Award number
1953350

Reduced-order modeling
of
turbulent reacting flows
using data-driven approaches

Kamila Zdybał

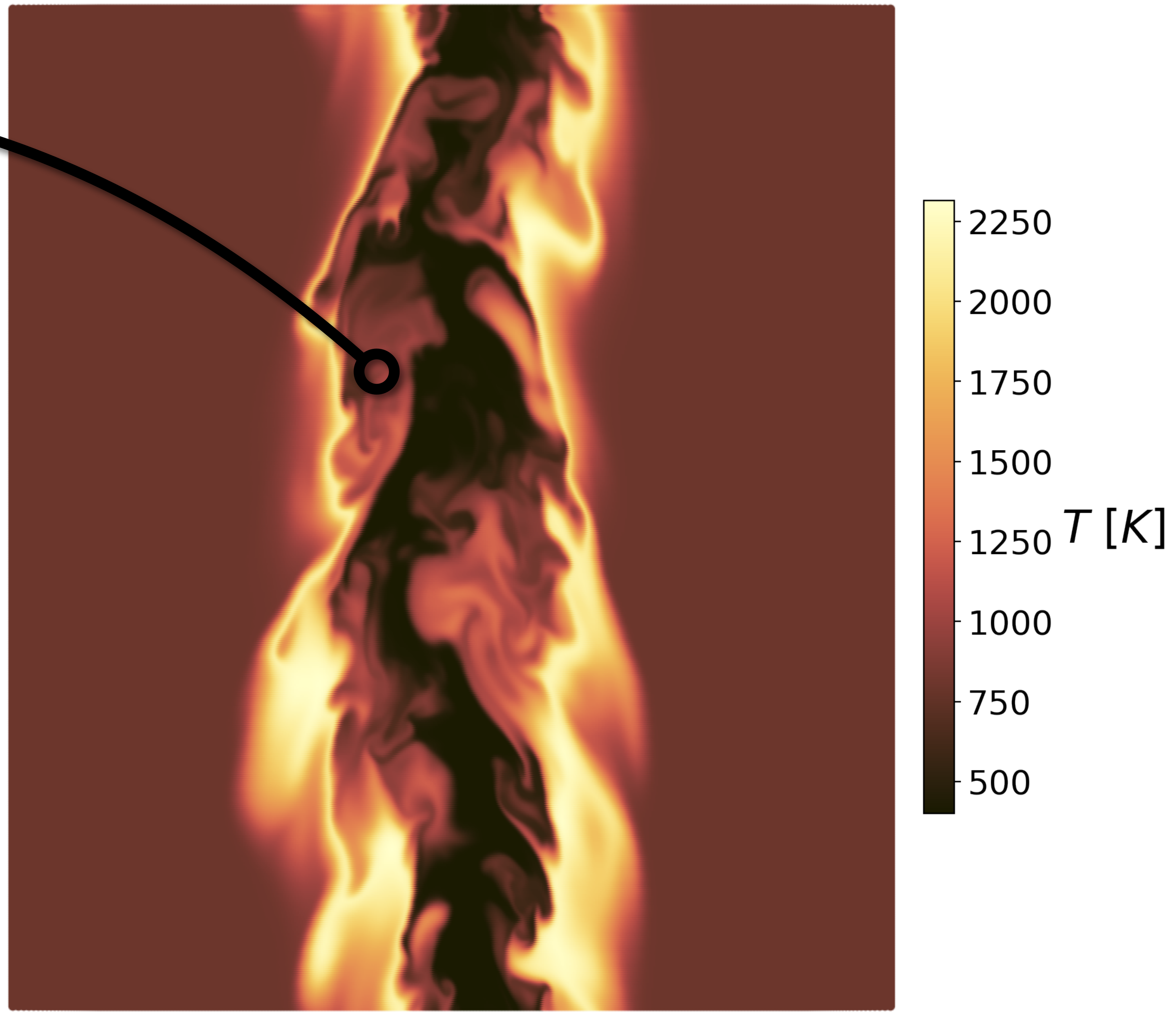
Supervisors: Prof. Alessandro Parente, Prof. James C. Sutherland

12 October 2023
18th ERCOFTAC Autumn Festival, Liège

The goal of a reacting flow simulation.

$$\{T, \underbrace{Y_1, Y_2, \ldots, Y_{n-1}}_{\text{Chemical composition}}\}$$

Temperature



DNS simulation of an *n*-heptane/air jet flame

A. Attili, F. Bisetti, M.E. Mueller, H. Pitsch. Formation, growth, and transport of soot in a three-dimensional turbulent non-premixed jet flame.
A. Attili, F. Bisetti, M.E. Mueller, H. Pitsch. Effects of non-unity Lewis number of gas-phase species in turbulent non-premixed sooting flames.

