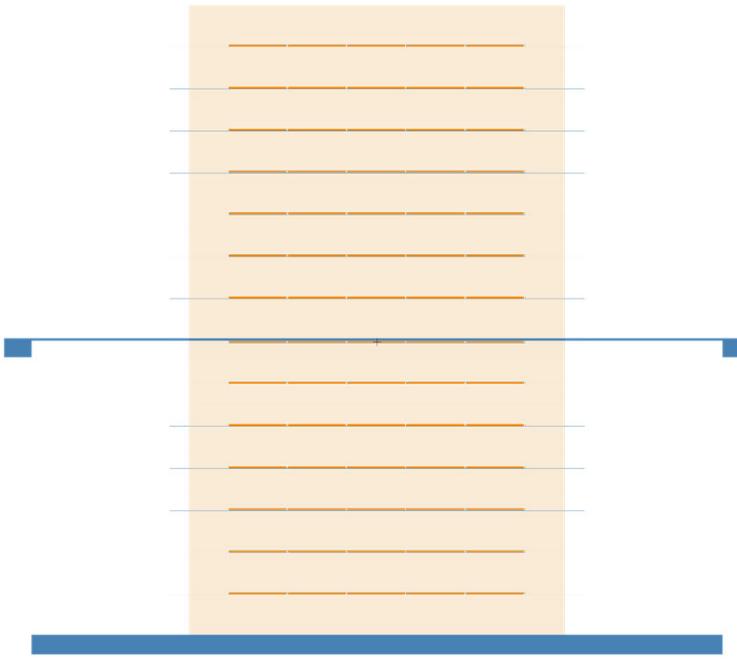
# Create a new configuration Now, subcritical ( $k < 1$ )



# Final gradient evaluations

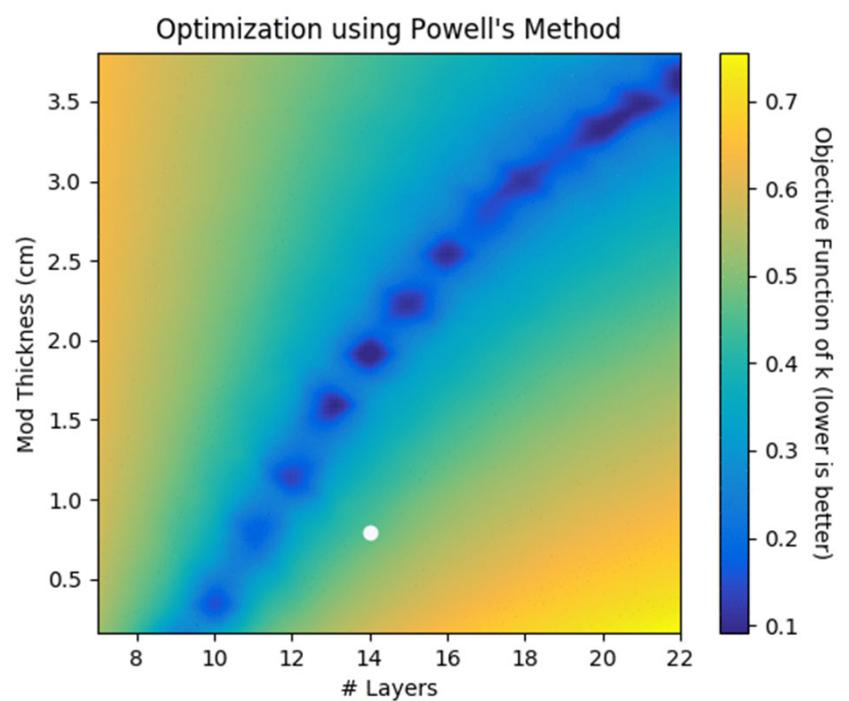


Select the minimum as the configuration closest to critical



# Optimizing the Objective Function

- Example of a linear search using Powell's Method
- These are the actual steps that were taken to determine some of the reported critical configurations



# Results

## **$^{239}\text{Pu}/\text{Alumina TEX}$**

- 8 critical assemblies selected
  - Intermediate fraction: 0.68
  - No thermal fission (<1%)
- Alumina moderator can be used to fine tune the neutron energy spectrum

## **$^{233}\text{U}/\text{Polyethylene TEX}$**

- 14 critical assemblies selected for CED-2
  - Thermal fraction: 0.81
  - Intermediate fraction: 0.57
- No critical assemblies with a majority fast fission were found



# $^{233}\text{U}/\text{Polyethylene}$ Critical Configurations

$N_x$	$N_y$	$N_z$	Moderator Thickness $t_M$ (cm)	Reflector Thickness $t_R$ (cm)	Fission Fractions		
					Thermal	Inter	Fast
6	4	11	0.794	2.54	0.53	0.41	0.06
6	4	18	0.476	2.54	0.41	0.51	0.08
6	4	11	0.635	3.81	0.52	0.42	0.06
6	4	15	0.476	3.81	0.46	0.47	0.08
8	6	13	0.476	2.54	0.41	0.51	0.08
8	6	19	0.318	2.54	0.32	0.57	0.11
9	6	13	0.476	2.54	0.41	0.51	0.08
9	6	18	0.318	2.54	0.32	0.57	0.11
7	5	6	4.76	2.54	0.81	0.16	0.03



# $^{233}\text{U}/\text{Polyethylene}$ Critical Configurations

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6	4	15	0.476	3.81	0.46	0.47	0.08
8	6	13	0.476	2.54	0.41	0.51	0.08
8	6	19	0.318	2.54	0.32	0.57	0.11
9	6	13	0.476	2.54	0.41	0.51	0.08
9	6	18	0.318	2.54	0.32	0.57	0.11
7	5	6	4.76	2.54	0.81	0.16	0.03



