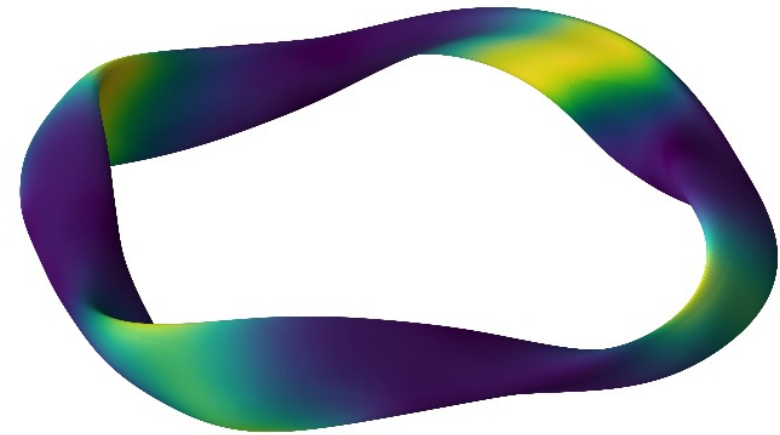
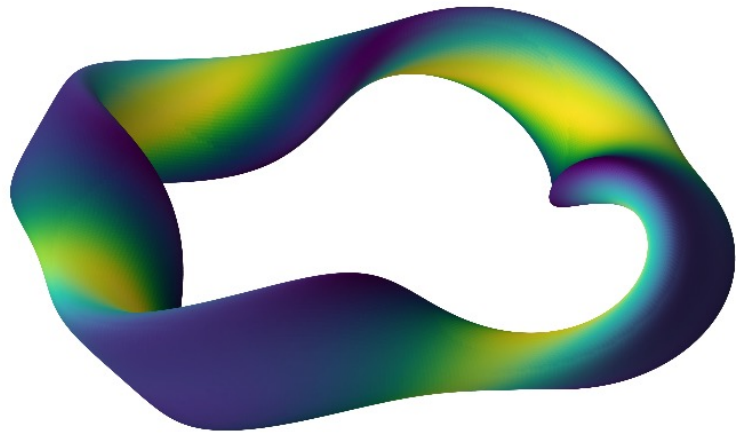


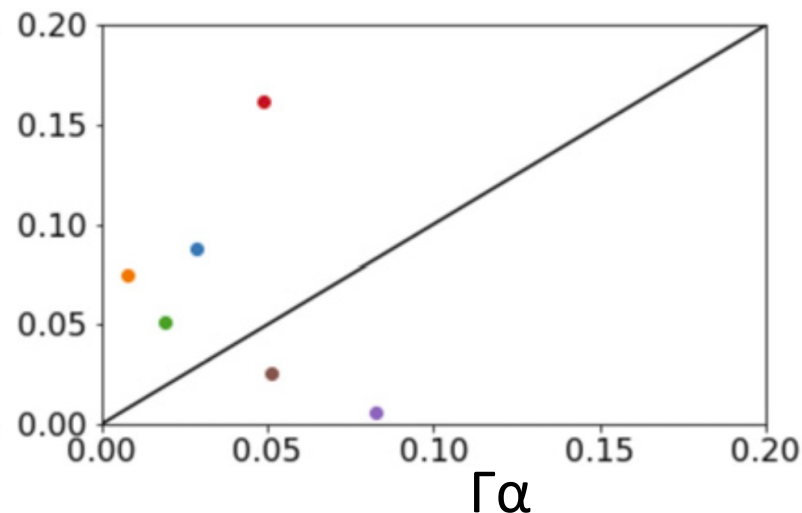
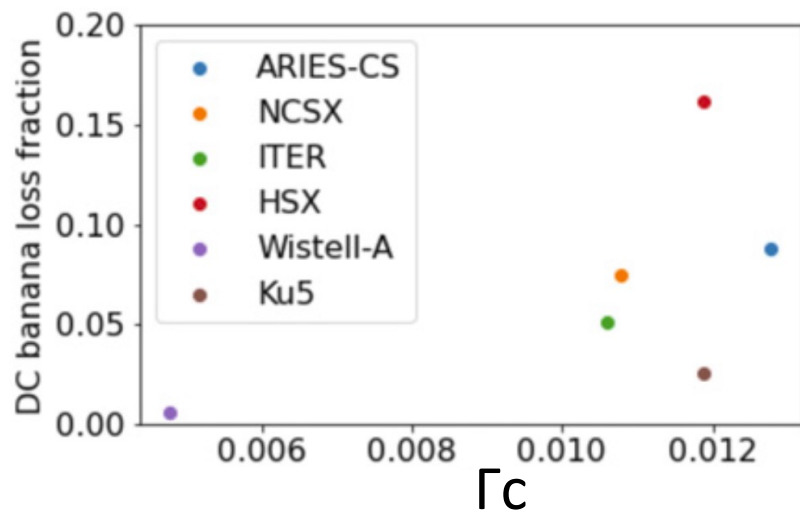
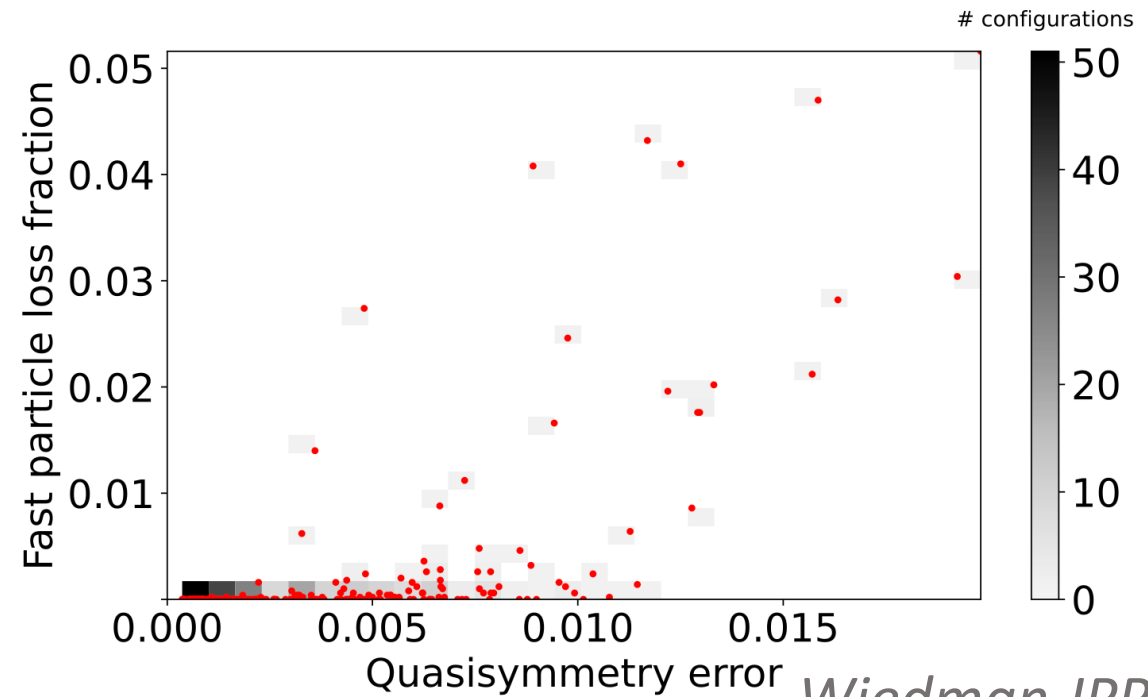
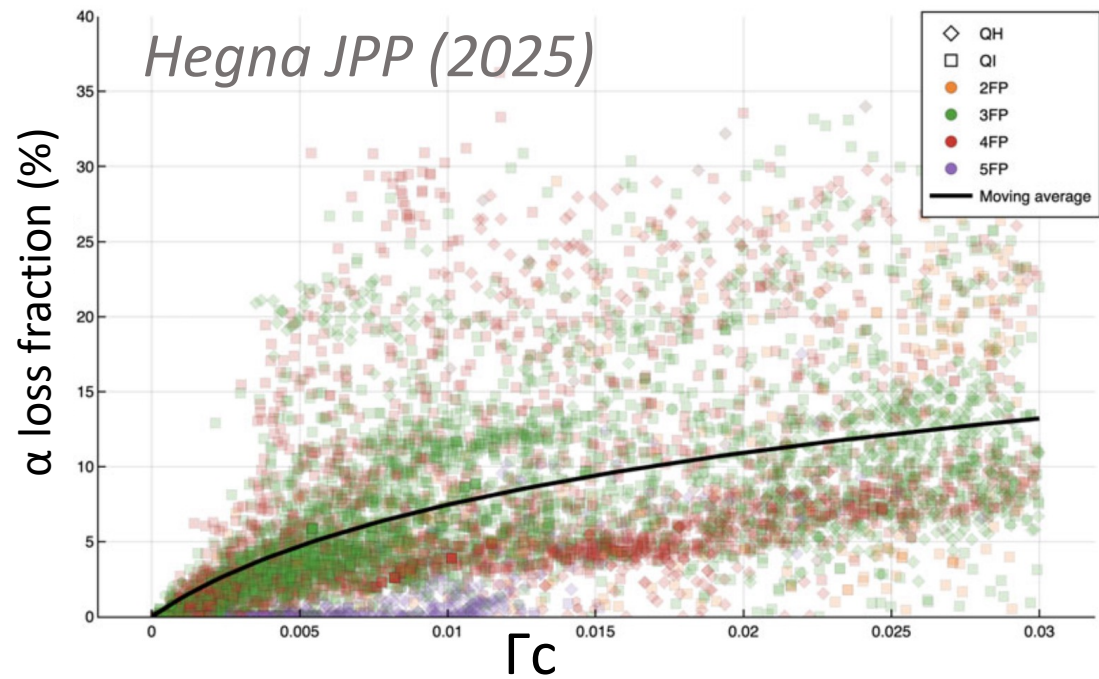
Bayesian optimization of stellarator α -particle confinement using data-informed parameter spaces & dimensionality reduction



Matt Landreman¹, Michael Czekanski², Andrew Giuliani³,
Byoungchan Jang¹, Rory Conlin¹

1. University of Maryland 2. Cornell University 3. Flatiron Institute

Physics-based surrogates like quasisymmetry & Γ_c aren't that well correlated with α confinement

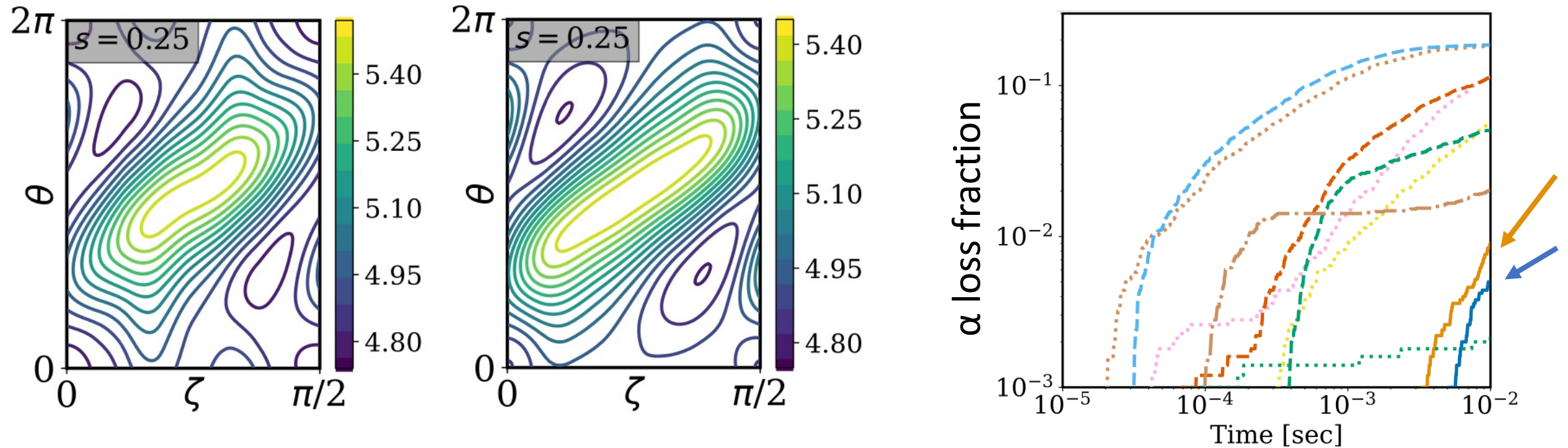


Wiedman JPP (2024)

Paul NF (2022)

We should try harder at directly tracing alpha particles inside optimization

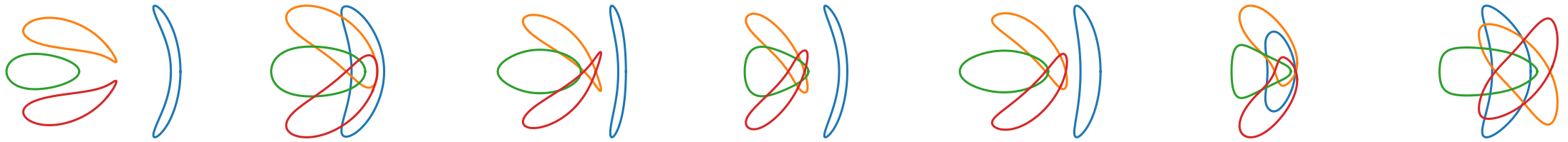
- Bindel, Landreman, & Padidar (2023) traced alphas in the optimization loop, found promising new configurations with significant departures from QS/QI in the loop.



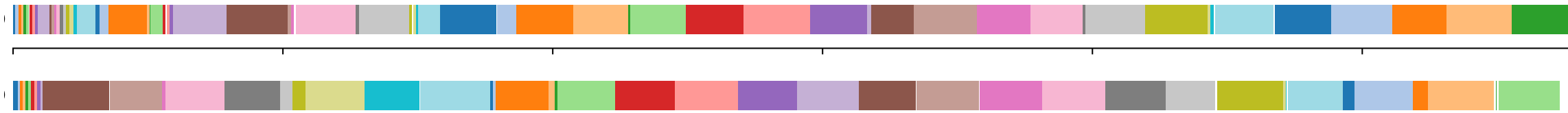
- Related work on piecewise omnigenity (Velasco, Zhu, Fernández-Pacheco, Liu, ...)
- GPUs now allow tracing 25,000 particles for 0.1 s (physical time) in only ~4 minutes wallclock. Affordable in the loop.

Outline

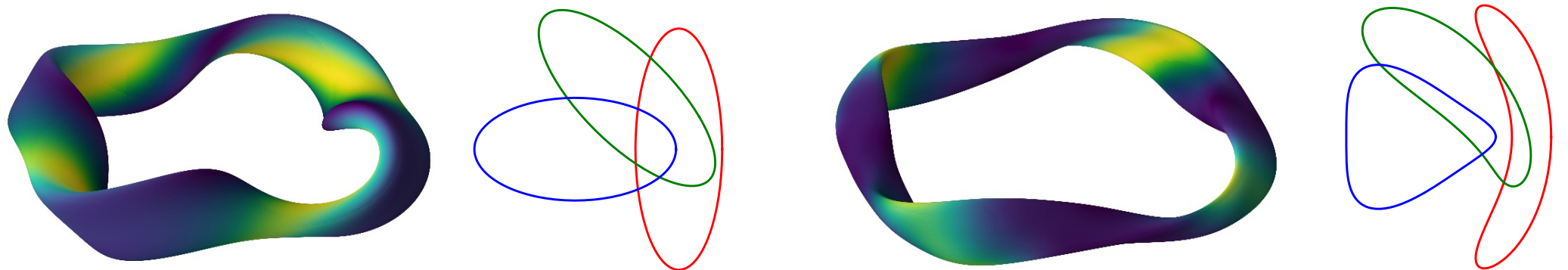
1. New parameter spaces to optimize in



2. Bayesian optimization of α -particle confinement



3. Resulting new configurations

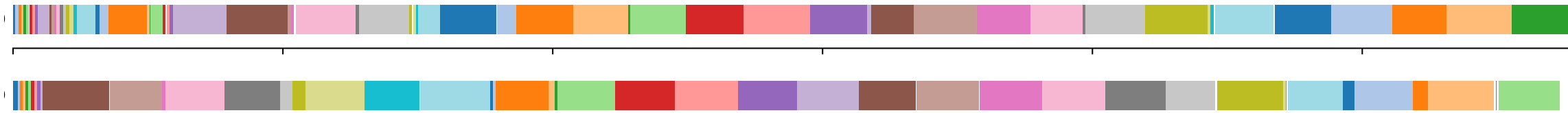


Outline

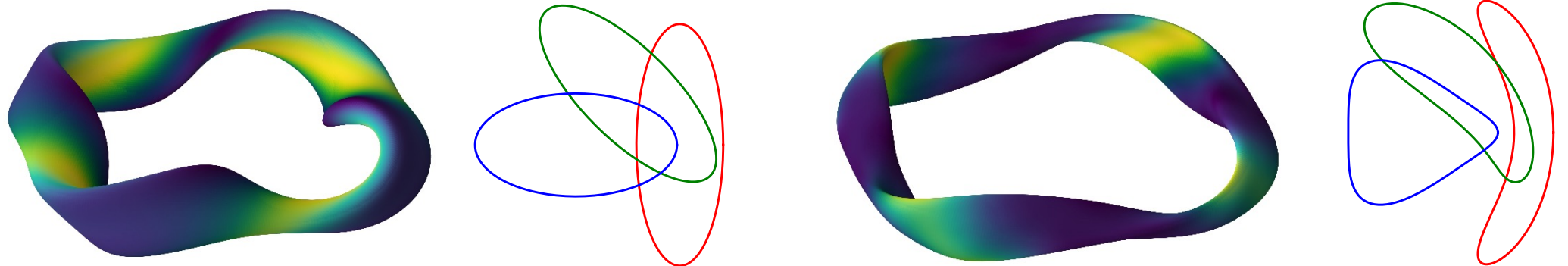
1. New parameter spaces to optimize in



2. Bayesian optimization of α -particle confinement



3. Resulting new configurations



For alphas in the loop, need a well-scaled parameter space

- Due to Monte-Carlo noise & chaos, focus on derivative-free optimization algorithms.
- Many algorithms (e.g. Bayesian) need bound constraints. Hard to pick these with the usual Fourier representation.
- Need d.o.f.s to be scaled comparably.
- Derivative-free methods don't scale well with # of dimensions. Try dimensionality reduction.
- Here: 2 new parameter spaces, both based on dataset of boundary shapes.

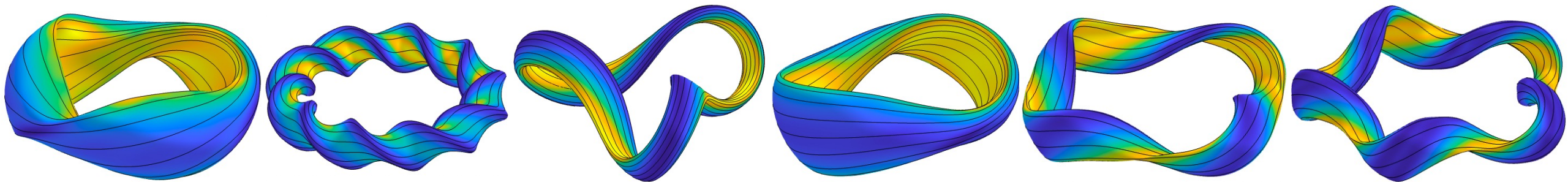
Diverse dataset of known stellarator boundaries

Combine 3 groups:

- 1) Famous devices (W7-X, LHD, HSX, NCSX, TJ-II, CTH, CNT, ...)
- 2) QUASR (QA & QH). Pick configs with lowest QS error at each aspect ≤ 10 , iota, nfp. Filter: vmec++ converges at $\beta=2\%$
- 3) ConStellation (QI). Filter for aspect ≤ 10 , vmec++ converges at $\beta=2\%$, Mercier-stable or nearly so.

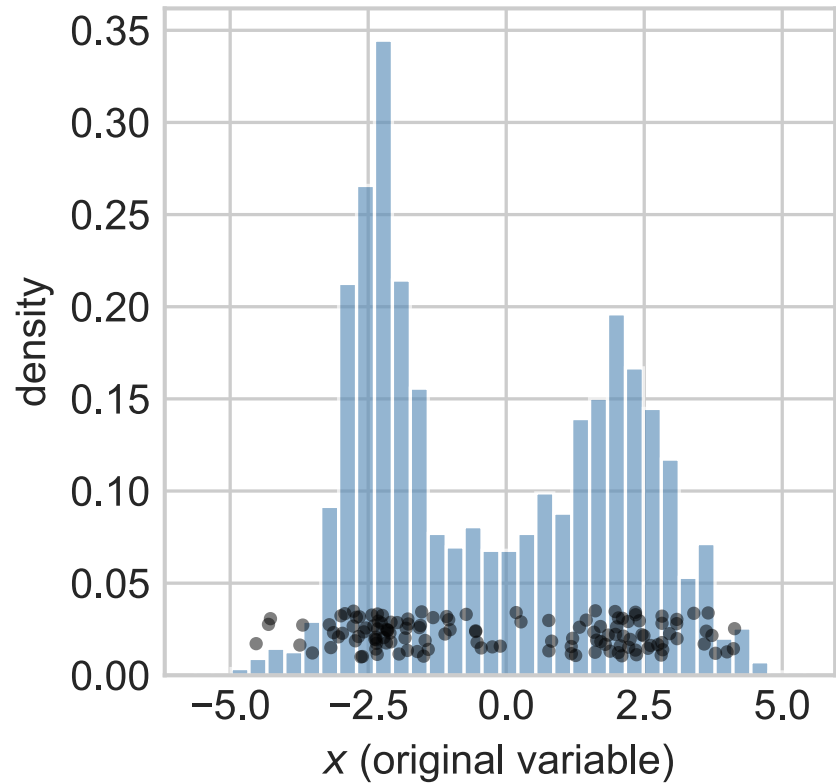
Systematize orientation ($\theta=0$ at outboard, bean at $\phi=0$, etc.)