The ~~goal~~ of a reacting flow simulation.

challenge

$$\{T, \underbrace{Y_1, Y_2, \ldots, Y_{n-1}}_{\text{Chemical composition}}\}$$

Temperature

$$\frac{\partial \rho T}{\partial t} = \ldots$$

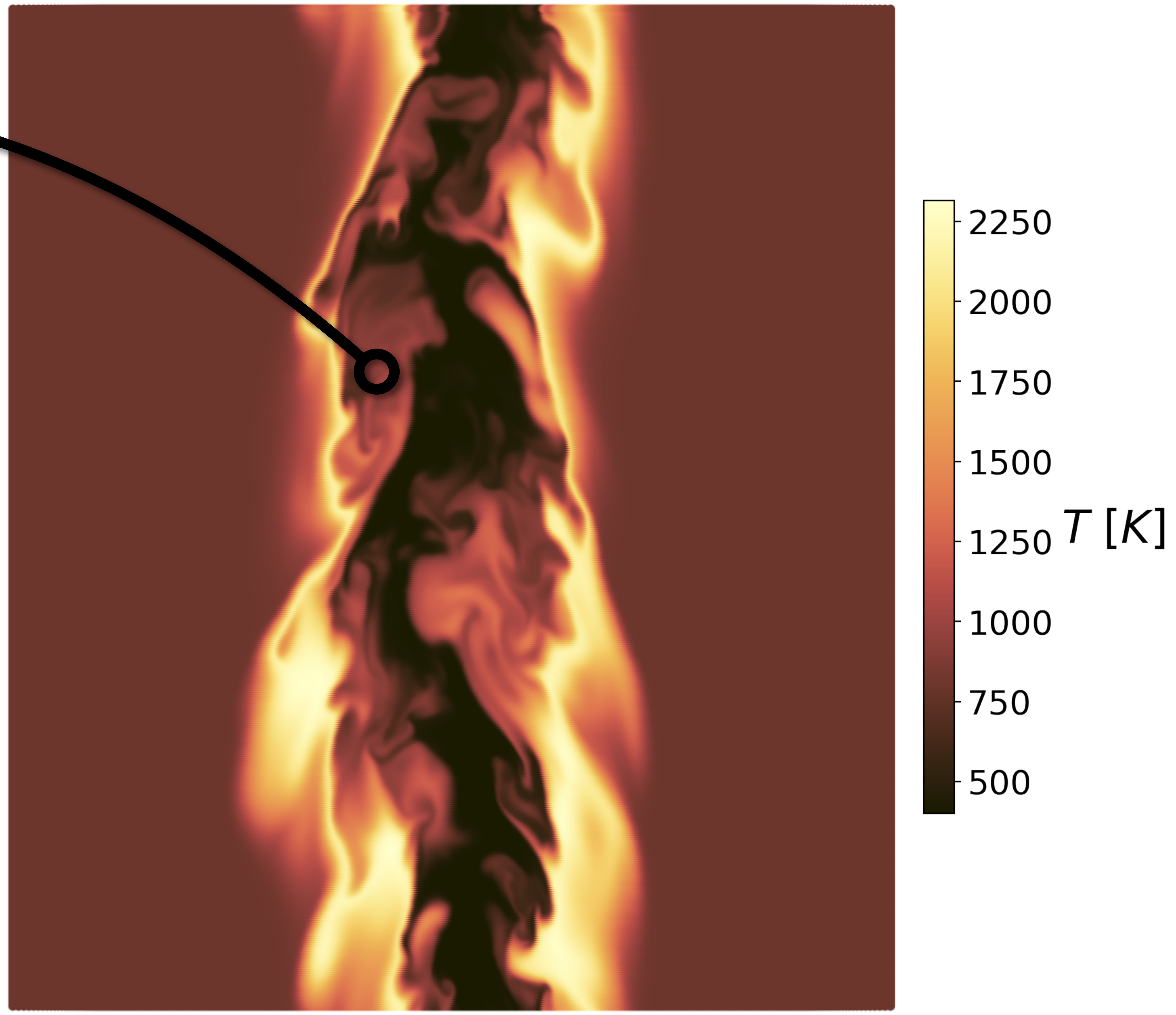
$$\frac{\partial \rho Y_1}{\partial t} = \ldots$$

$$\frac{\partial \rho Y_2}{\partial t} = \ldots$$

$$\vdots$$

$$\frac{\partial \rho Y_{n-1}}{\partial t} = \ldots$$

Large system
of coupled PDEs!