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6	4	18	0.476	2.54	0.41	0.51	0.08
6	4	11	0.635	3.81	0.52	0.42	0.06
6	4	15	0.476	3.81	0.46	0.47	0.08
8	6	13	0.476	2.54	0.41	0.51	0.08
8	6	19	0.318	2.54	0.32	0.57	0.11
9	6	13	0.476	2.54	0.41	0.51	0.08
9	6	18	0.318	2.54	0.32	0.57	0.11
7	5	6	4.76	2.54	0.81	0.16	0.03



# $^{233}\text{U}/\text{Polyethylene}$ Critical Configurations

$N_x$	$N_y$	$N_z$	Moderator Thickness $t_M$ (cm)	Reflector Thickness $t_R$ (cm)	Fission Fractions		
					Thermal	Inter	Fast
6	4	11	0.794	2.54	0.53	0.41	0.06
6	4	18	0.476	2.54	0.41	0.51	0.08
6	4	11	0.635	3.81	0.52	0.42	0.06
6	4	15	0.476	3.81	0.46	0.47	0.08
8	6	13	0.476	2.54	0.41	0.51	0.08
8	6	19	0.318	2.54	0.32	0.57	0.11
9	6	13	0.476	2.54	0.41	0.51	0.08
9	6	18	0.318	2.54	0.32	0.57	0.11
7	5	6	4.76	2.54	0.81	0.16	0.03



# $^{239}\text{Pu}/\text{Alumina}$ Critical Configurations

<b>Nx</b>	<b b="" ny<=""></b>	<b b="" nz<=""></b>	<b>Moderator Thickness <math>t_M</math> (cm)</b>	<b reflector="" thickness<br=""></b> $t_R$ (cm)	<b>Fission Fractions</b>	
					<b>Inter</b>	<b>Fast</b>
9	6	19	2.54	7.60	0.51	0.49
9	6	20	4.45	12.7	0.66	0.34
10	6	17	2.38	7.60	0.50	0.50
10	6	17	4.60	12.7	0.66	0.33
11	7	12	2.22	10.2	0.50	0.50
11	7	15	4.76	10.2	0.67	0.33
12	8	11	2.86	10.2	0.56	0.44
12	8	12	5.56	10.2	0.68	0.31



# $^{239}\text{Pu}/\text{Alumina}$ Critical Configurations

<b>Nx</b>	<b b="" ny<=""></b>	<b b="" nz<=""></b>	<b>Moderator Thickness <math>t_M</math> (cm)</b>	<b reflector="" thickness<br=""></b> $t_R$ (cm)	<b>Fission Fractions</b>	
					<b>Inter</b>	<b>Fast</b>
9	6	19	2.54	7.60	0.51	0.49
9	6	20	4.45	12.7	0.66	0.34
10	6	17	2.38	7.60	0.50	0.50
10	6	17	4.60	12.7	0.66	0.33
11	7	12	2.22	10.2	0.50	0.50
11	7	15	4.76	10.2	0.67	0.33
12	8	11	2.86	10.2	0.56	0.44
12	8	12	5.56	10.2	0.68	0.31



# $^{239}\text{Pu}/\text{Alumina}$ Critical Configurations

<b>Nx</b>	<b b="" ny<=""></b>	<b b="" nz<=""></b>	<b>Moderator Thickness <math>t_M</math> (cm)</b>	<b reflector="" thickness<br=""></b> $t_R$ (cm)	<b>Fission Fractions</b>	
					<b>Inter</b>	<b>Fast</b>
9	6	19	2.54	7.60	0.51	0.49
9	6	20	4.45	12.7	0.66	0.34
10	6	17	2.38	7.60	0.50	0.50
10	6	17	4.60	12.7	0.66	0.33
11	7	12	2.22	10.2	0.50	0.50
11	7	15	4.76	10.2	0.67	0.33
12	8	11	2.86	10.2	0.56	0.44
12	8	12	5.56	10.2	0.68	0.31



# $^{239}\text{Pu}/\text{Alumina}$ Critical Configurations

<b>Nx</b>	<b b="" ny<=""></b>	<b b="" nz<=""></b>	<b>Moderator Thickness <math>t_M</math> (cm)</b>	<b reflector="" thickness<br=""></b> $t_R$ (cm)	<b>Fission Fractions</b>	
					<b>Inter</b>	<b>Fast</b>
9	6	19	2.54	7.60	0.51	0.49
9	6	20	4.45	12.7	0.66	0.34
10	6	17	2.38	7.60	0.50	0.50
10	6	17	4.60	12.7	0.66	0.33
11	7	12	2.22	10.2	0.50	0.50
11	7	15	4.76	10.2	0.67	0.33
12	8	11	2.86	10.2	0.56	0.44
12	8	12	5.56	10.2	0.68	0.31



# Conclusions and Future Work

- These critical configurations will help to verify and validate nuclear data for neutron-induced fission with  $^{239}\text{Pu}$  and  $^{233}\text{U}$  by maximizing the relative fission fraction in the intermediate energy range
- Optimus offers a significant time savings during the design and search process for critical configurations
- IER-329 ( $^{233}\text{U}/\text{Polyethylene}$ ) will further study these 14 configurations in the CED-2 report



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- Thanks to our colleagues at the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) for their technical expertise and the collaboration that inspired the test cases and development of the Optimus software package
  - IRSN maintains a similar and much more mature code called Prométhée: <http://promethee.irsn.fr>



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# Questions?

Thanks for attending!