Apply spectral condensation to all, to systematize θ .

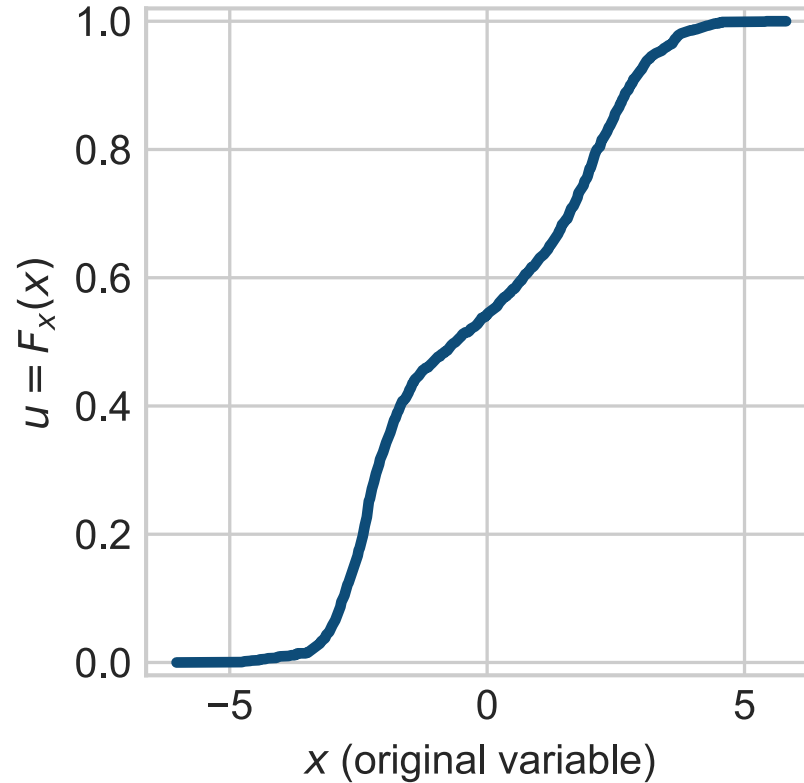


Use quantile transformation to map between distribution & [0,1]

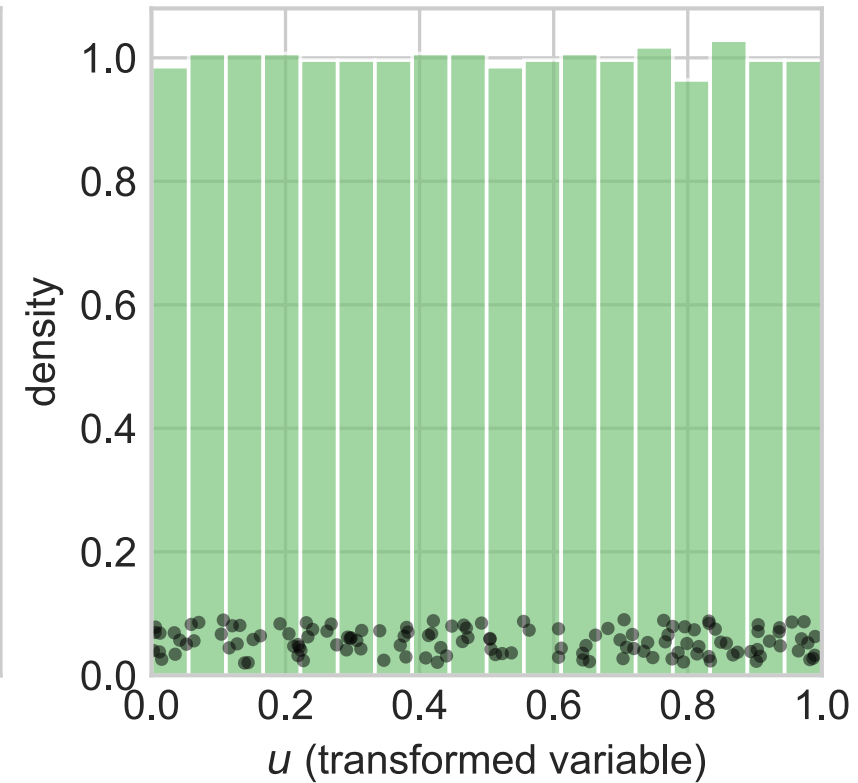
Original Distribution



Empirical CDF



Transformed Distribution

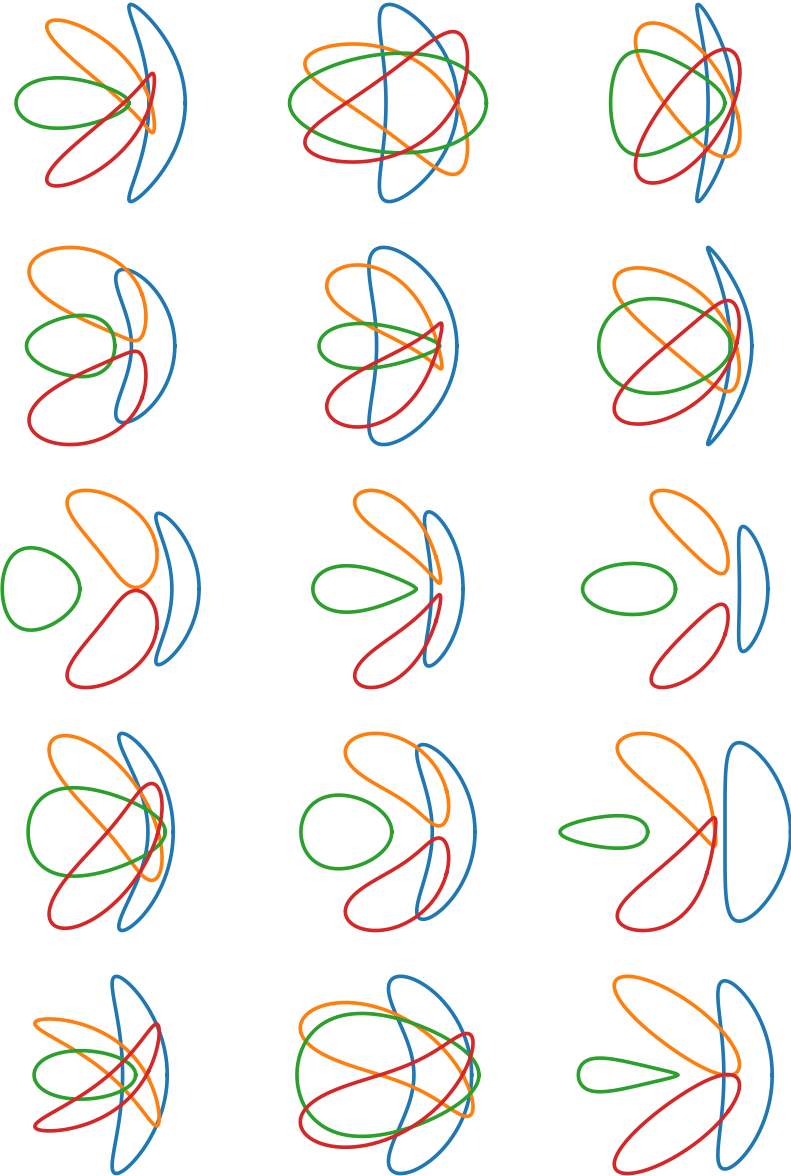


← Inverse map

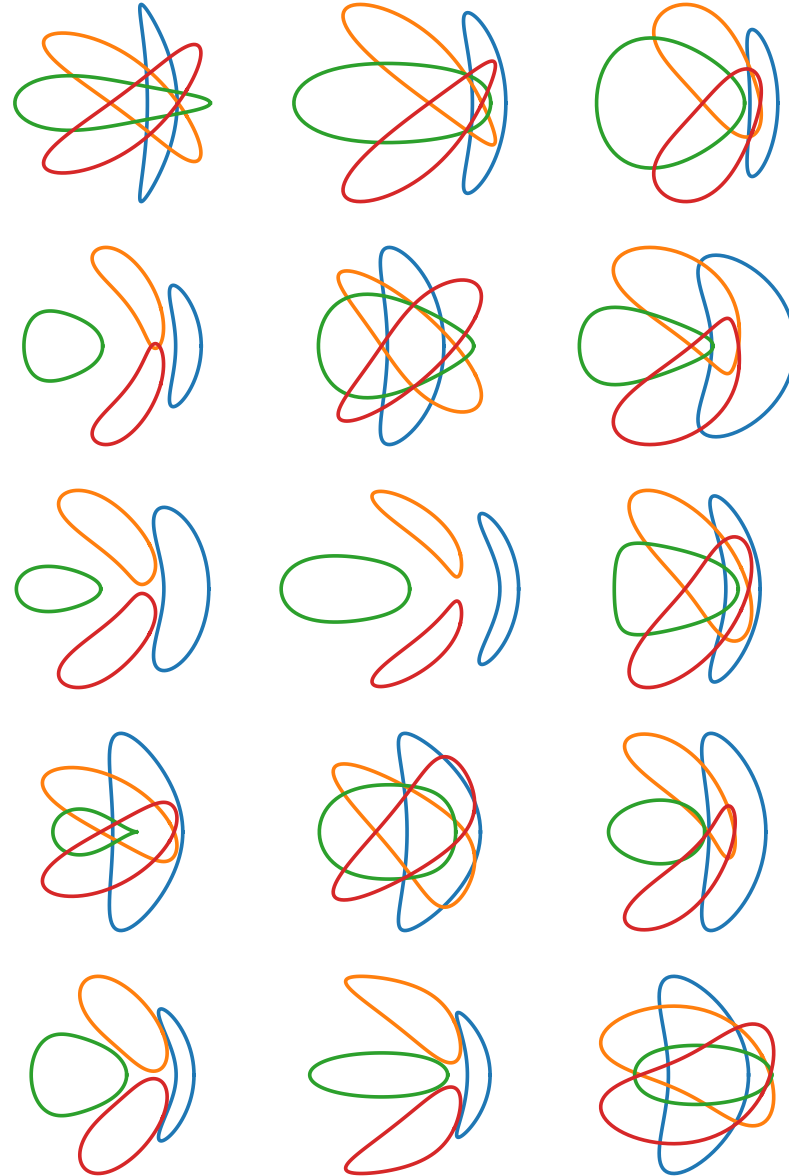
d.o.f.s for optimization

New space 1: Apply Quantile Transform to Garabedian Δ_{mn} 's

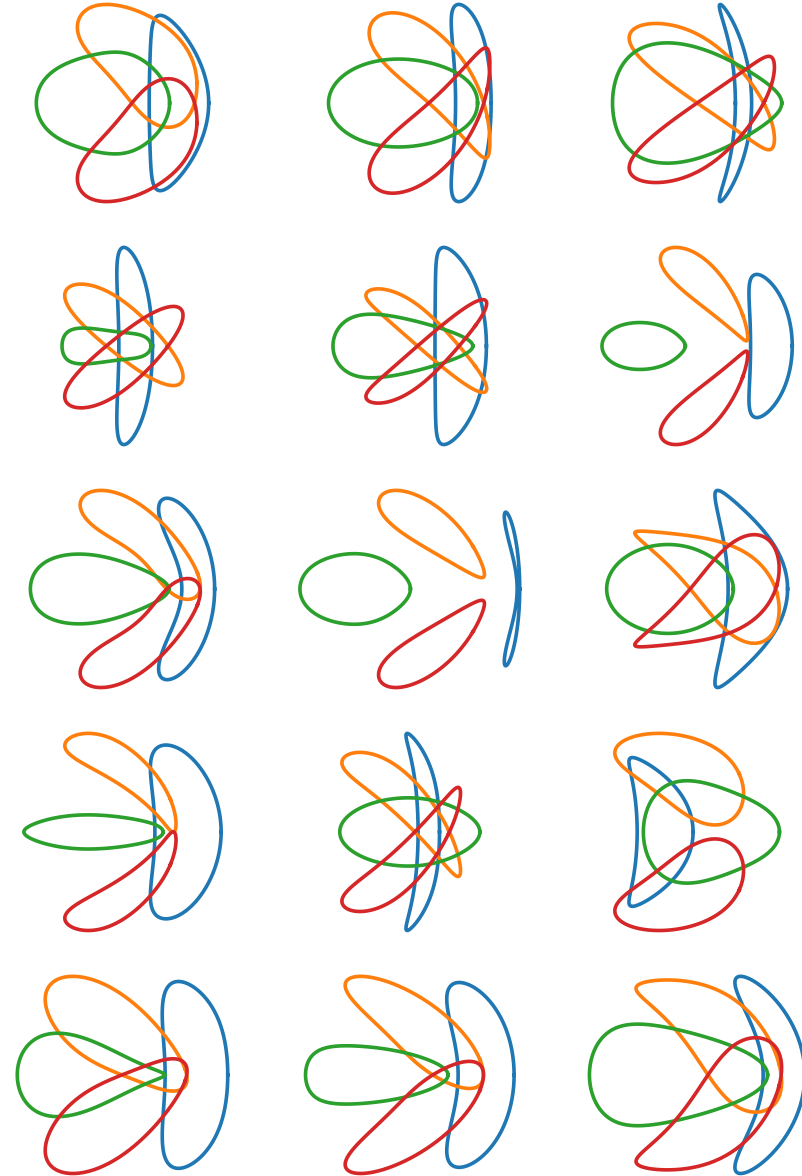
$|m| \leq 2, |n| \leq 2$



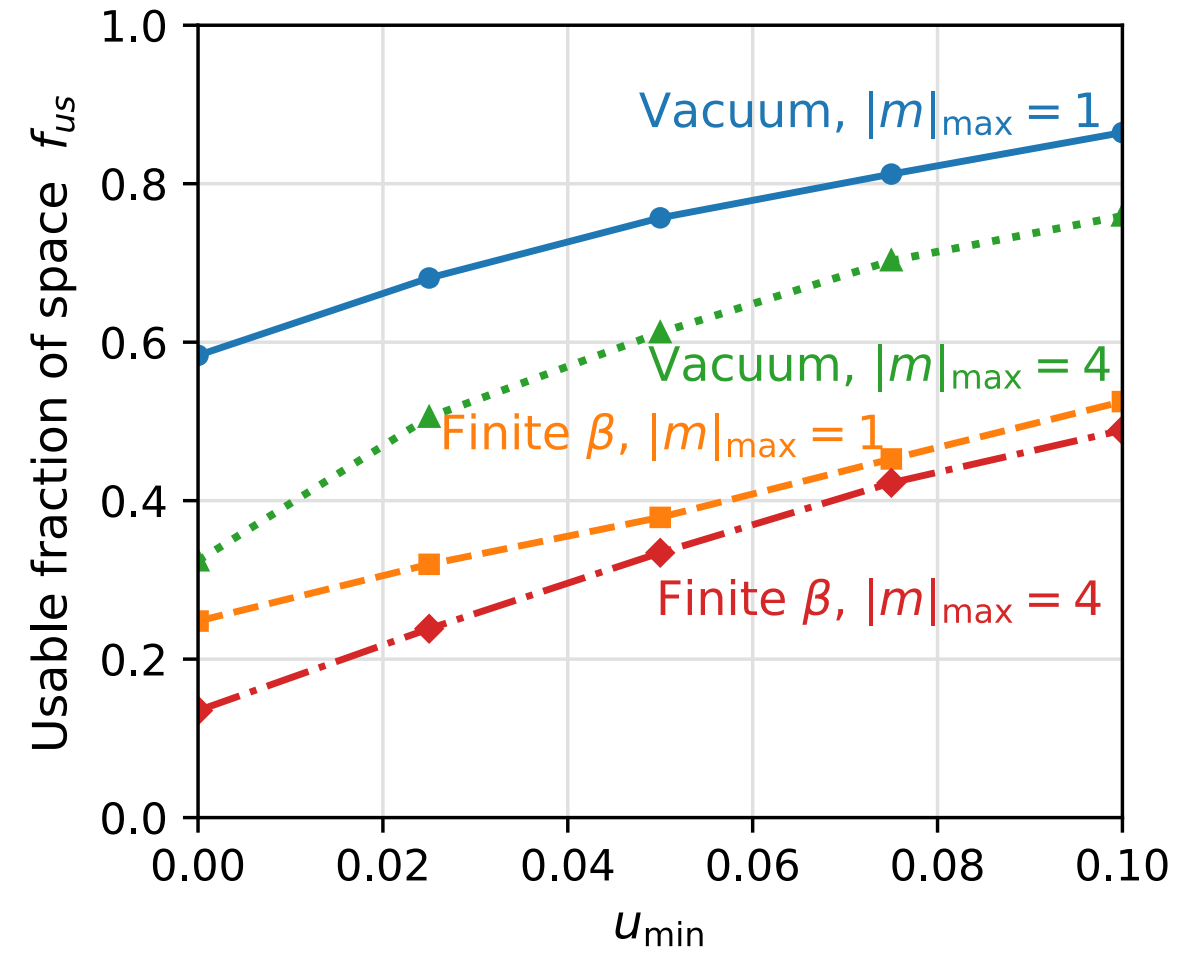
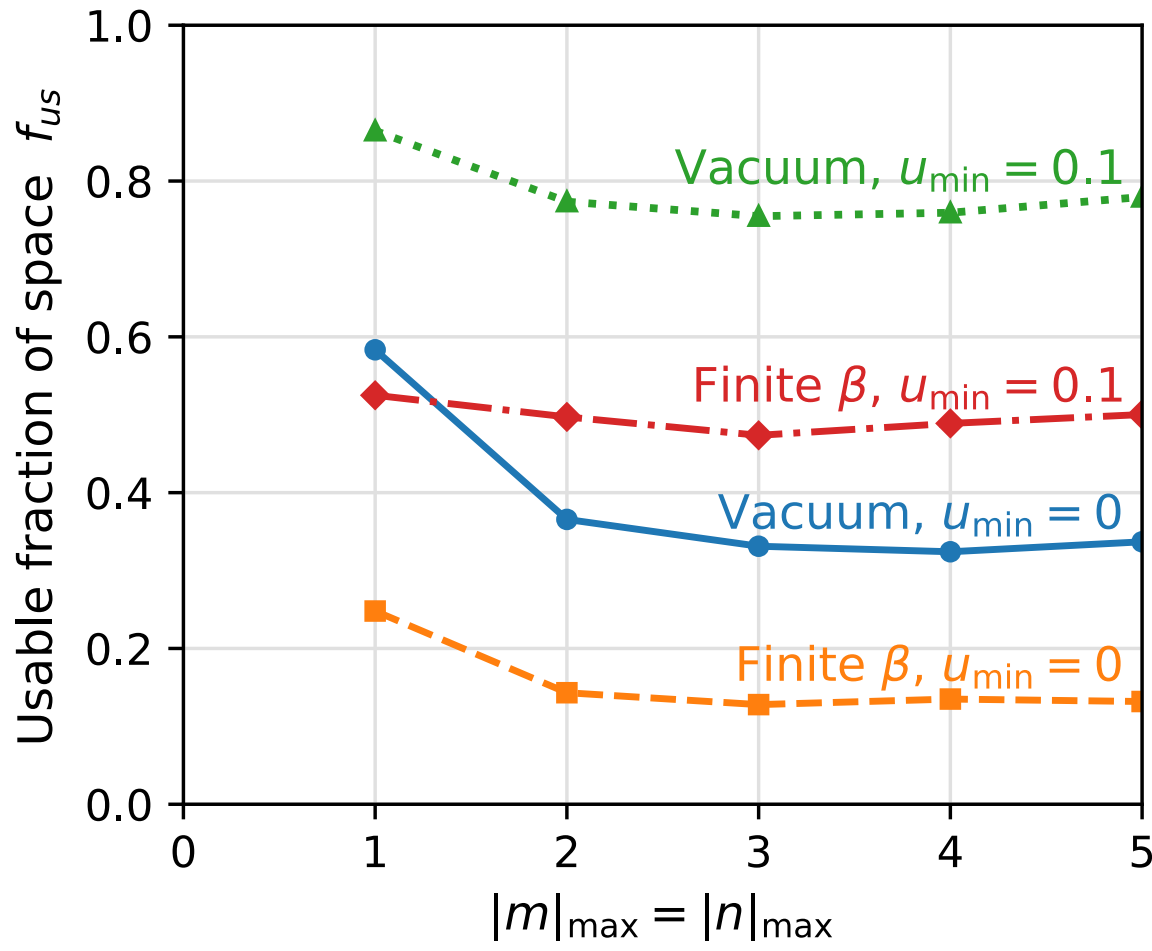
$|m| \leq 3, |n| \leq 3$