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In my doctoral thesis, I've built tools to help improve **reduced-order models.**

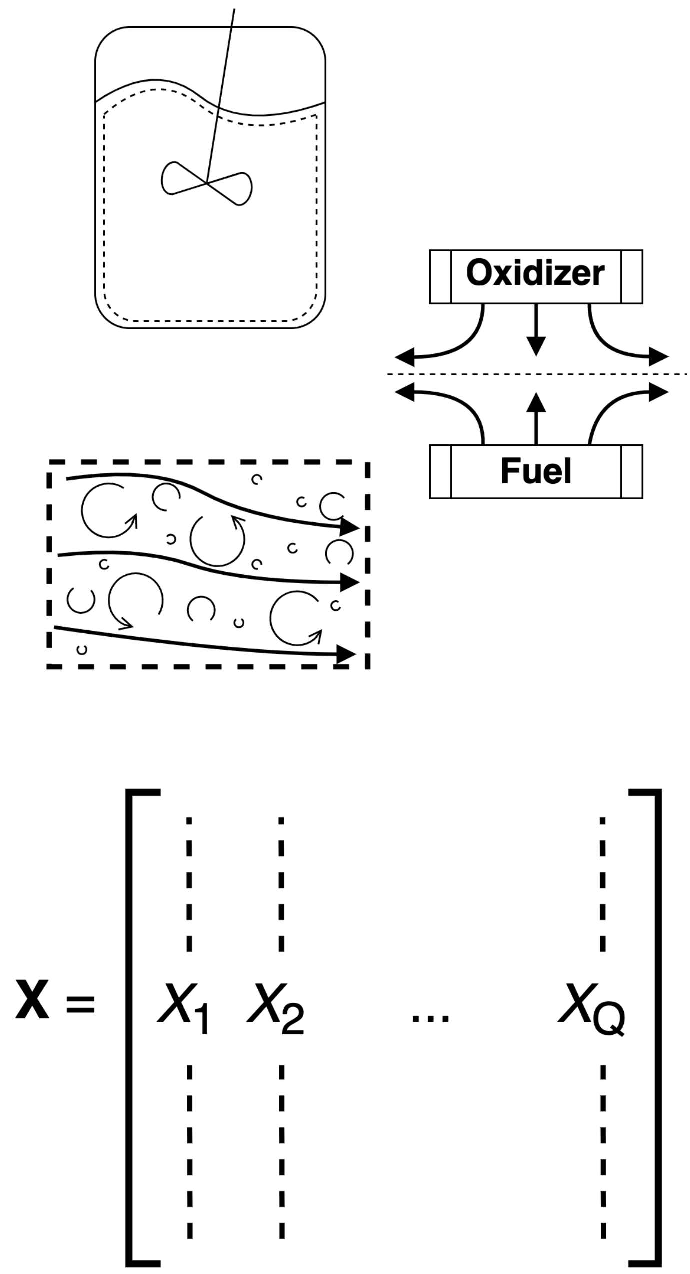
$$
\begin{cases}
\dfrac{\partial \rho T}{\partial t} = \dots \\
\dfrac{\partial \rho Y_1}{\partial t} = \dots \\
\dfrac{\partial \rho Y_2}{\partial t} = \dots \\
\vdots \\
\dfrac{\partial \rho Y_{n-1}}{\partial t} = \dots
\end{cases}
$$