$|m| \leq 4, |n| \leq 4$



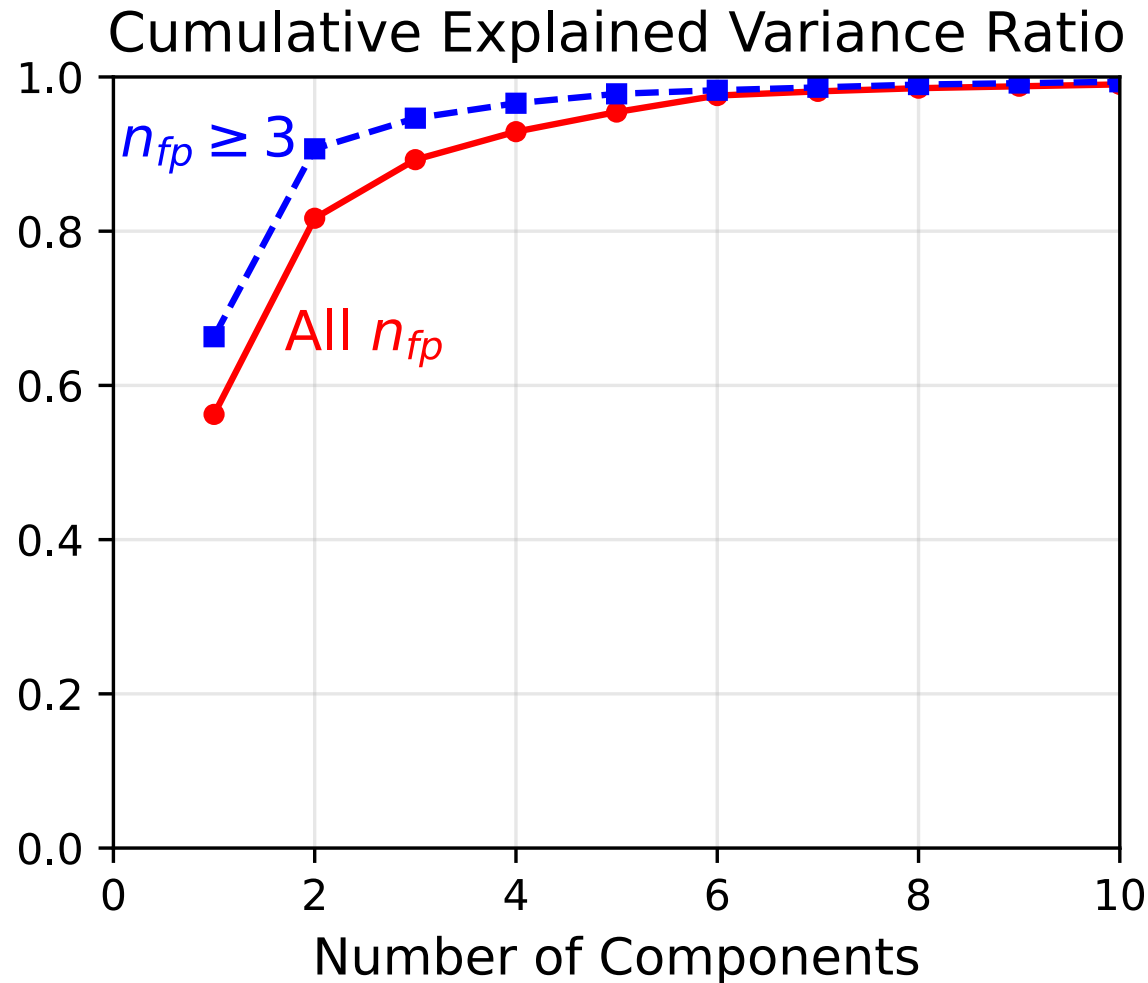
MHD equilibrium converges for a reasonable fraction of the space



Vmec++, each d.o.f. sampled uniformly on $[u_{\min}, 1 - u_{\min}]$

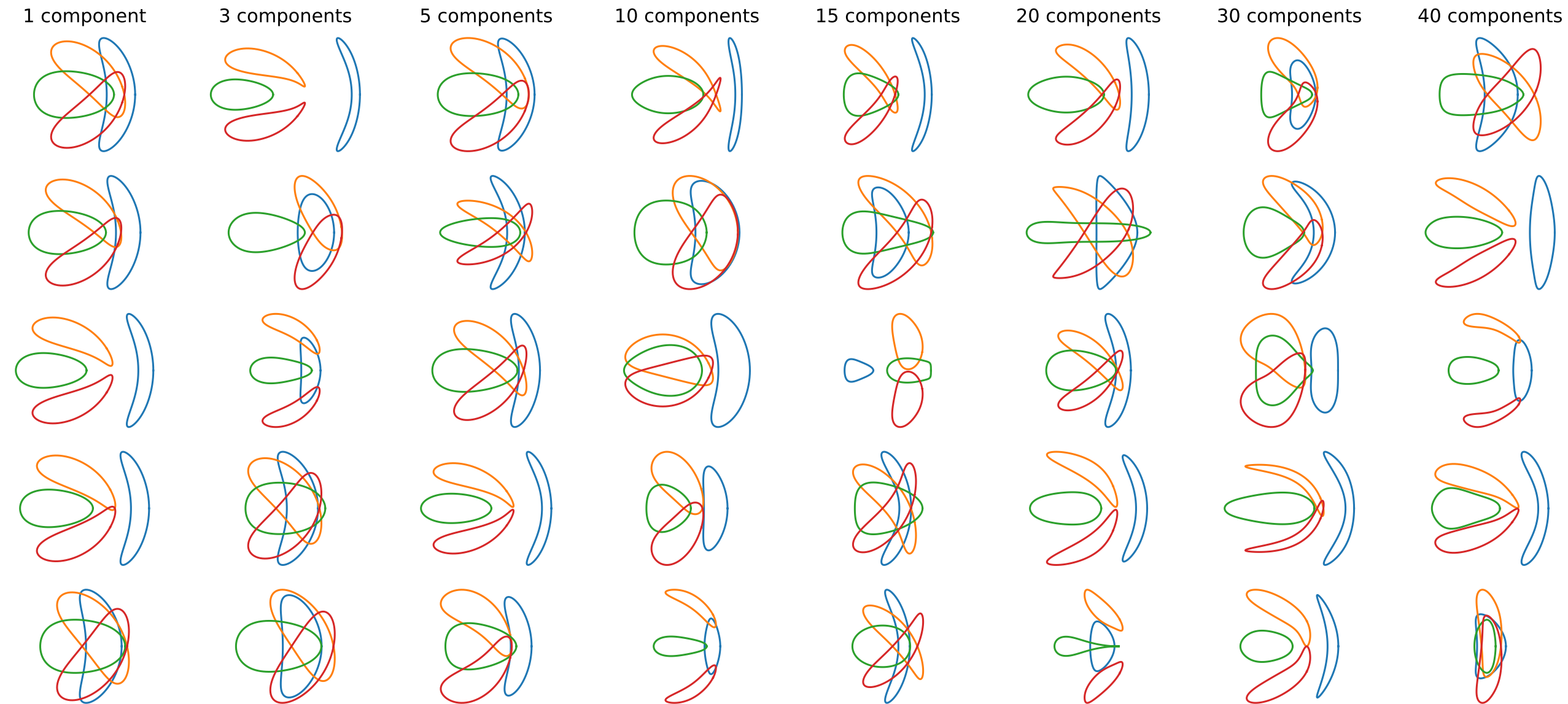
New space 2: principal components

- Apply PCA to boundary (R,Z) values, then apply quantile transform to PC amplitudes.
- Same advantages as space 1, & also dimensionality reduction.

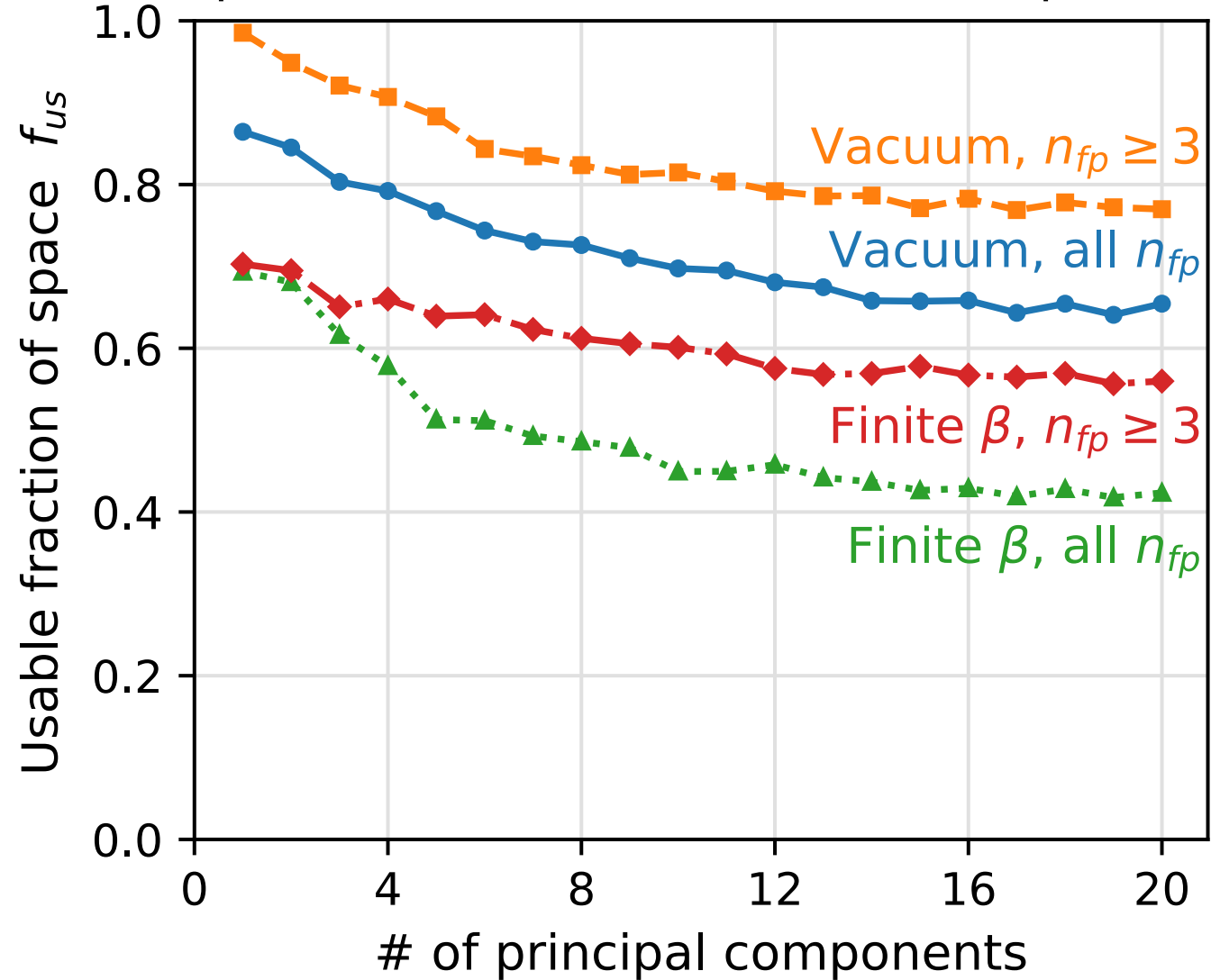


New space 2: principal components

- Apply PCA to boundary (R,Z) values, then apply QuantileTransform to PC amplitudes.



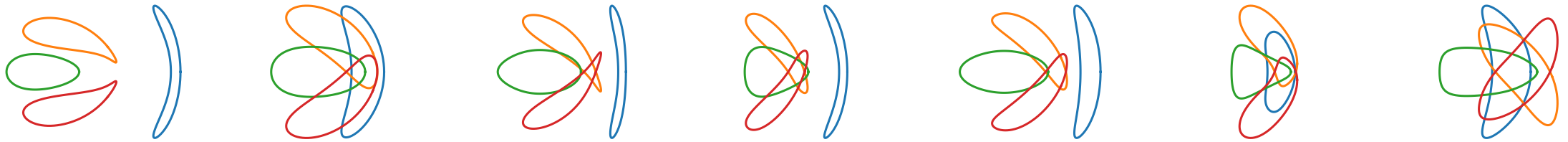
MHD equilibrium converges for a reasonable fraction of the space



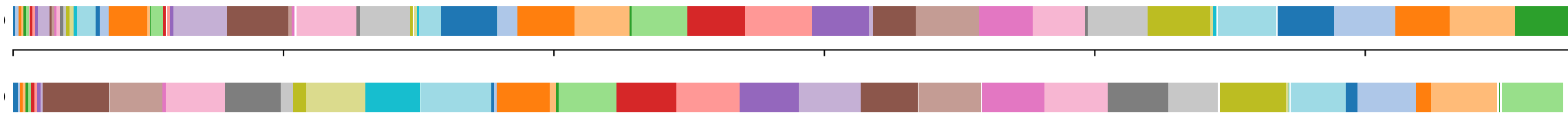
Vmec++, each d.o.f. sampled uniformly on $[0, 1]$

Outline

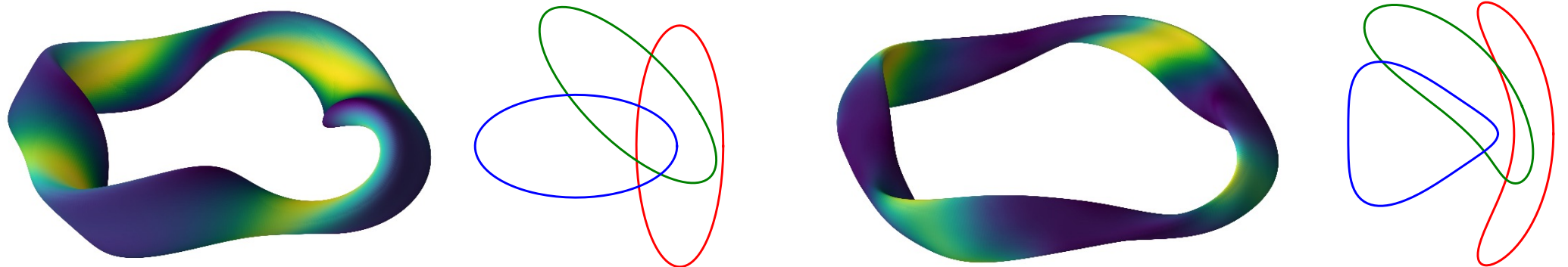
1. New parameter spaces to optimize in



2. Bayesian optimization of α -particle confinement



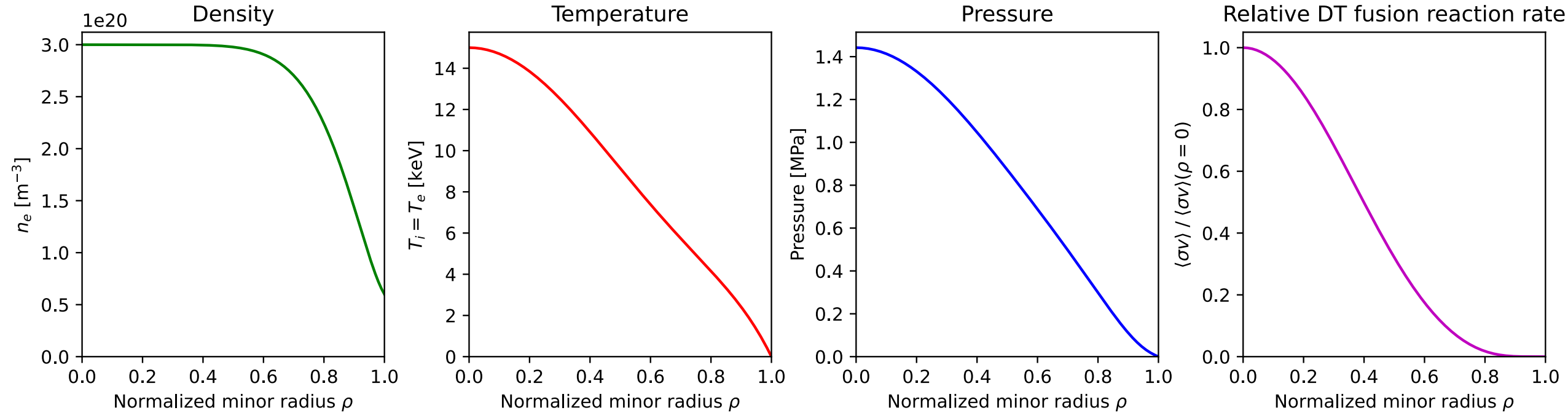
3. Resulting new configurations



Plausible profiles & scaling for alpha tracing

$$n_e(\rho) = (3 \times 10^{20} \text{ m}^{-3})(1 - 2\rho^8 + 1.2\rho^{12})$$

$$T_i(\rho) = T_e(\rho) = (15 \text{ keV})(1 - 2\rho^2 + 2\rho^4 - \rho^6)$$



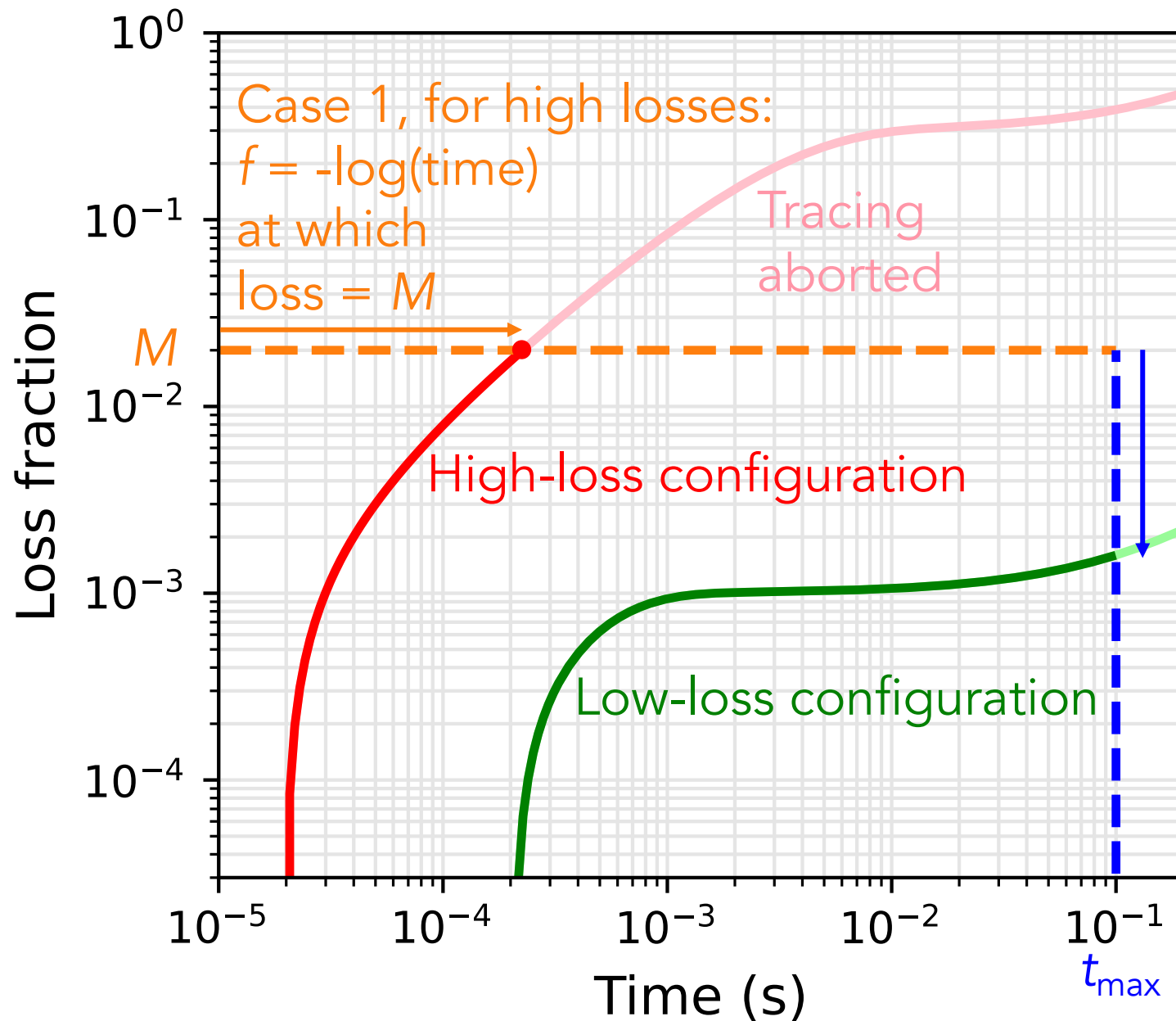
$$\text{Size scaling: } a = (0.31 \text{ m}) / (\text{aspect})^{0.38}$$

Fits Stellaris ($a=1.3\text{m}$), Infinity Two ($a=1.3\text{m}$), Helios ($a=1.8\text{m}$), ARIES-CS ($a=1.7\text{m}$)

Scale B so $B_{\text{max}} = 12 \text{ T}$. Comparable to Stellaris & Infinity Two.

B_{max} more meaningful constraint than $\langle B \rangle$. Gives $\langle \beta \rangle = 1.5\% - 3\%$.

The objective function saves computation for the best configurations



Case 1, for high losses:
 $f = -\log(\text{time})$
at which
loss = M

Tracing
aborted

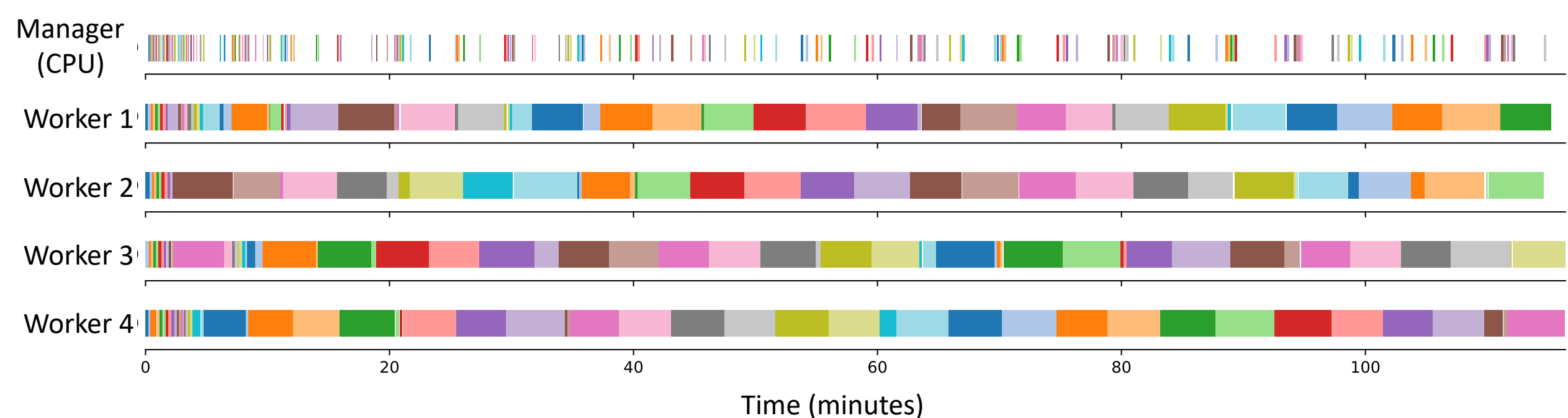
High-loss configuration

Low-loss configuration

Case 2, for low losses:
 $f = \text{constant} + \log(\text{loss})$ at t_{\max}

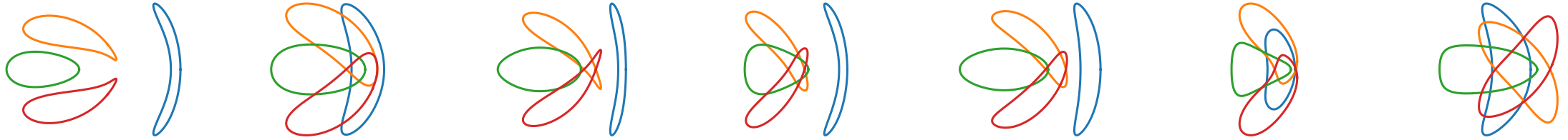
Asynchronous Bayesian optimization

- GPU guiding center tracing using FIRM3D/CATAPULT:
Czekanski arXiv:2604.07617,
`github.com/ColumbiaStellaratorTheory/firm3d`
- Trace 25,000 particles for 0.1 sec physical time, source \propto fusion rate.
- Use all 4 GPUs on 1 node of Perlmutter (Nvidia A100s) for 2 hrs.

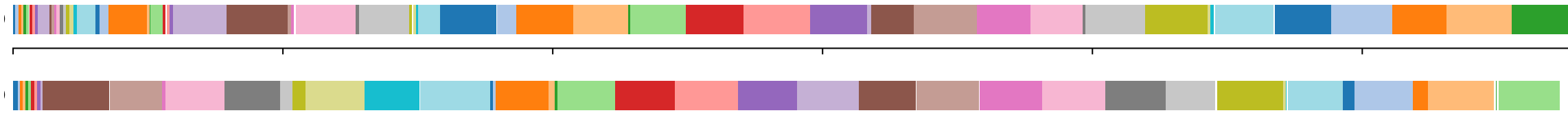


Outline

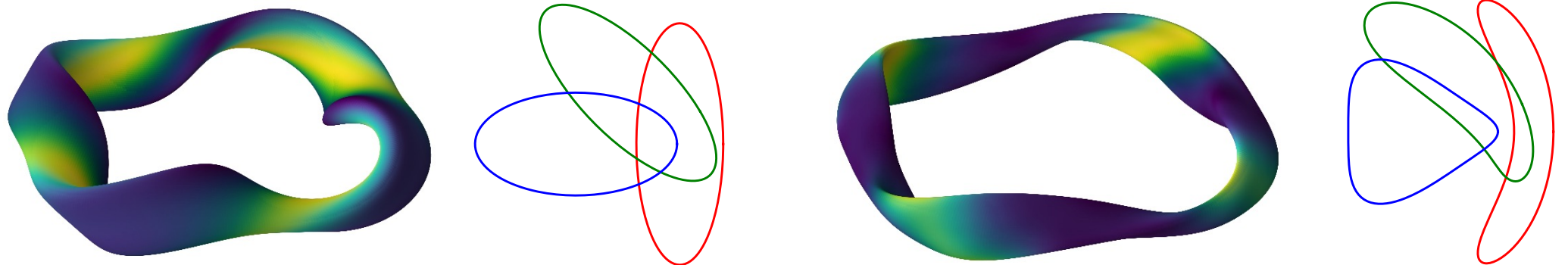
1. New parameter spaces to optimize in



2. Bayesian optimization of α -particle confinement



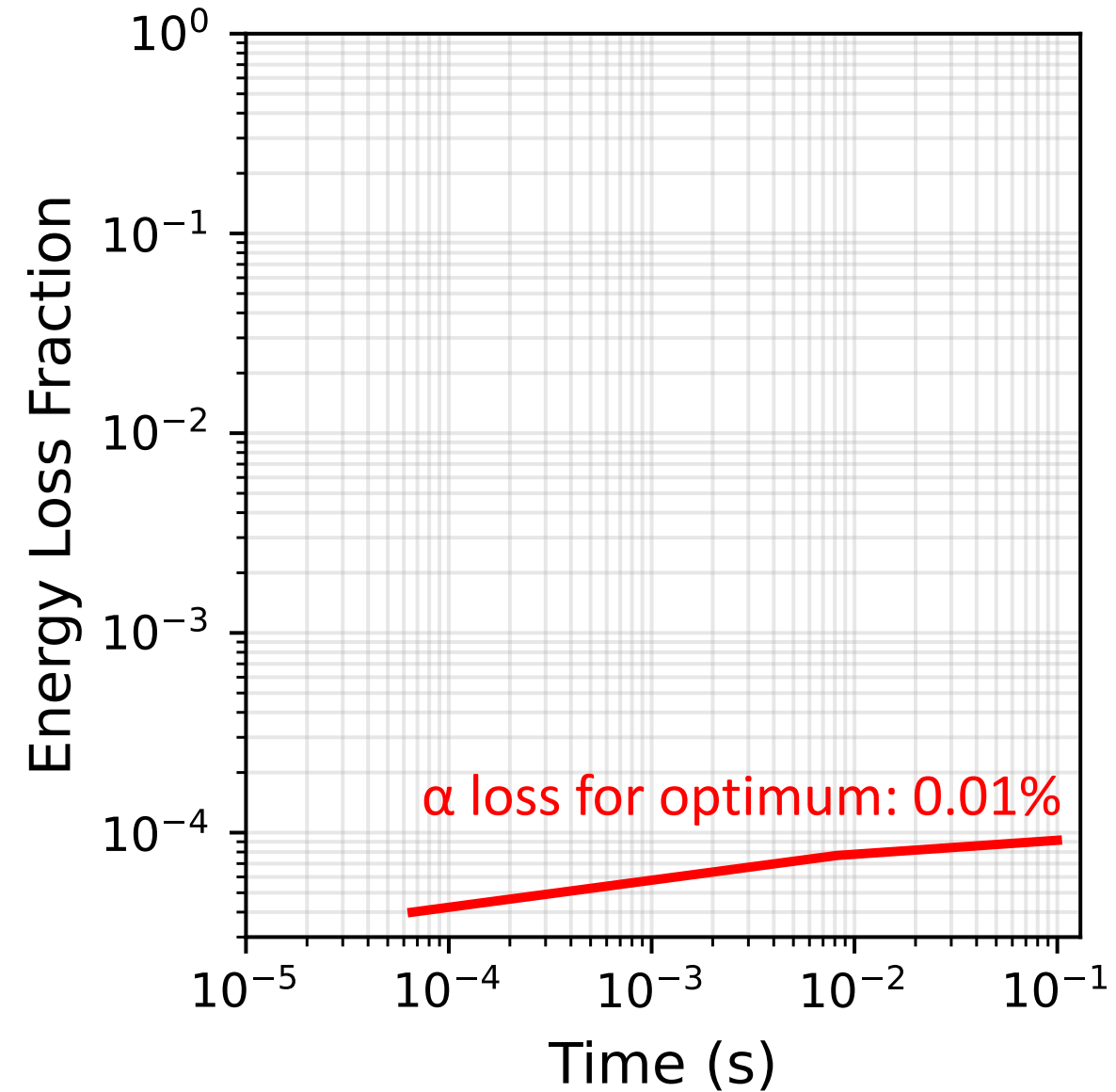
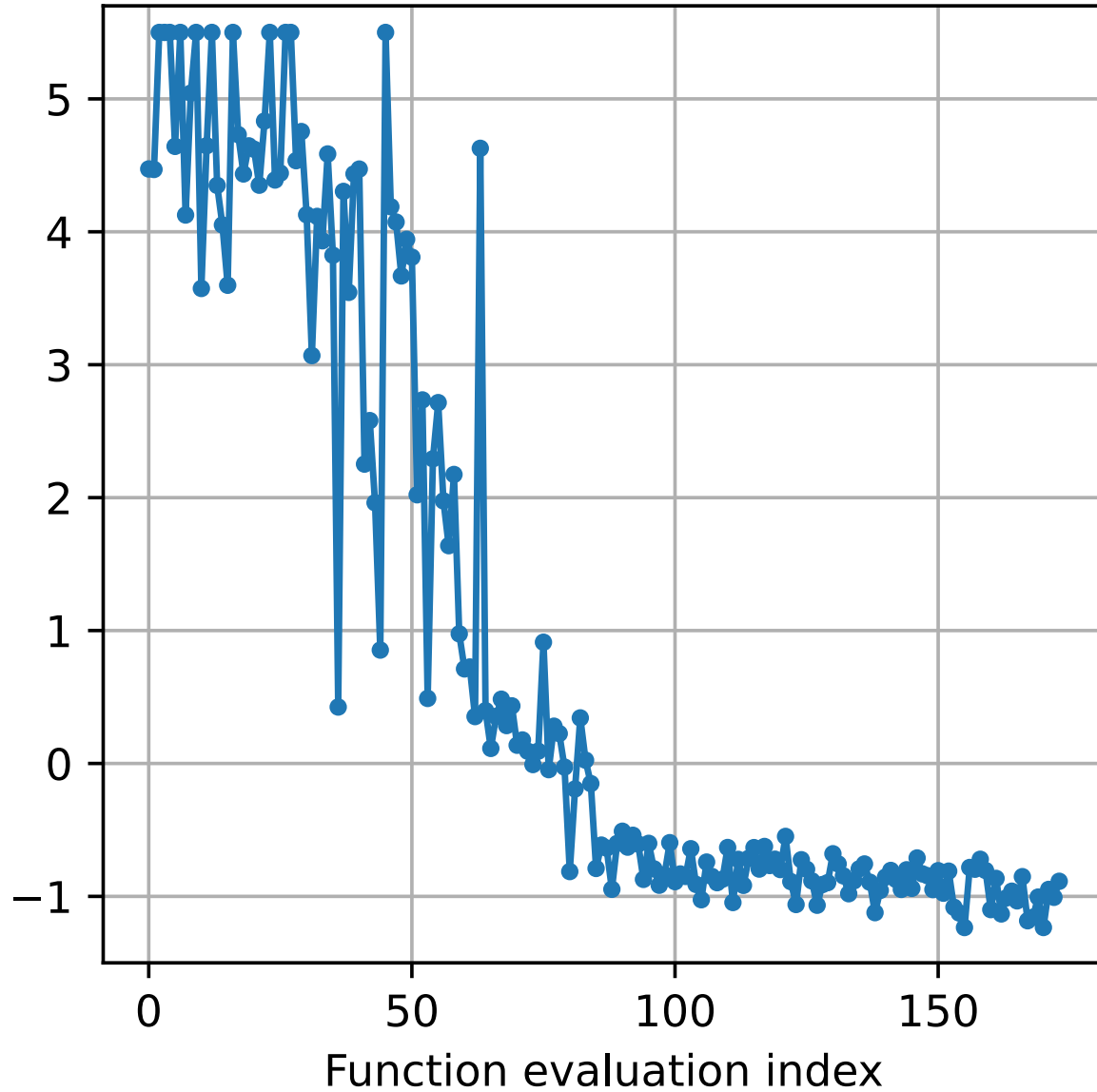
3. Resulting new configurations



New configuration 1

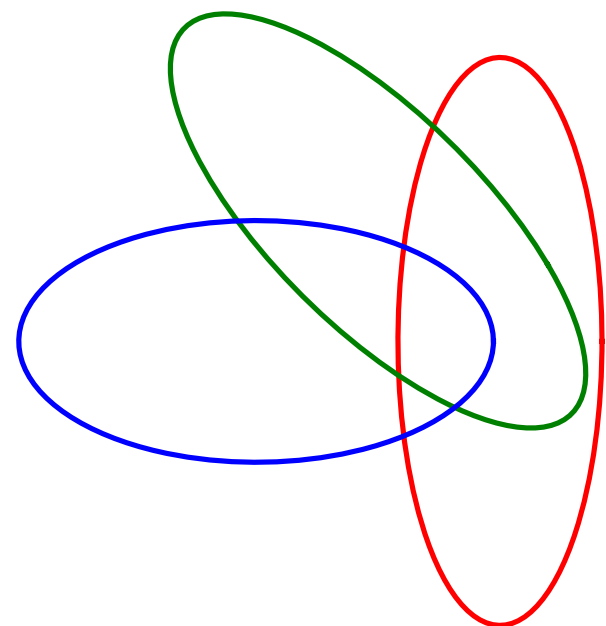
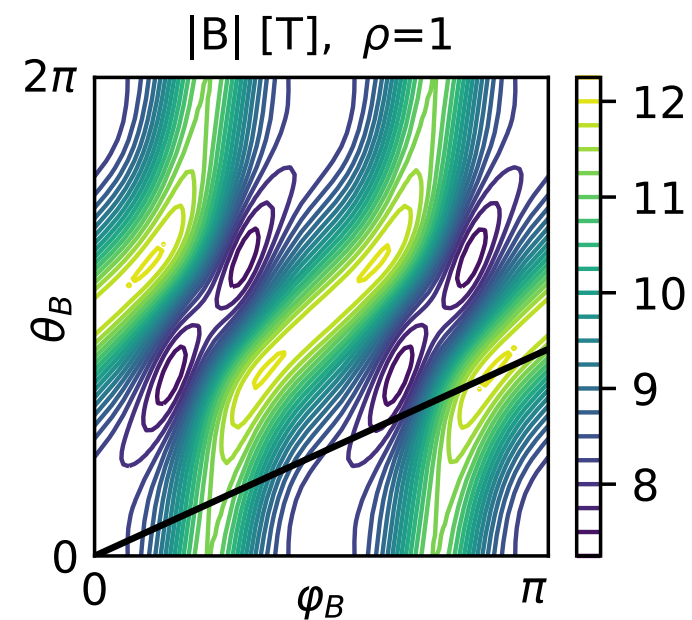
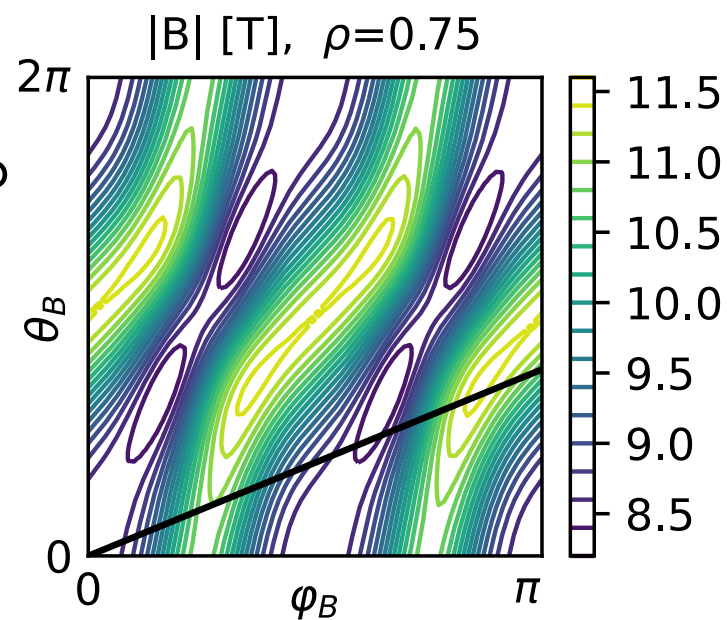
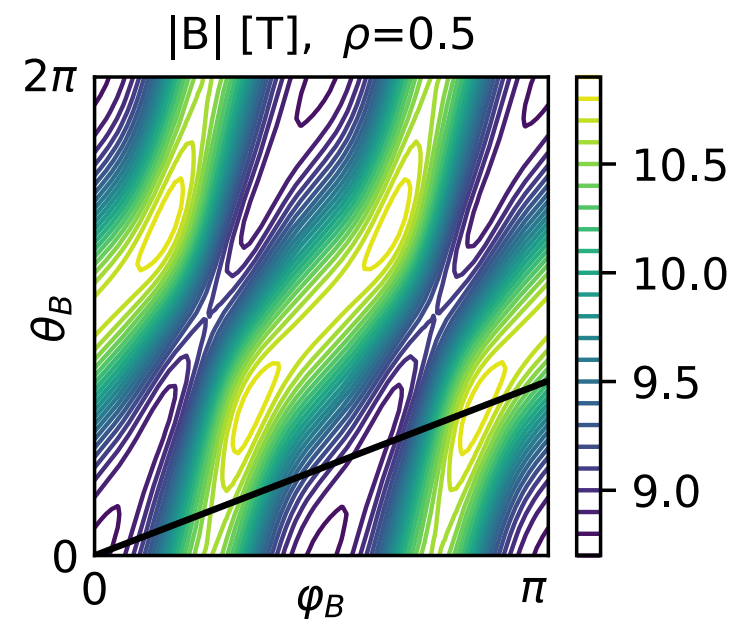
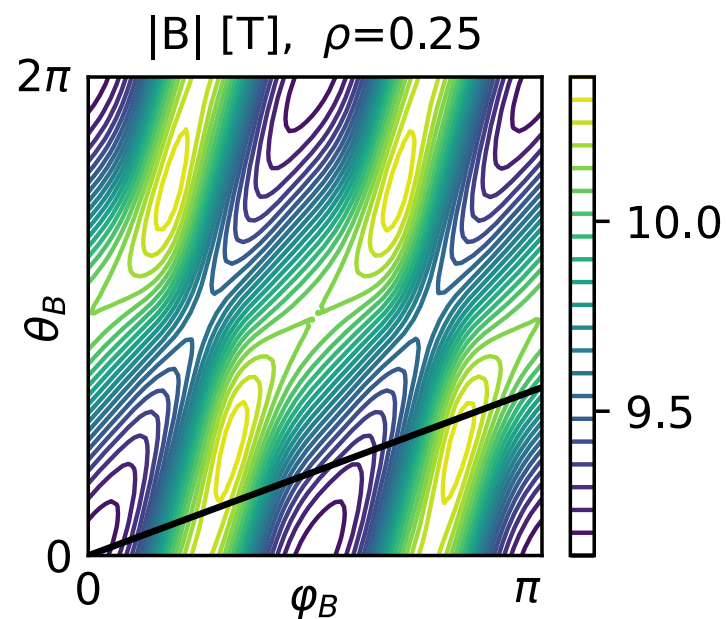
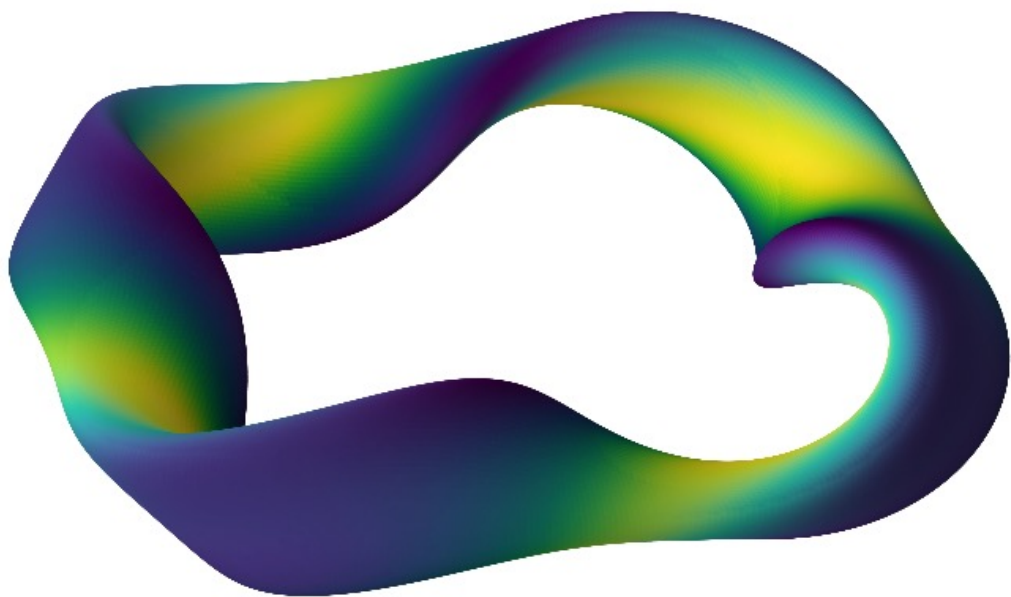
Garabedian space, $m, n \leq 1$. # dofs = 7

Optimization history



New configuration 1

QH-ish but far from ideal QH.