Dimensionality reduction

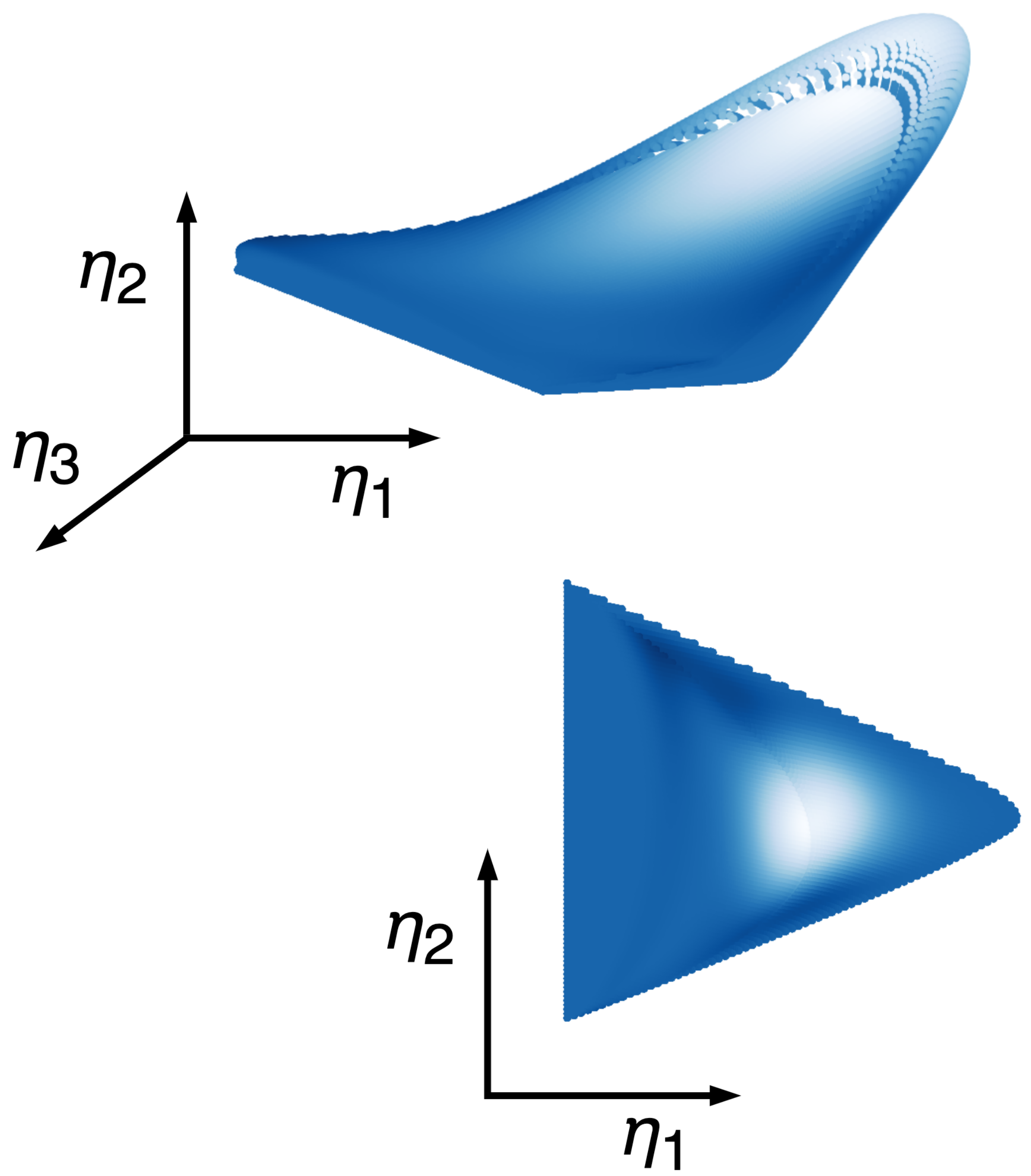
$$
\begin{cases}
\dfrac{\partial \eta_1}{\partial t} = \dots \\
\dfrac{\partial \eta_2}{\partial t} = \dots \\
\dfrac{\partial \eta_3}{\partial t} = \dots
\end{cases}
$$

There's four steps to building ROMs.