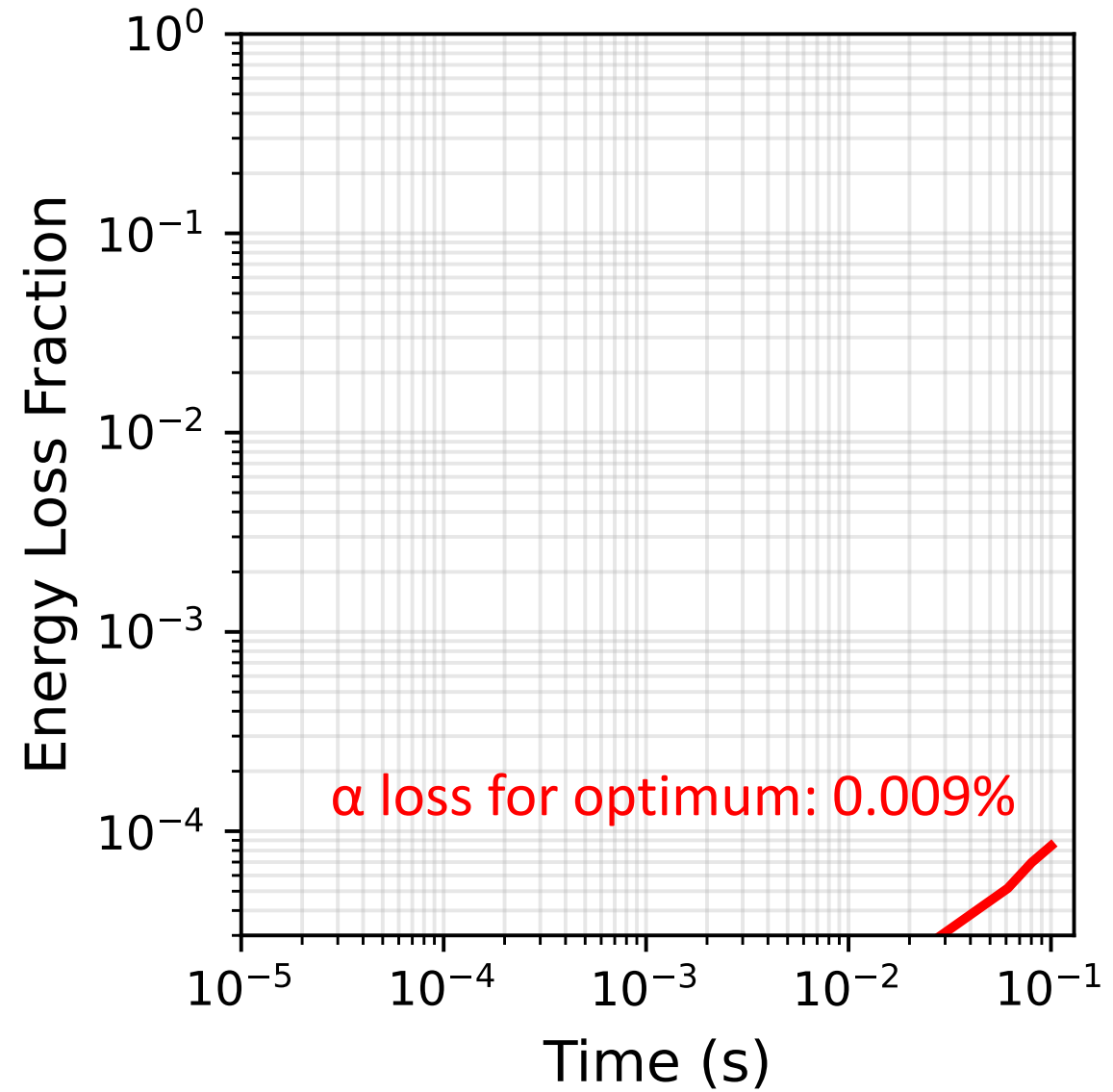
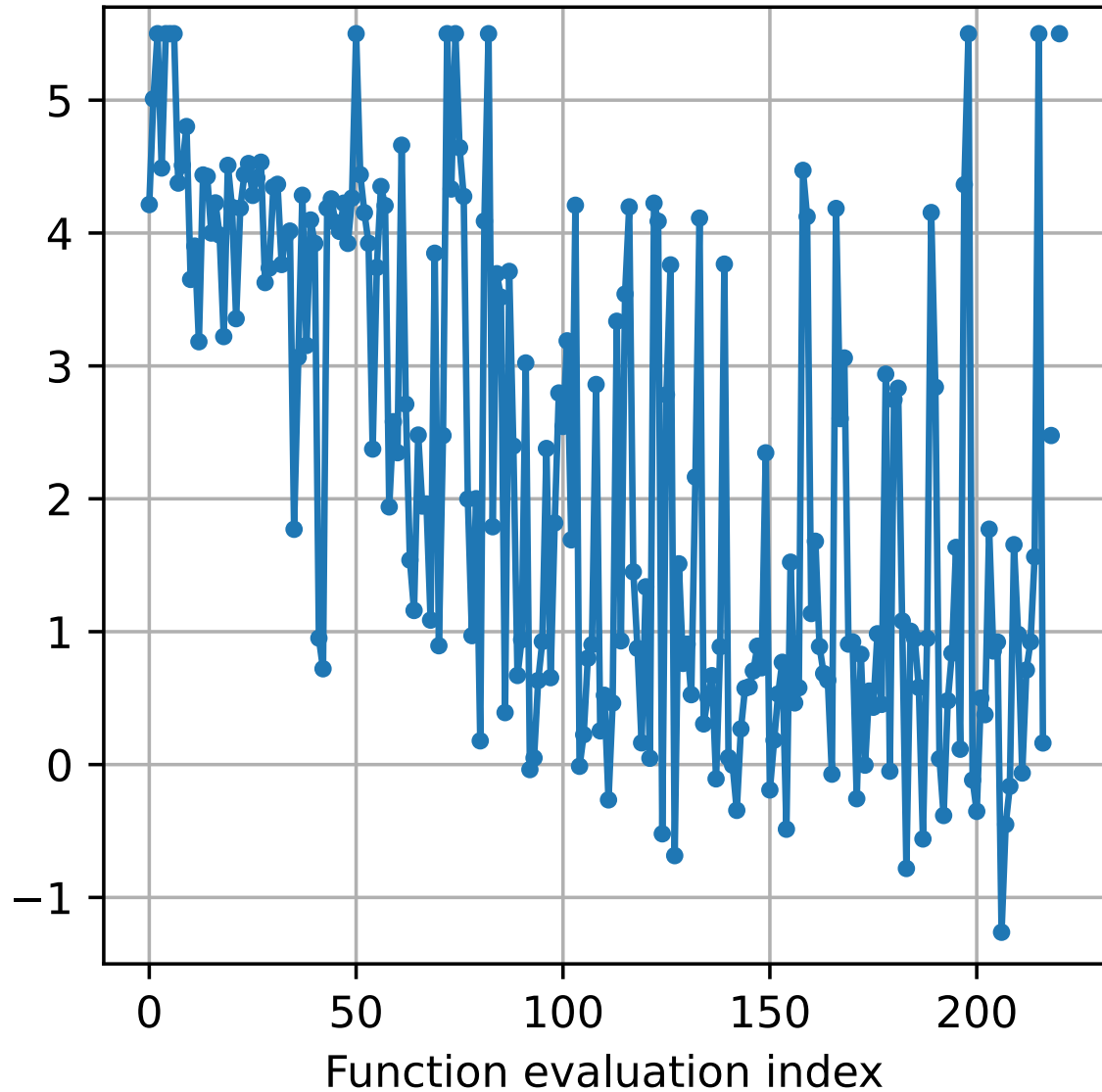


Aspect ratio = 6
 $\langle \beta \rangle = 1.5\%$

New configuration 2

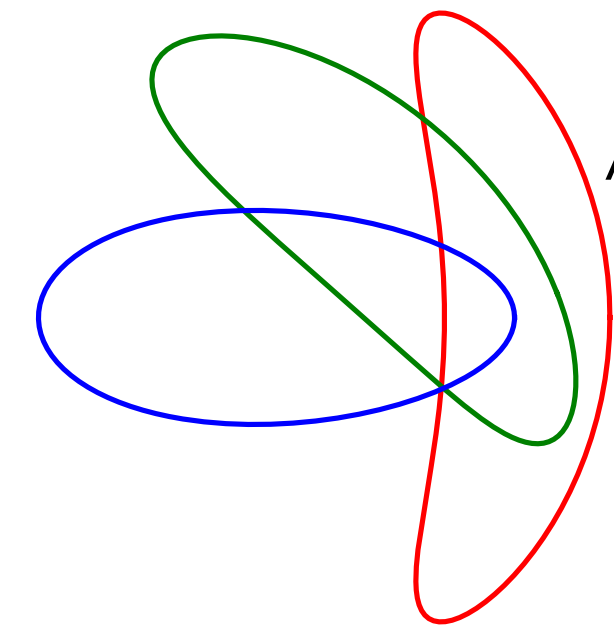
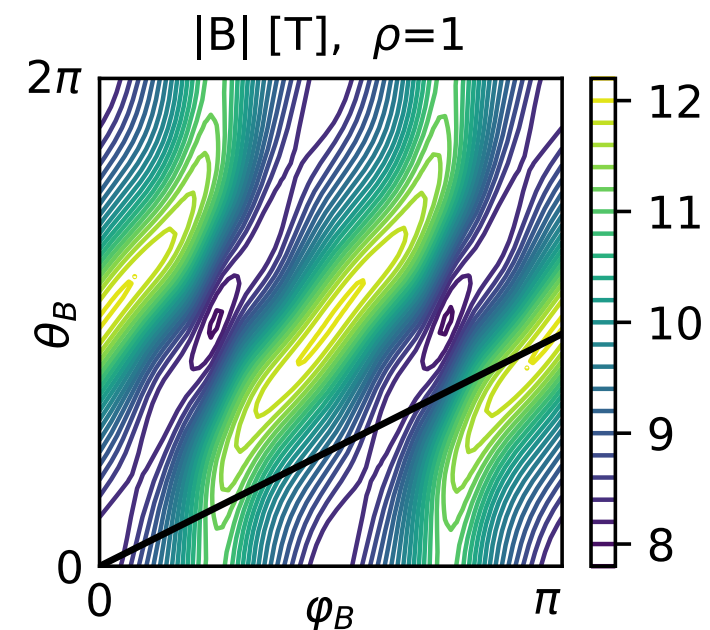
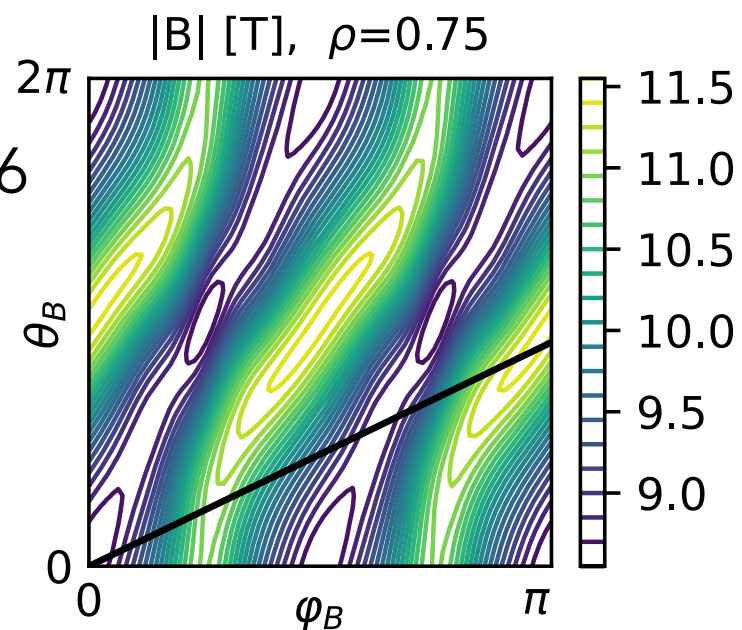
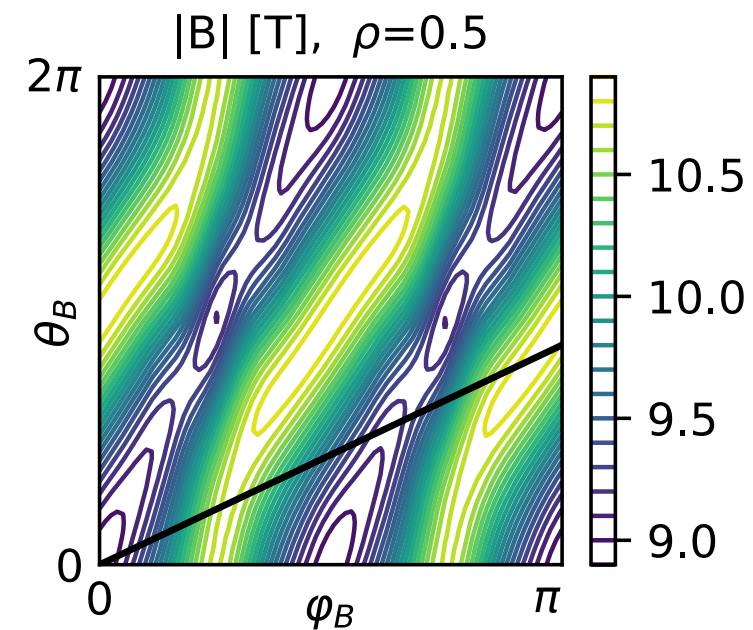
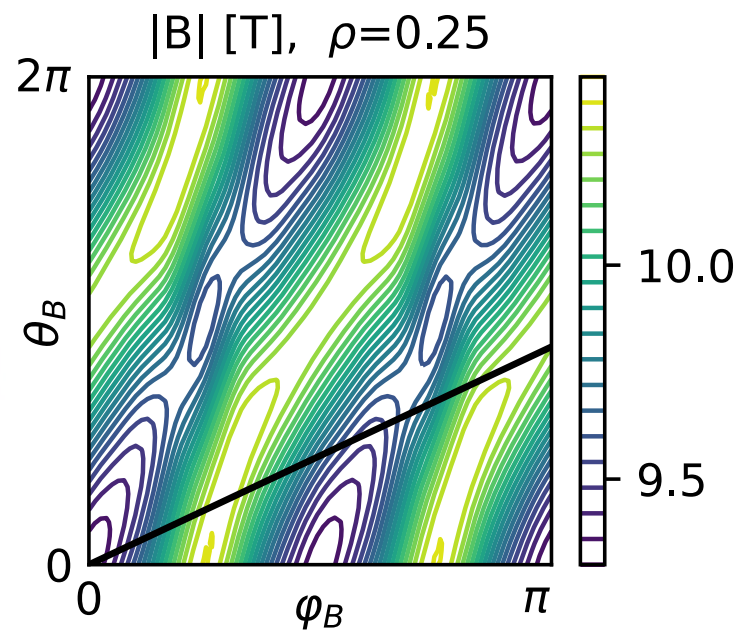
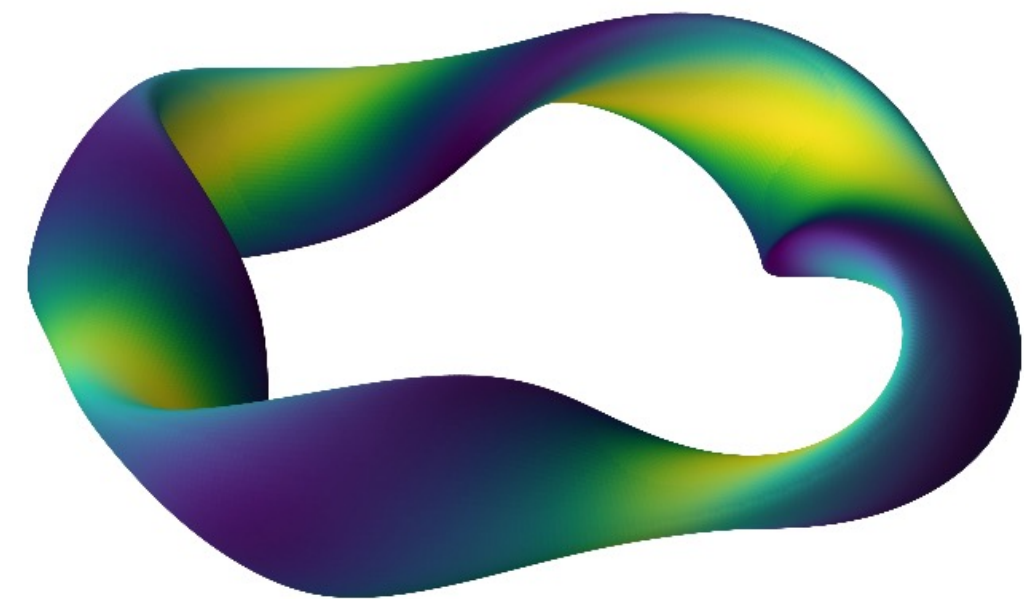
Garabedian space, $m, n \leq 2$. # dofs = 23

Optimization history



New configuration 2

QH-ish but far from ideal QH.

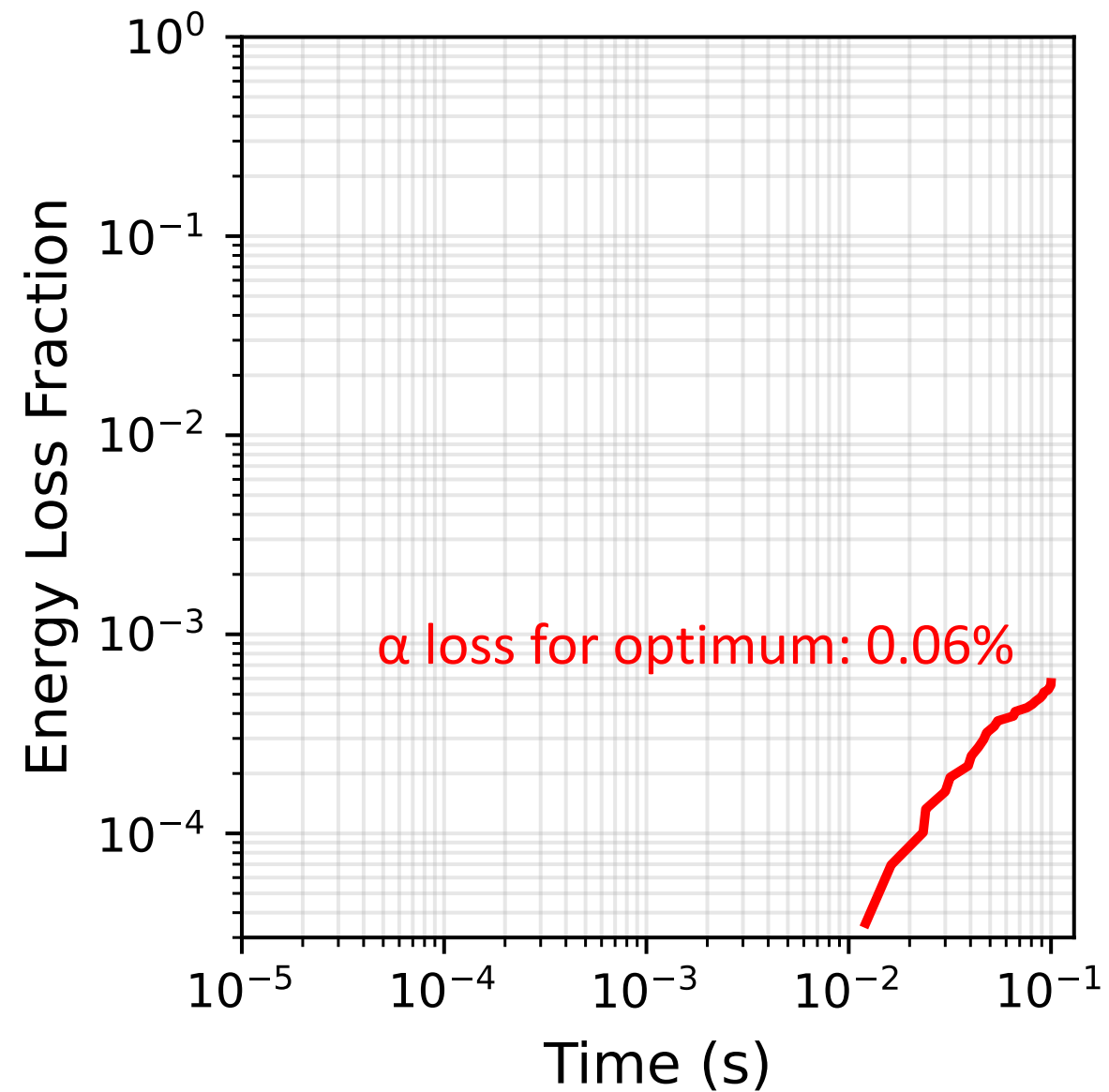
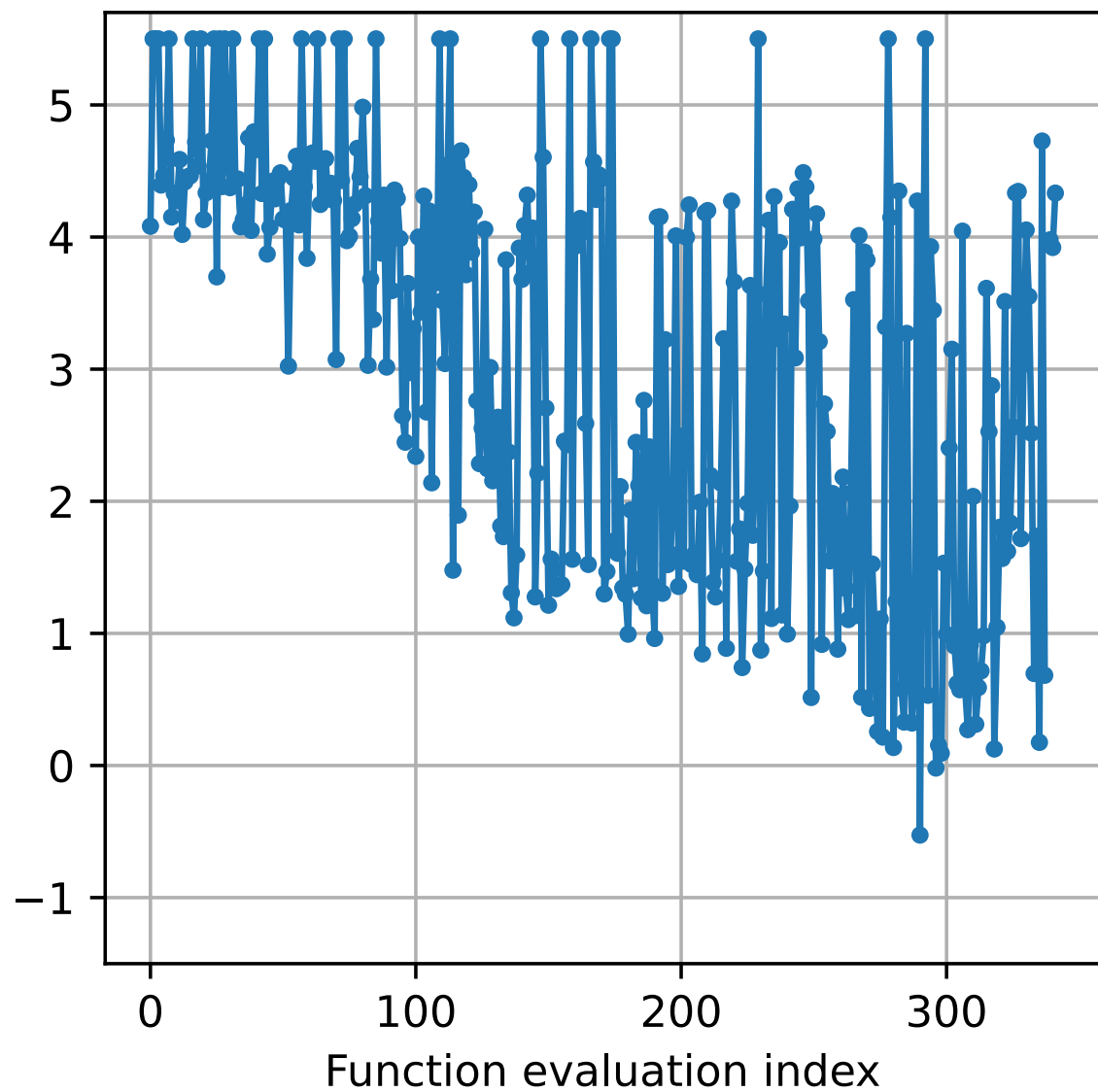


Aspect ratio = 6
 $\langle \beta \rangle = 1.4\%$

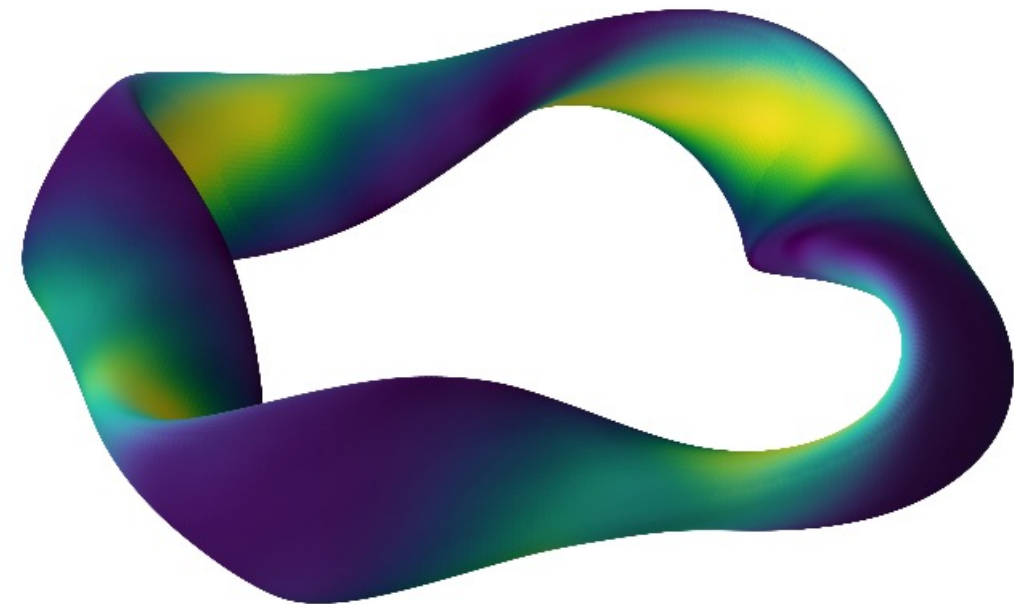
New configuration 3

PCA space, 20 components.

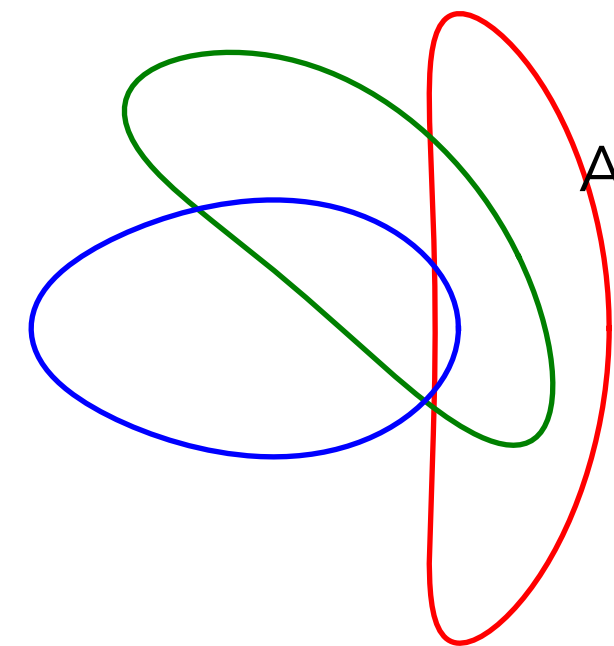
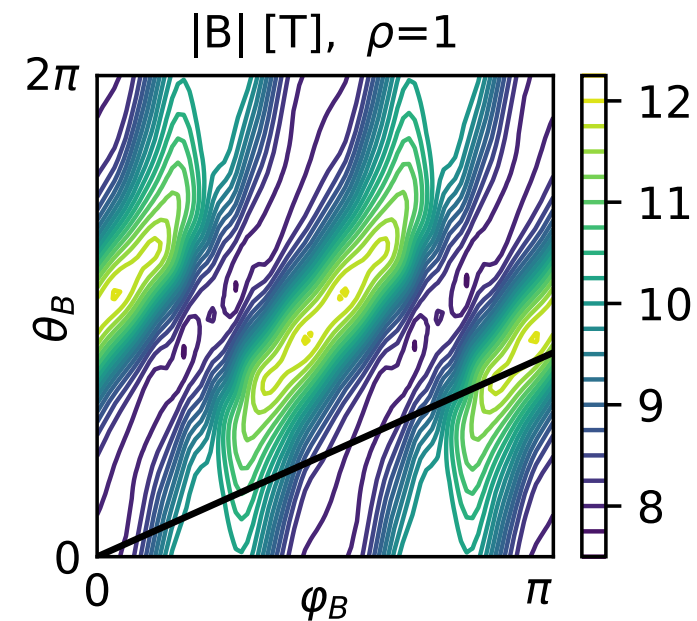
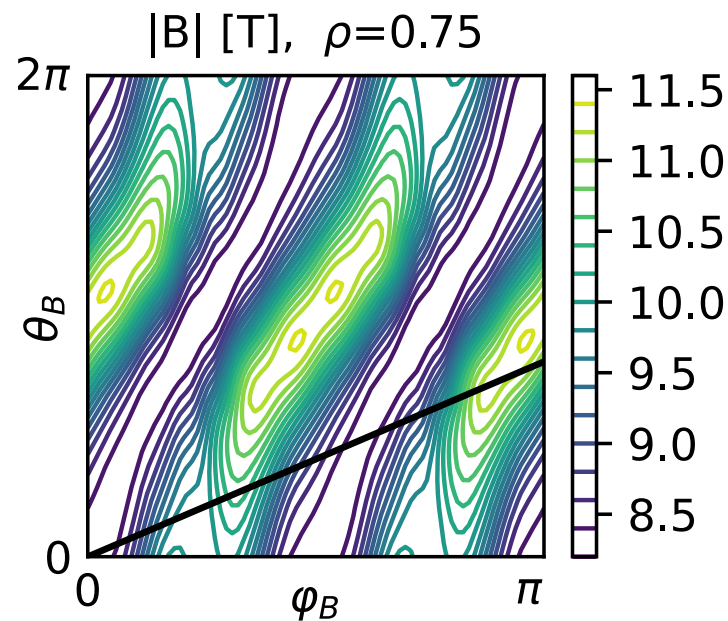
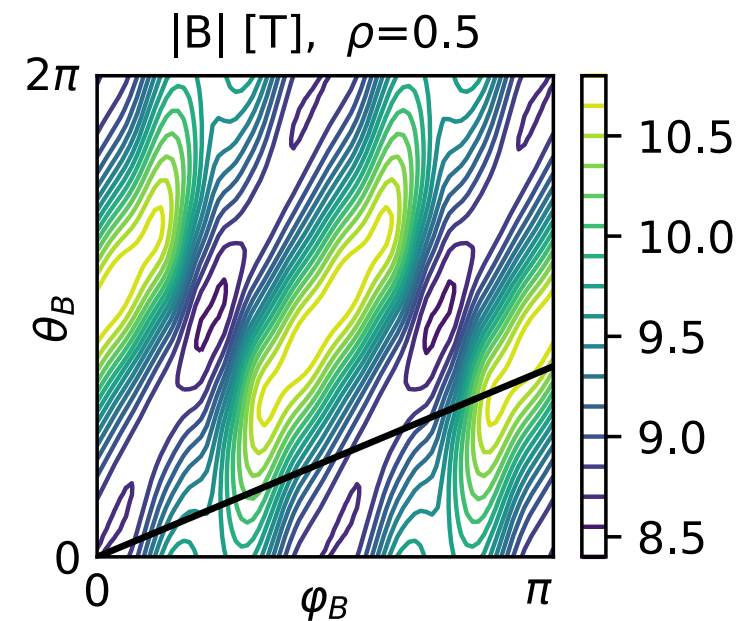
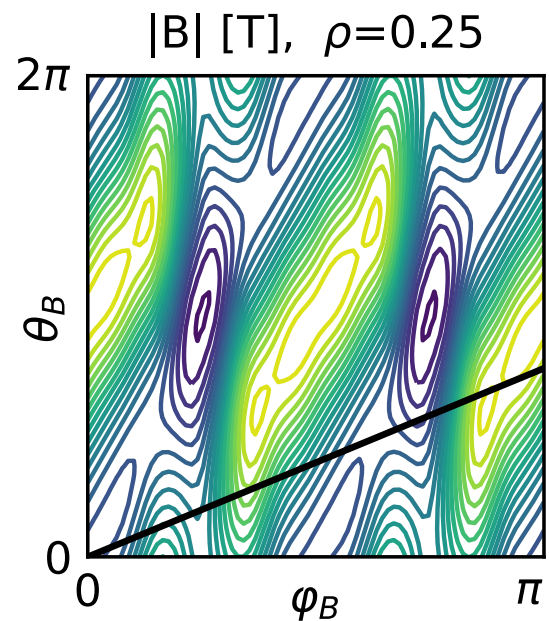
Optimization history



New configuration 3



Reminiscent of piecewise omnigenity

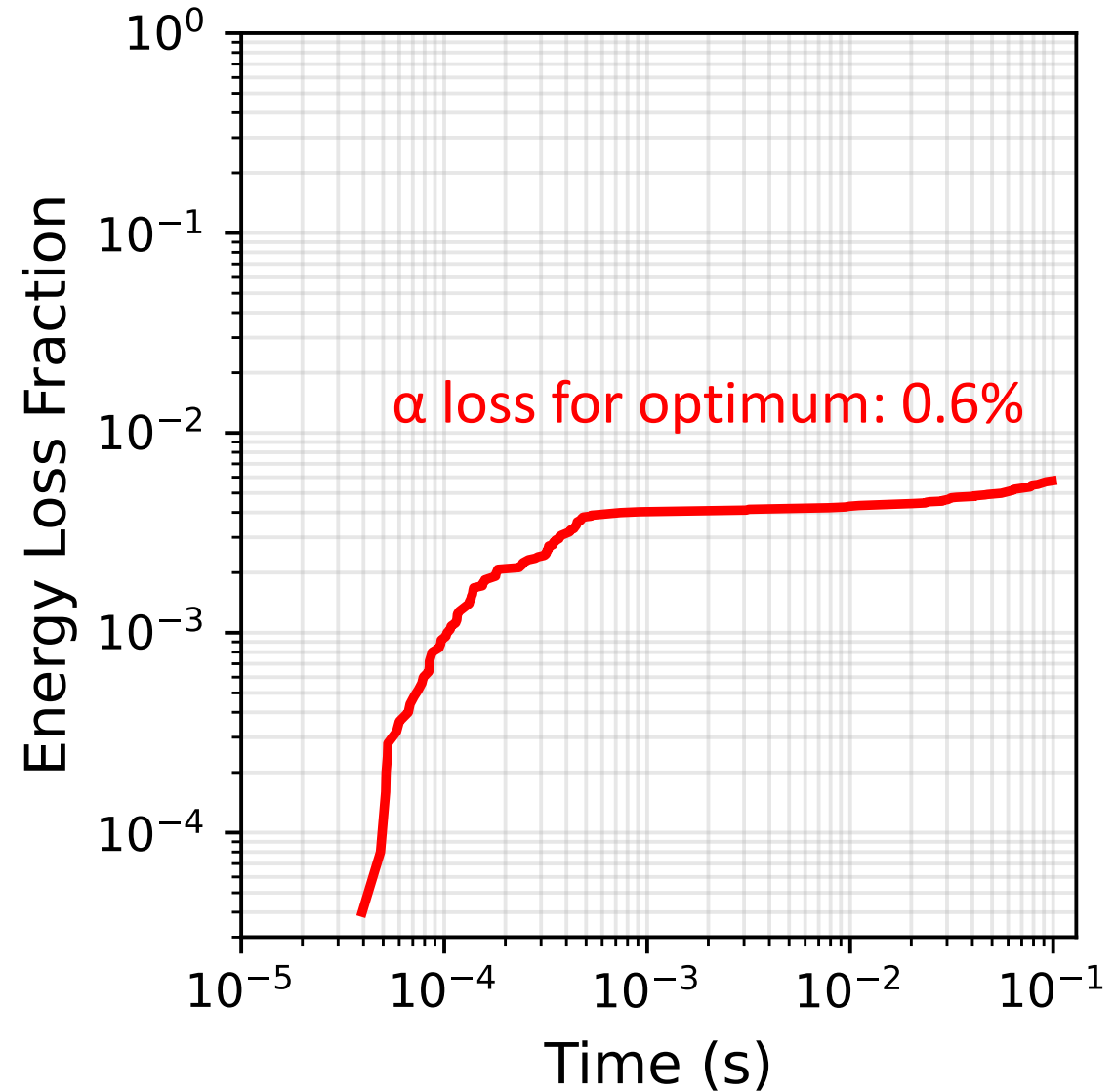
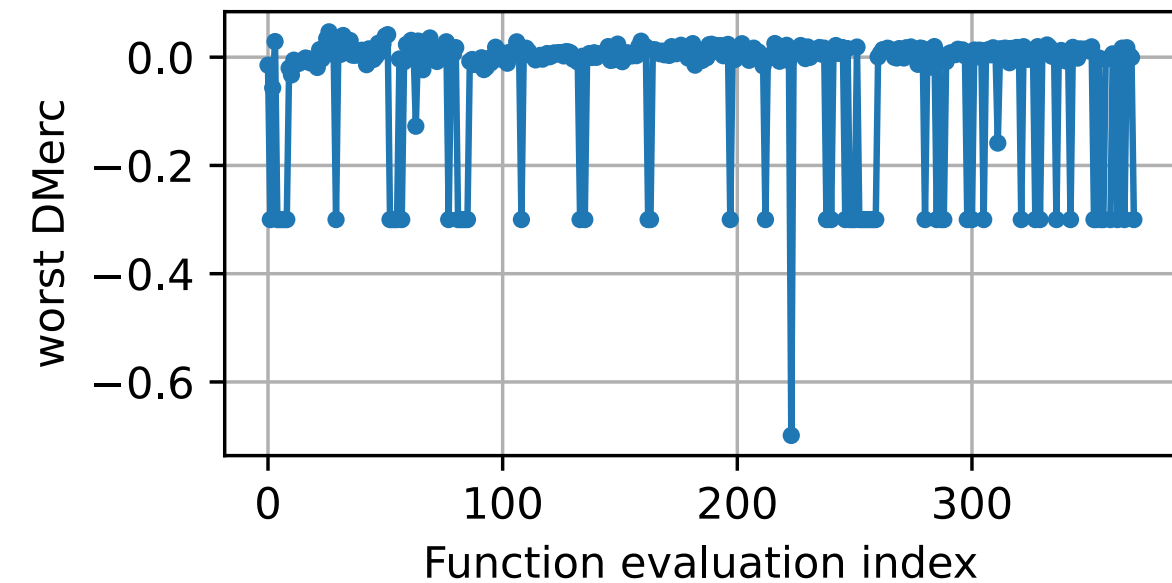
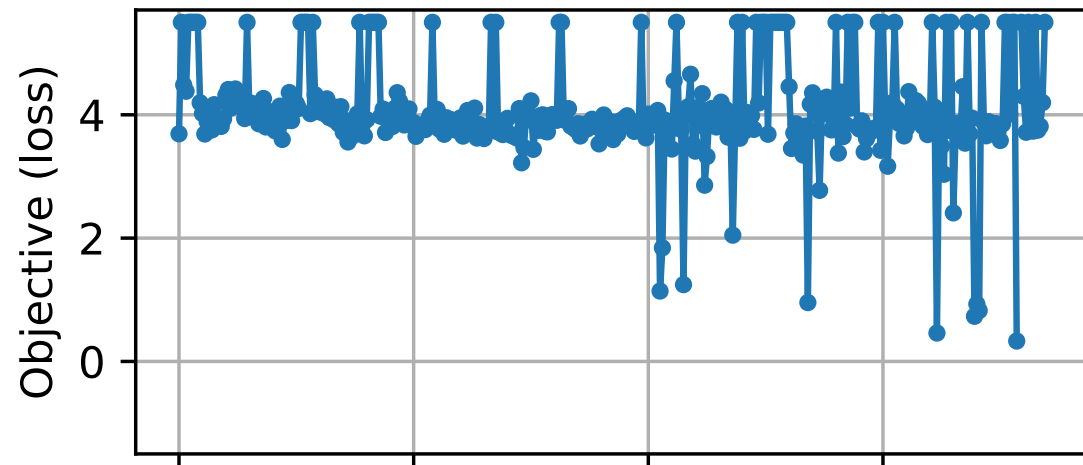


Aspect ratio = 6
 $\langle \beta \rangle = 1.5\%$

New configuration 4

Garabedian space, $m, n \leq 2$. # dofs = 23. Include Mercier stability constraint.