Training data



Dimensionality reduction

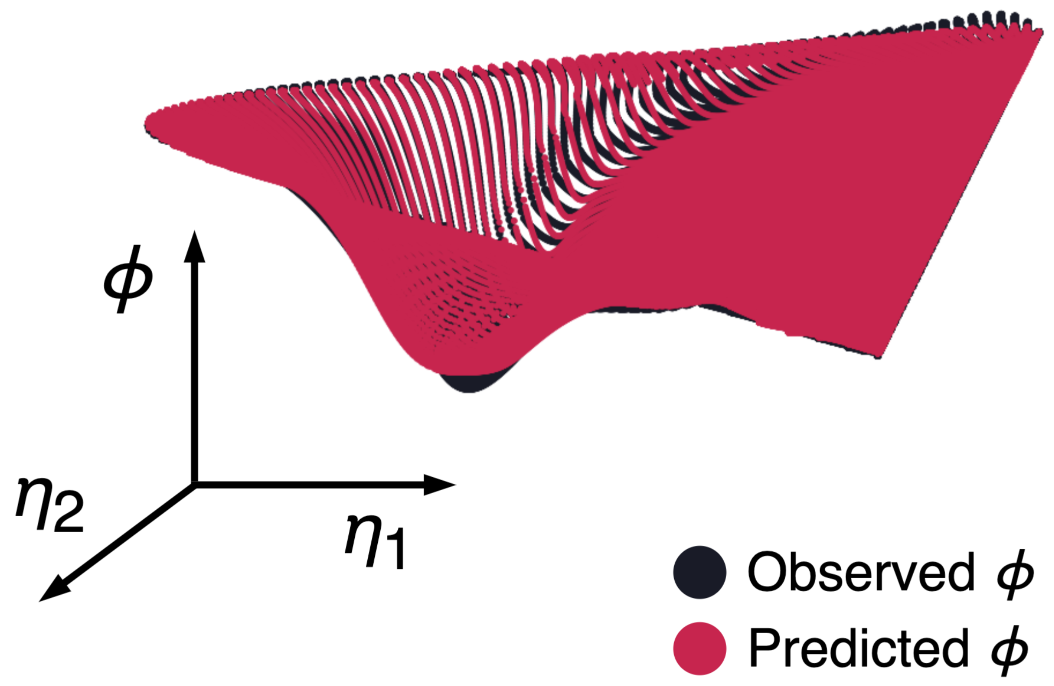


Building reduced-order models

$$\frac{\partial \mathbf{X}^\top}{\partial t} = -\nabla \cdot \mathbf{C}^\top - \nabla \cdot \mathbf{D}^\top + \mathbf{S}^\top$$

Projection of
the governing equations

$$\frac{\partial \boldsymbol{\eta}^\top}{\partial t} = -\nabla \cdot \mathbf{C}_{\boldsymbol{\eta}}^\top - \nabla \cdot \mathbf{D}_{\boldsymbol{\eta}}^\top + \mathbf{S}_{\boldsymbol{\eta}}^\top$$