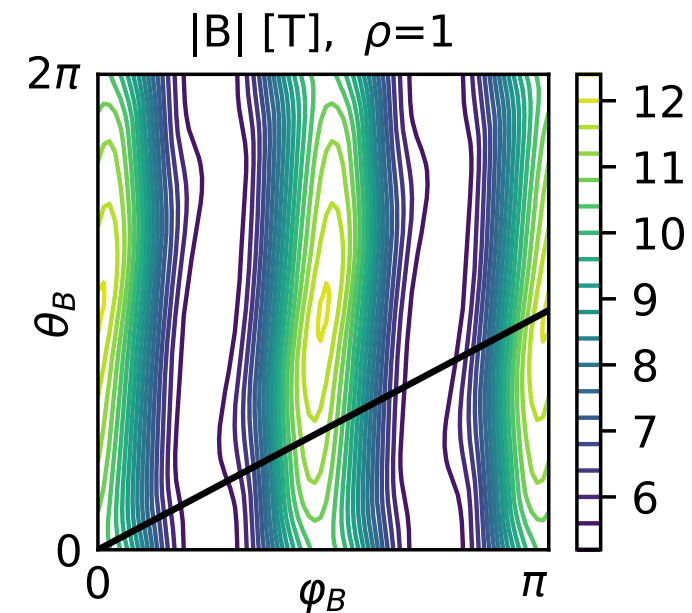
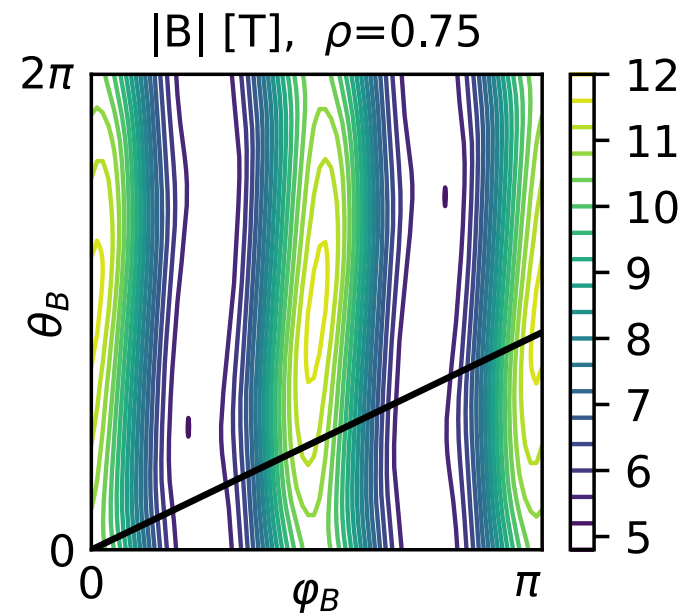
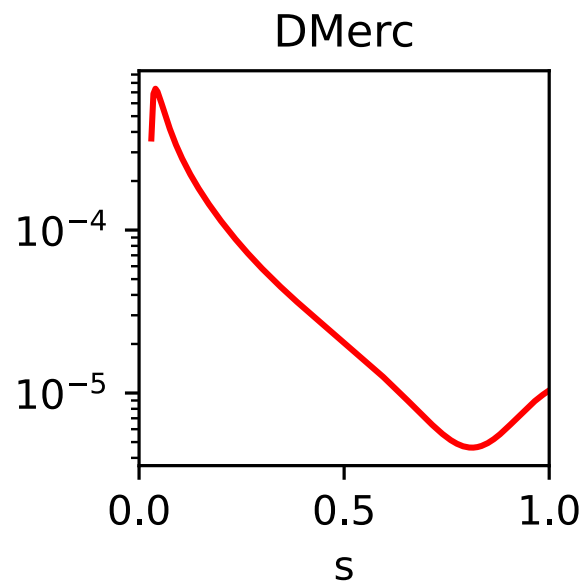
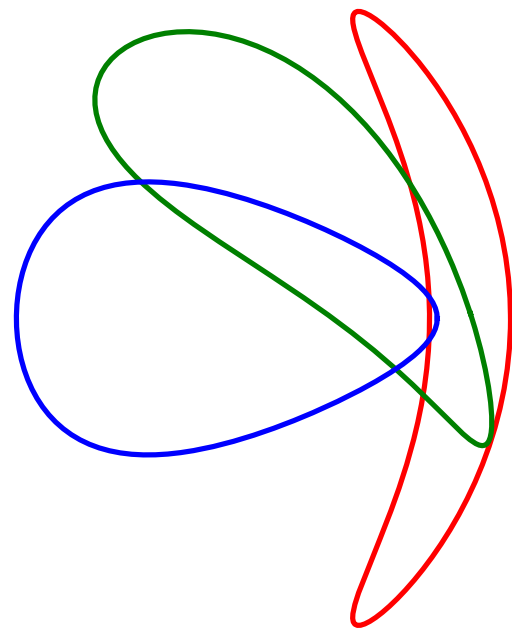
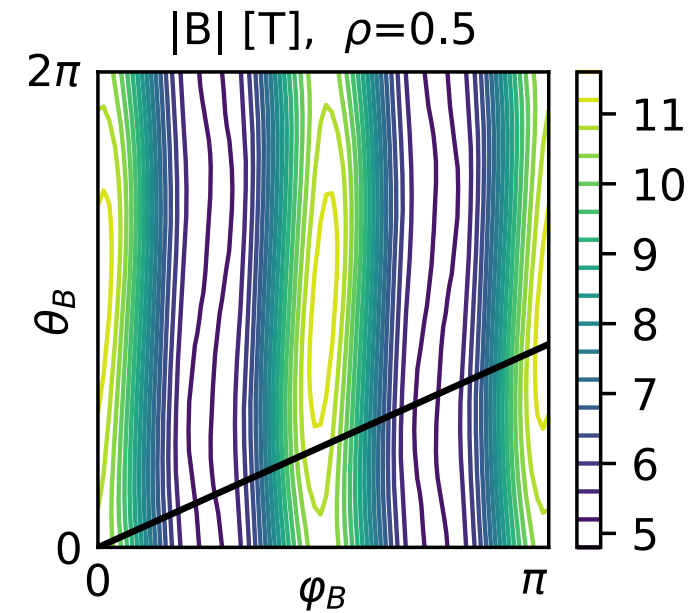
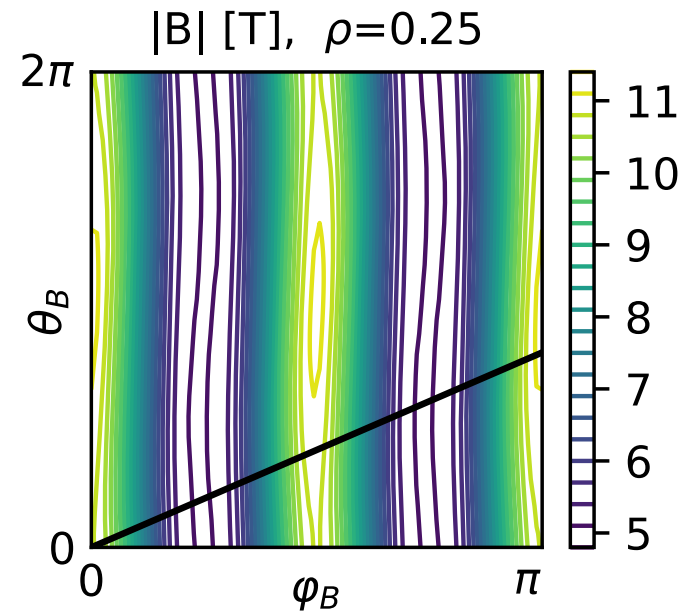
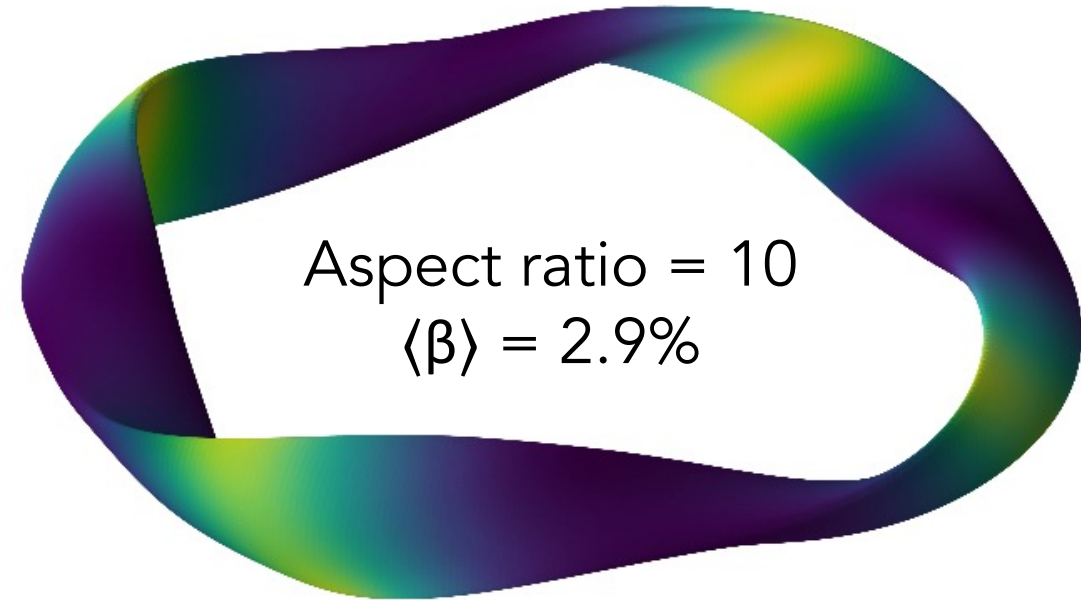
Optimization history



New configuration 4

α loss $\sim 0.6\%$

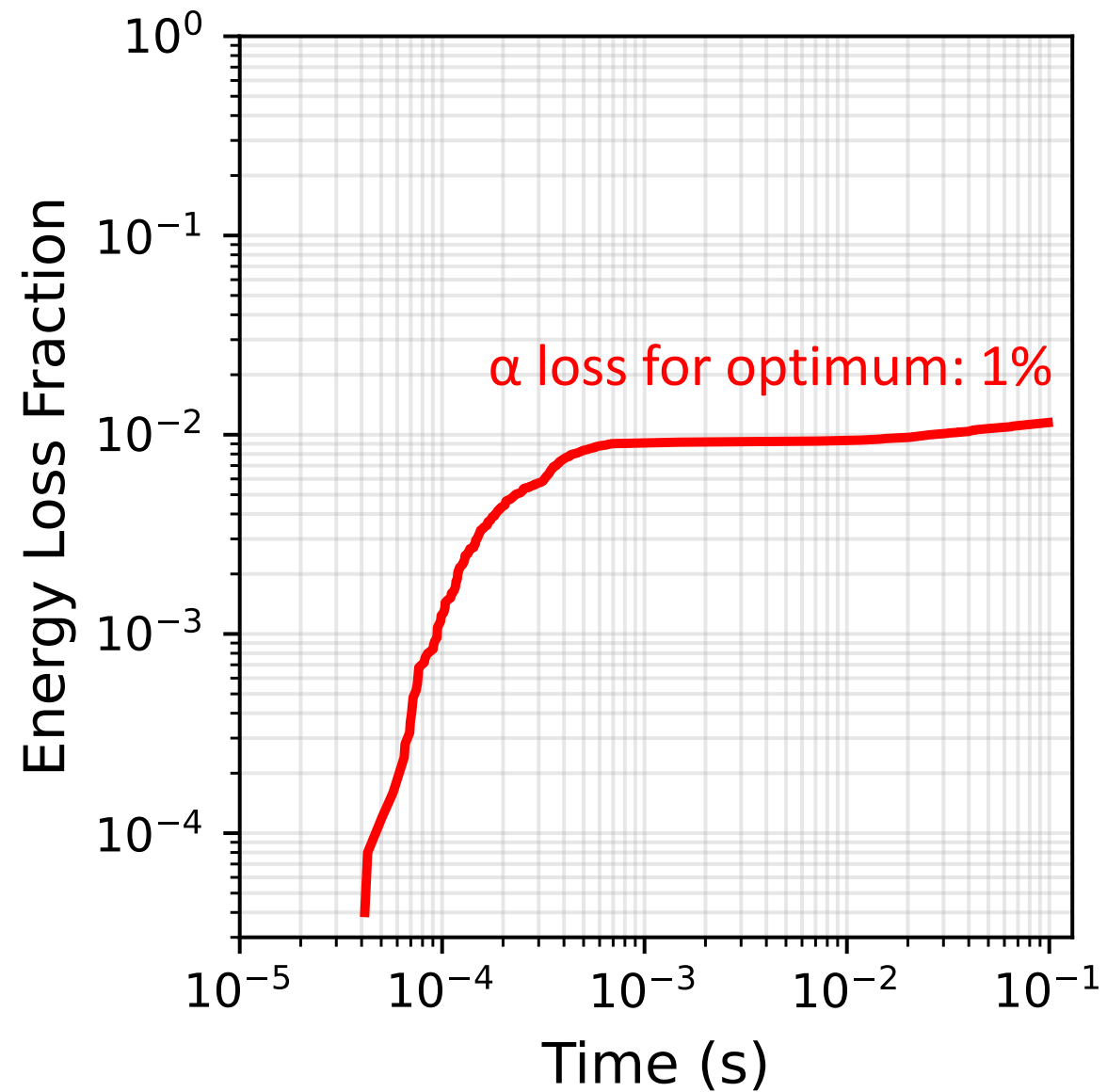
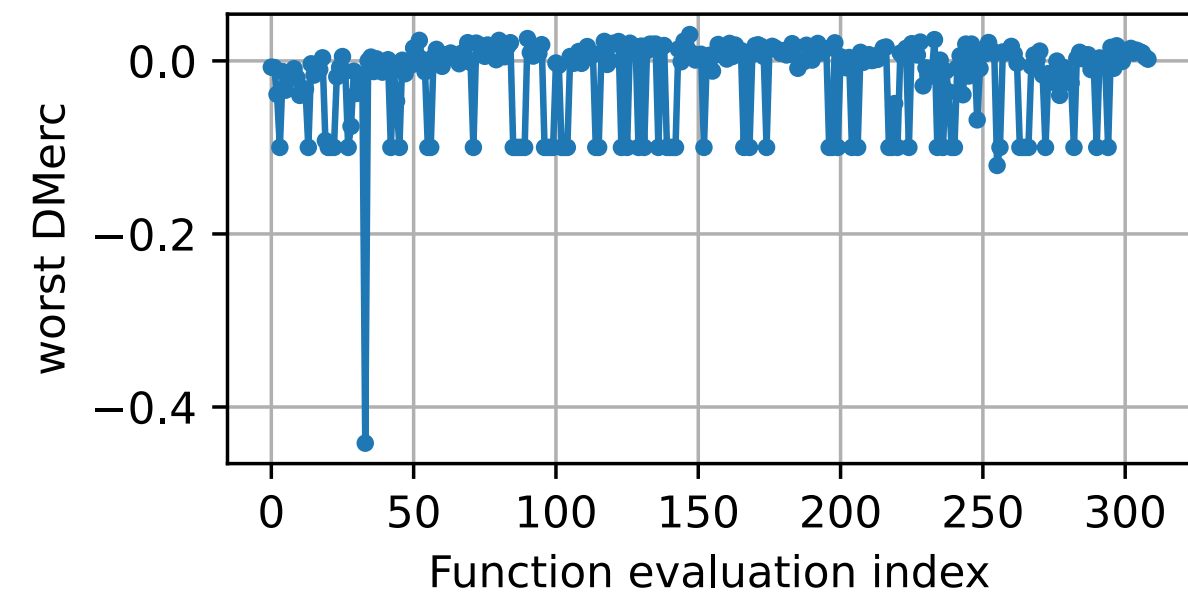
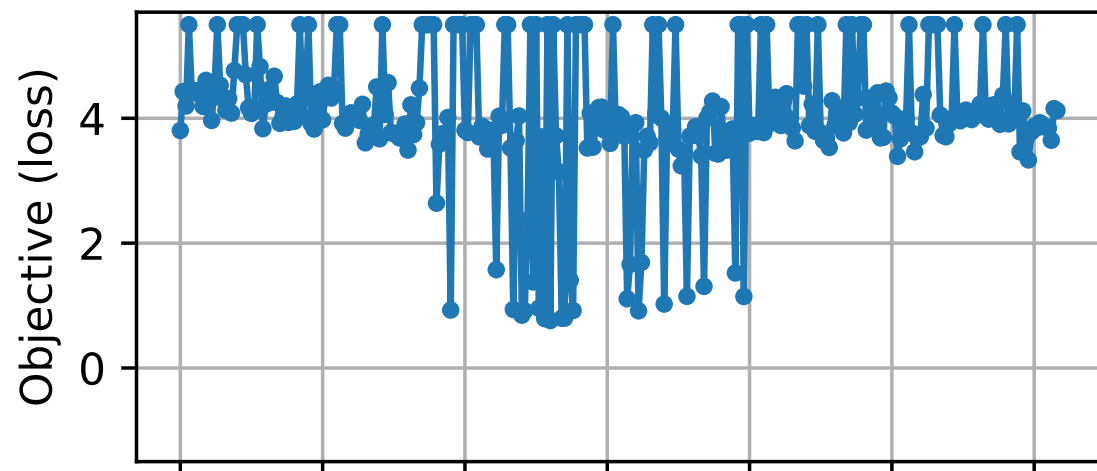
ConStellation configurations in dataset: $>15\%$ loss



New configuration 5

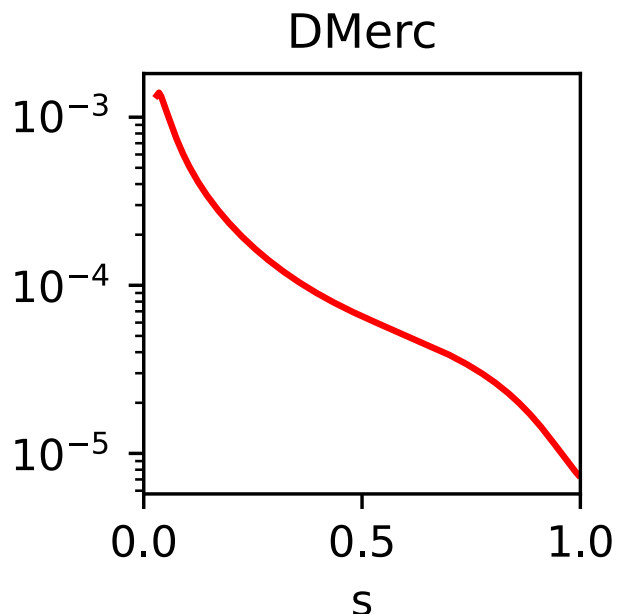
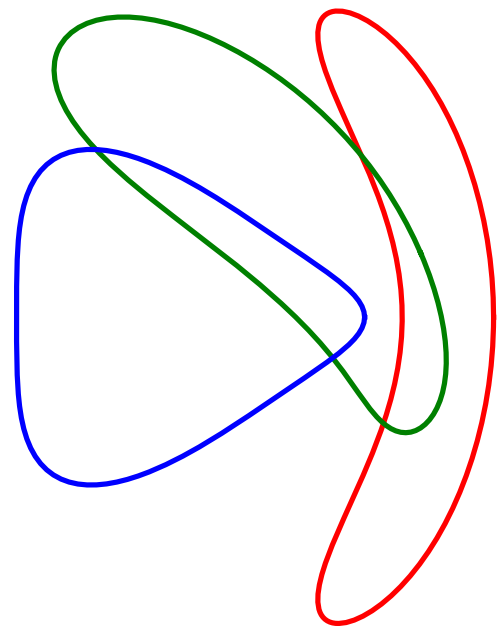
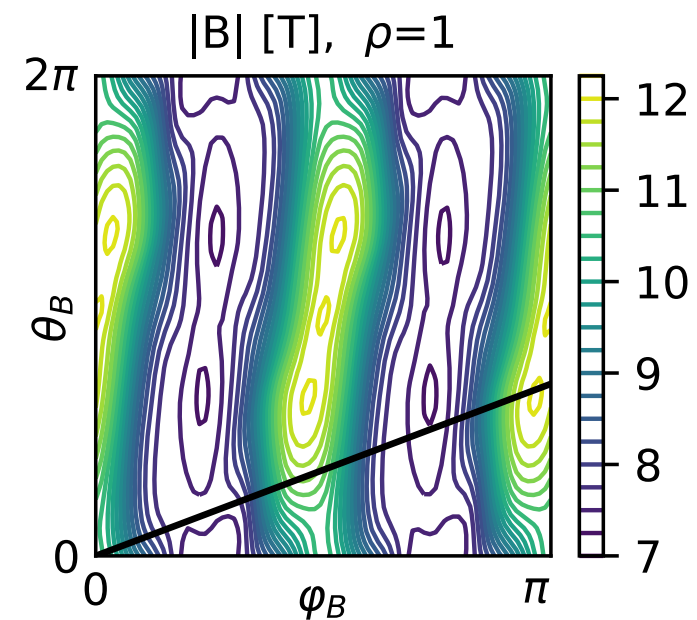
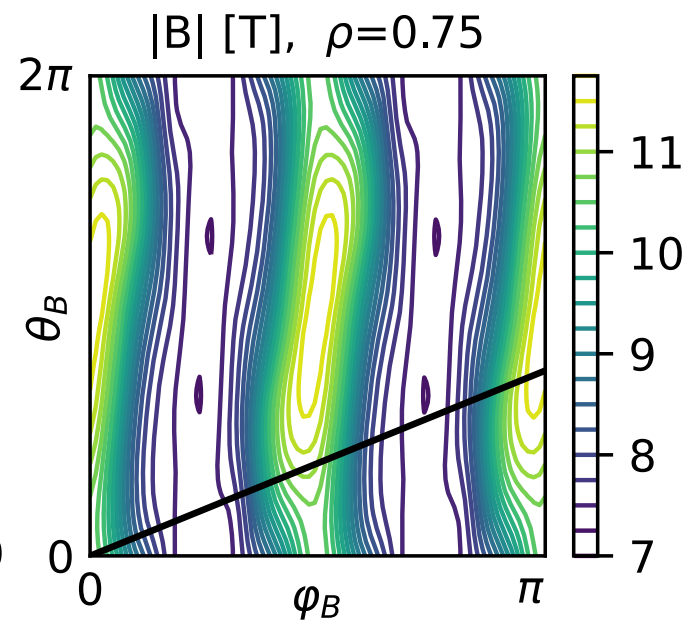
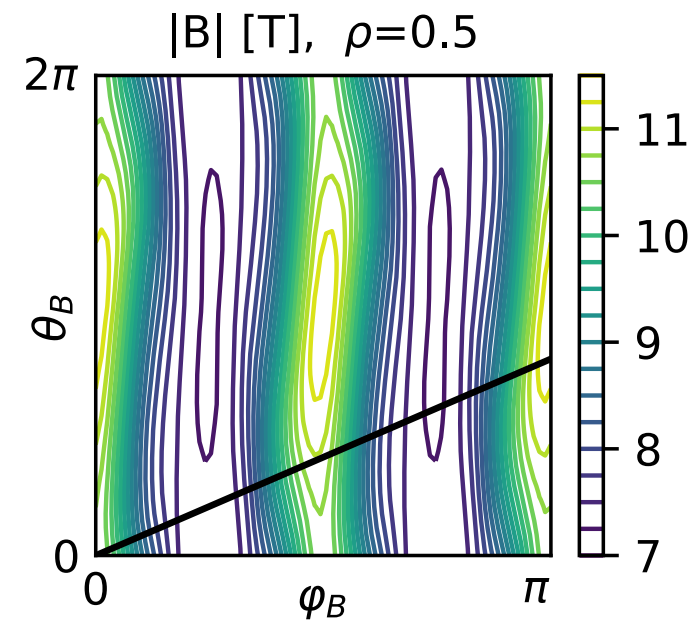
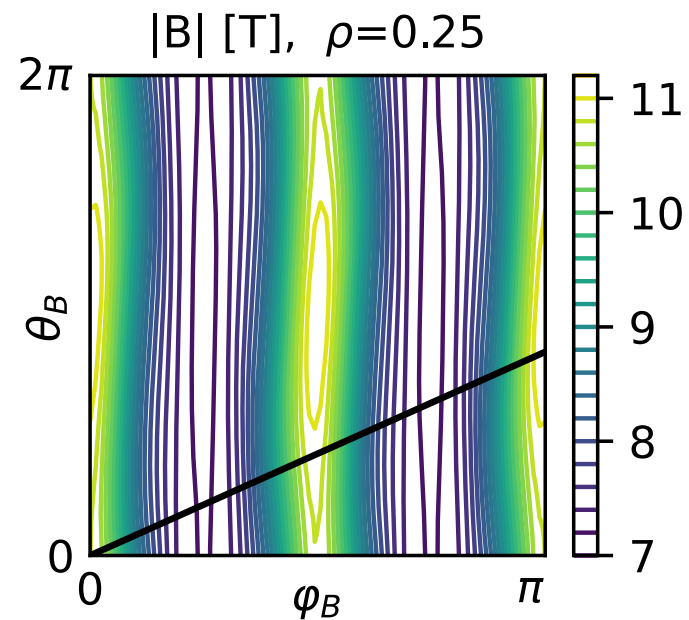
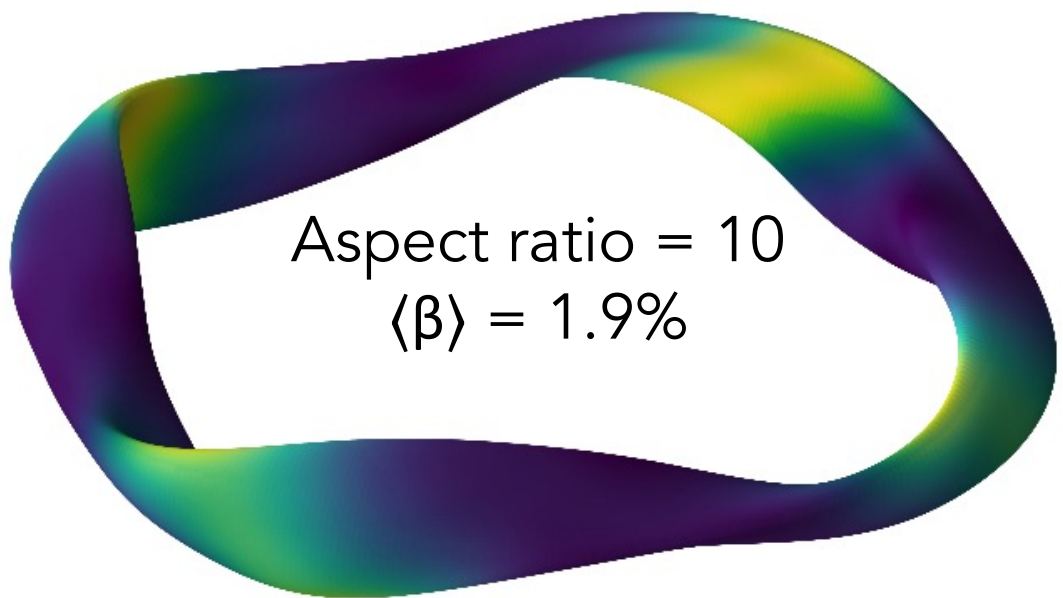
PCA space, 25 components. Include Mercier stability constraint.