Simulations

DNS simulation of an *n*-heptane/air jet flame

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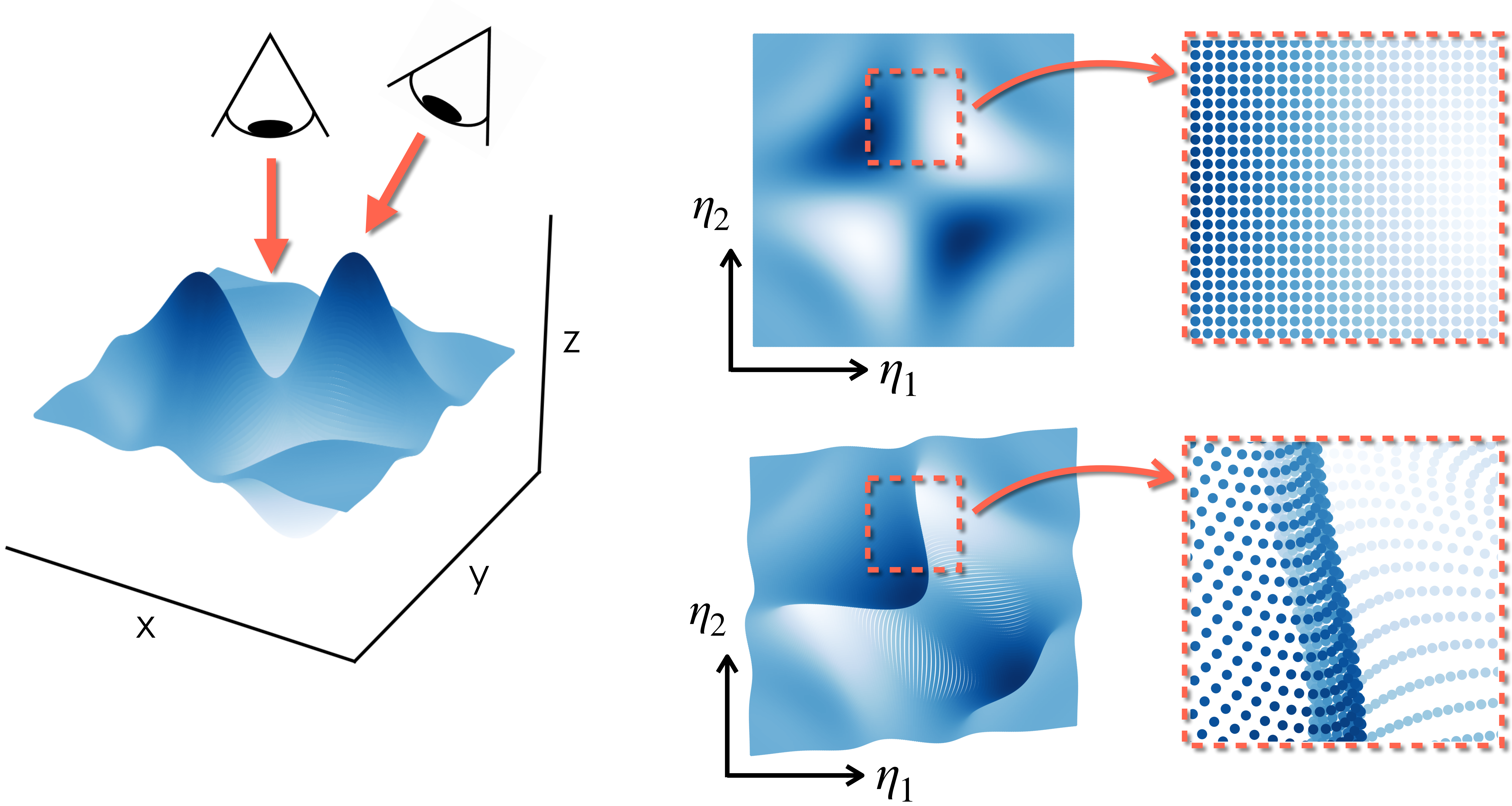
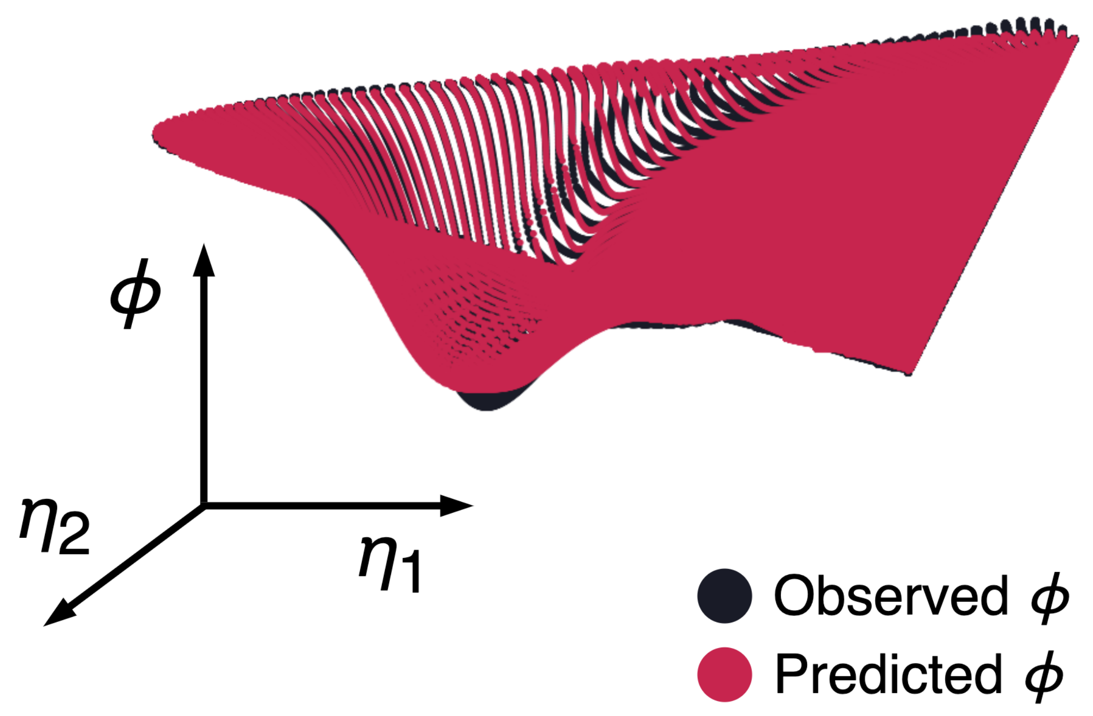
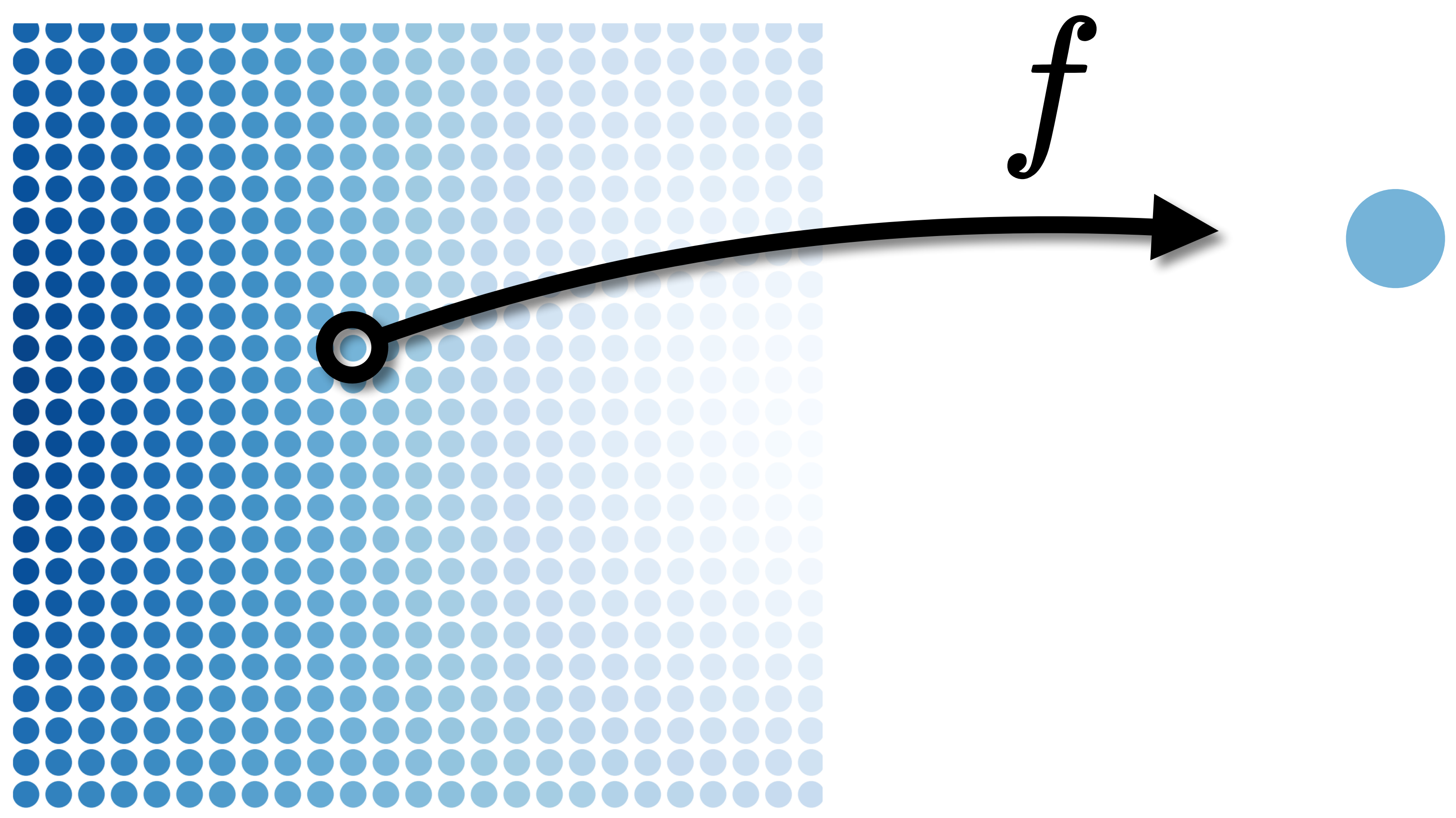
Projecting high-dimensional data onto lower dimensions can introduce non-uniqueness.