Optimization history



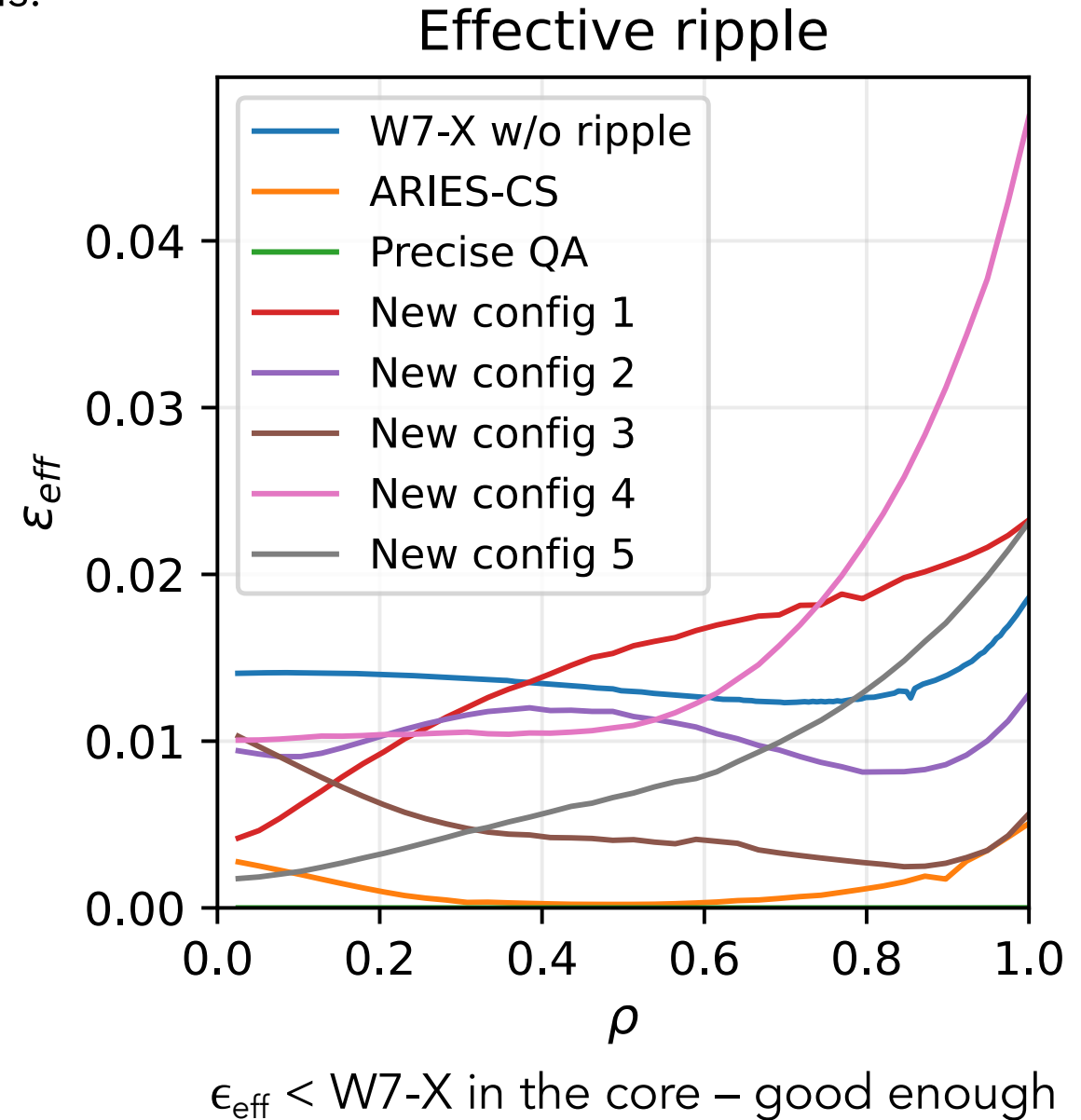
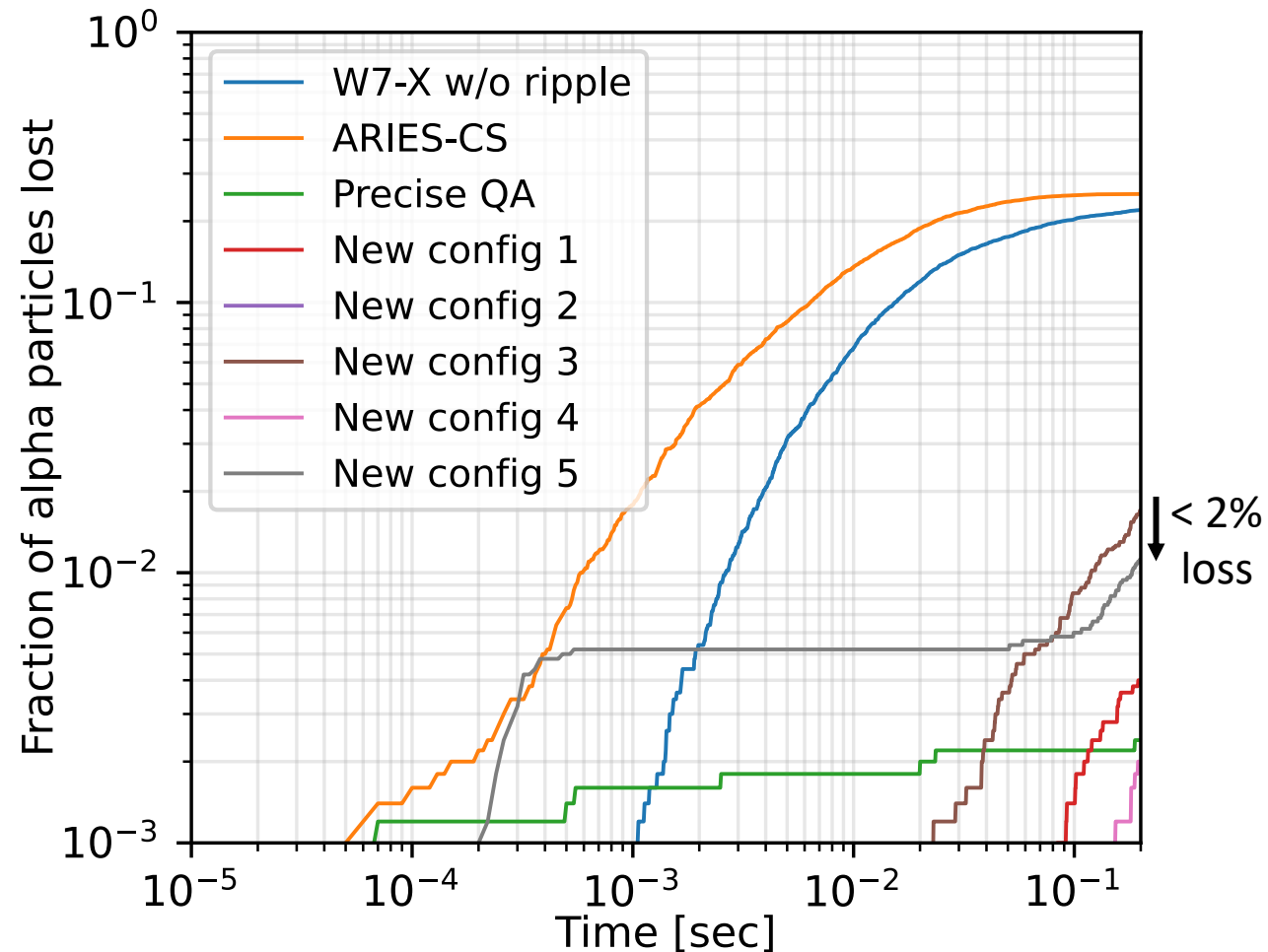
New configuration 5

Reminiscent of QI, but with no QI objective.



New configs also perform well on other benchmarks

- As in Landreman & Paul PRL (2022) & later publications.
- All configs scaled to ARIES-CS: $a = 1.7$ m, $\langle B \rangle = 5.9$ T
- Initialize particles at $s = 0.25$.



Conclusions

- These 2 new parameter spaces are nice for stage-1 optimization: few equilibrium failures despite strong shaping, & natural bound constraints.
- It's feasible to directly trace alphas inside the optimization loop.
- Configurations exist with excellent confinement that are far from ideal QA/QH/QI!

Future work

- Add constraints/objectives for iota, bootstrap current, $L_{\nabla B}$, ballooning, nonlinear gyrokinetics, etc.
- Fine-tune configurations using local optimization.
- Understand α trajectories in these fields – why aren't they lost?

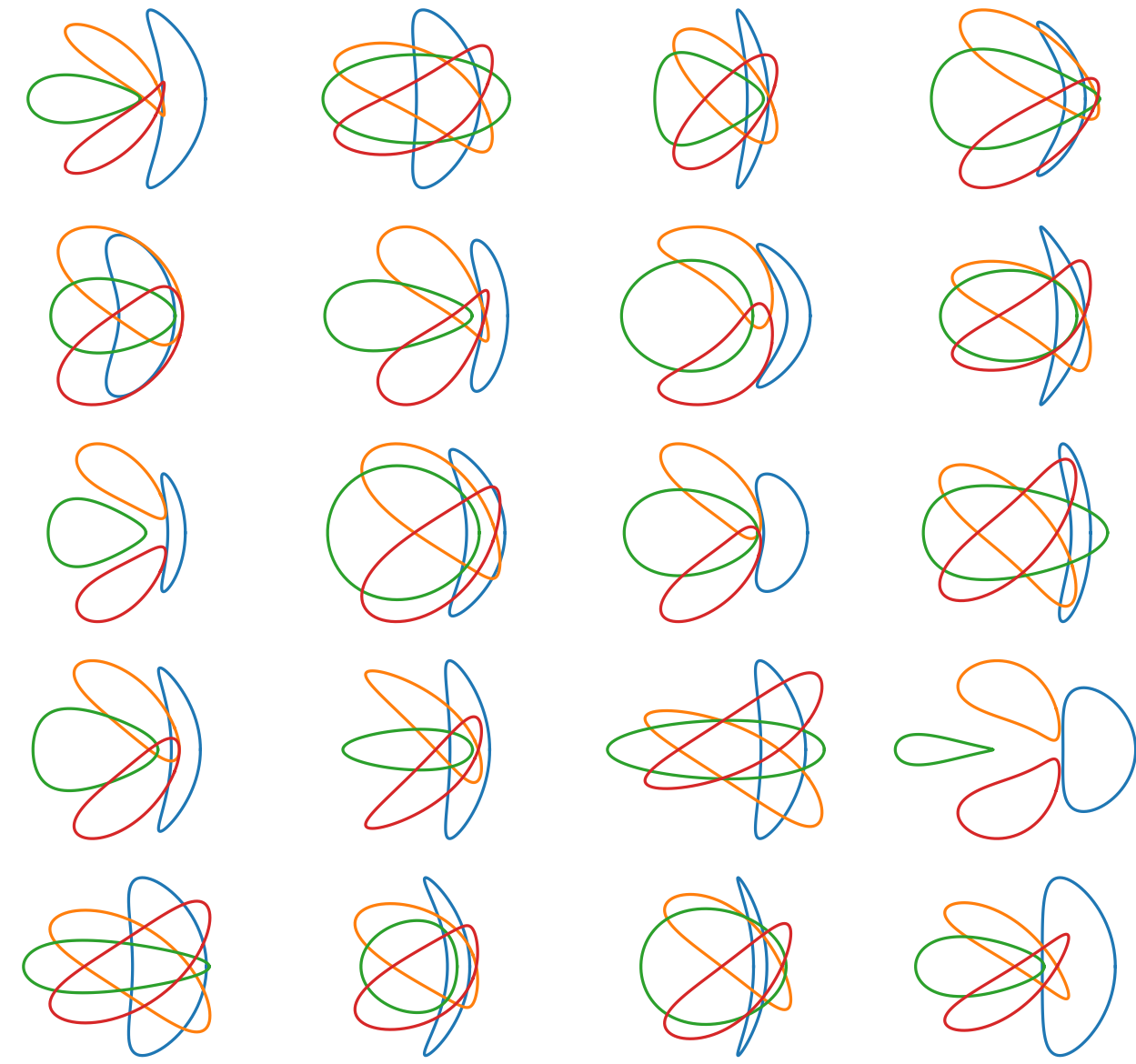
Extra slides

New space 1: Apply Quantile Transform to Garabedian Δ_{mn} 's

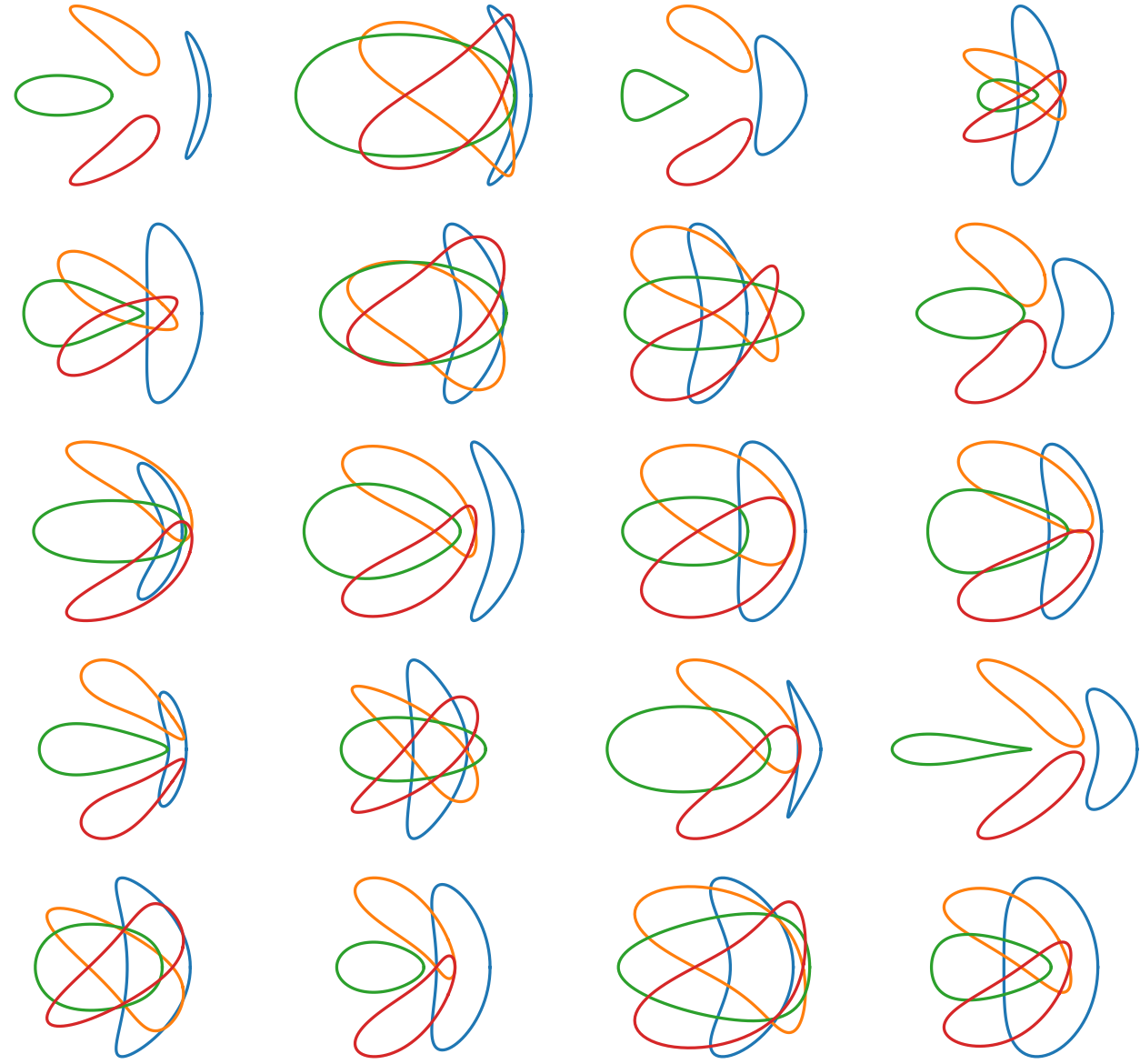
- Effective prior probability: uniform on unit hypercube.
- Natural bound constraints: extremes of the data.
- Robust to outliers in the data.
- Major & minor radius (hence aspect ratio) are matched exactly. No need for aspect penalty or constraint, 1 fewer d.o.f.
- Could apply method to VMEC or DESC Fourier amplitudes instead.
- Gives highly shaped boundaries ("expressive"), with few self-intersections or equilibrium failures.

New space 1: Apply Quantile Transform to Garabedian Δ_{mn} 's

$m_{\max} = n_{\max} = 2$

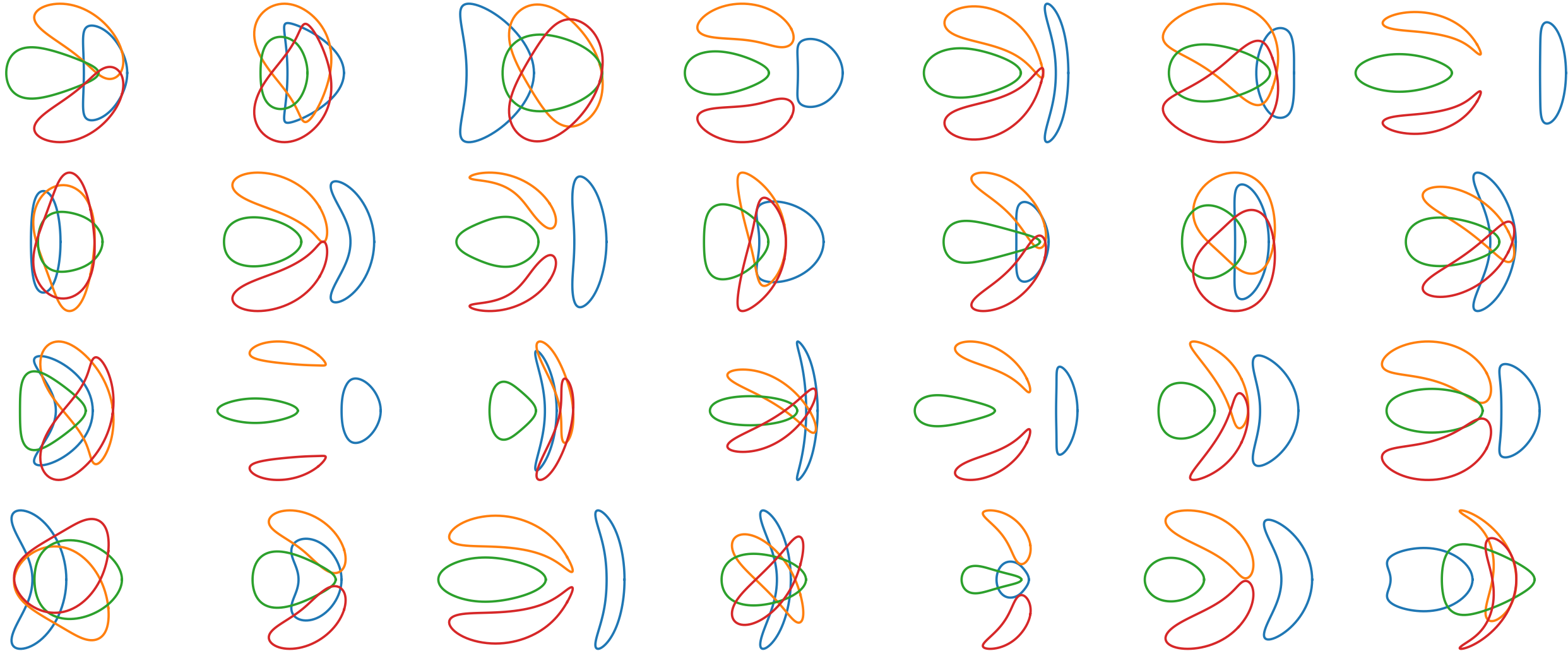


$m_{\max} = n_{\max} = 3$



New space 2: principal components

- Apply PCA to boundary (R,Z) values, then apply QuantileTransform to PC amplitudes.
- Same advantages as space 1, & also dimensionality reduction. 10 PCs shown here:



Optimization problem setup

- Alpha tracing using FIRM3D GPU "CATAPULT" method:
`github.com/ColumbiaStellaratorTheory/firm3d`.
- Trace 25,000 particles for 0.1 sec physical time, source \propto fusion rate, no collisions.
- Objective allows early termination if confinement is bad. Natural multi-fidelity method.

Time to reach loss of $M = 2\%$

$$f = \begin{cases} -\log_{10}(t_M) & \text{if } L(t_{max}) > M, \\ \log_{10}(L(t_{max}) + \epsilon) - \log_{10}(t_{max}) - \log_{10}(M + \epsilon) & \text{if } L(t_{max}) \leq M. \end{cases}$$

If loss $< 2\%$ at t_{max} , penalize loss at t_{max}

keep f continuous