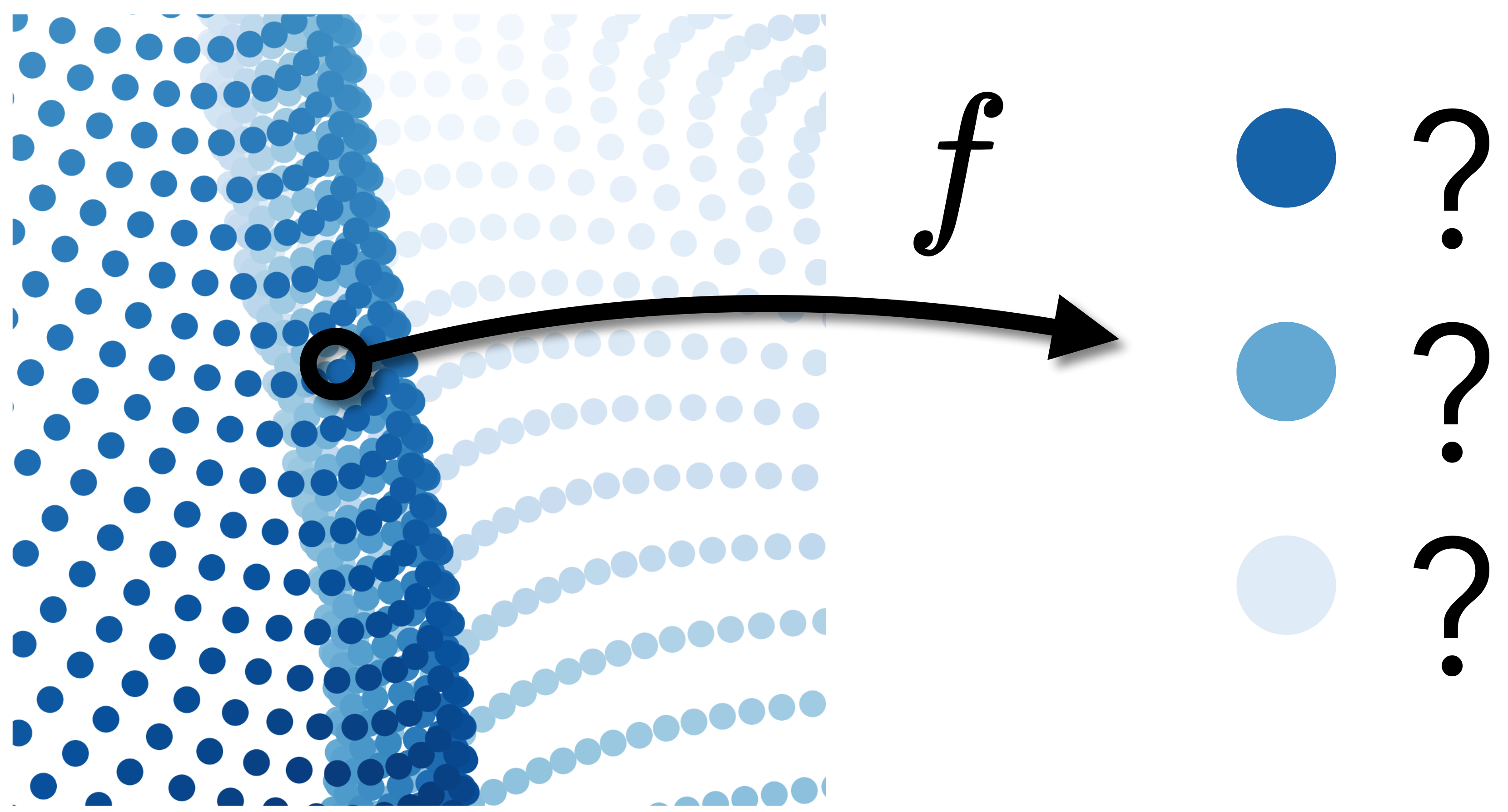


Regression model will likely struggle in the region of overlap.

$$\text{Quantity of interest} = f(\eta_1, \eta_2)$$





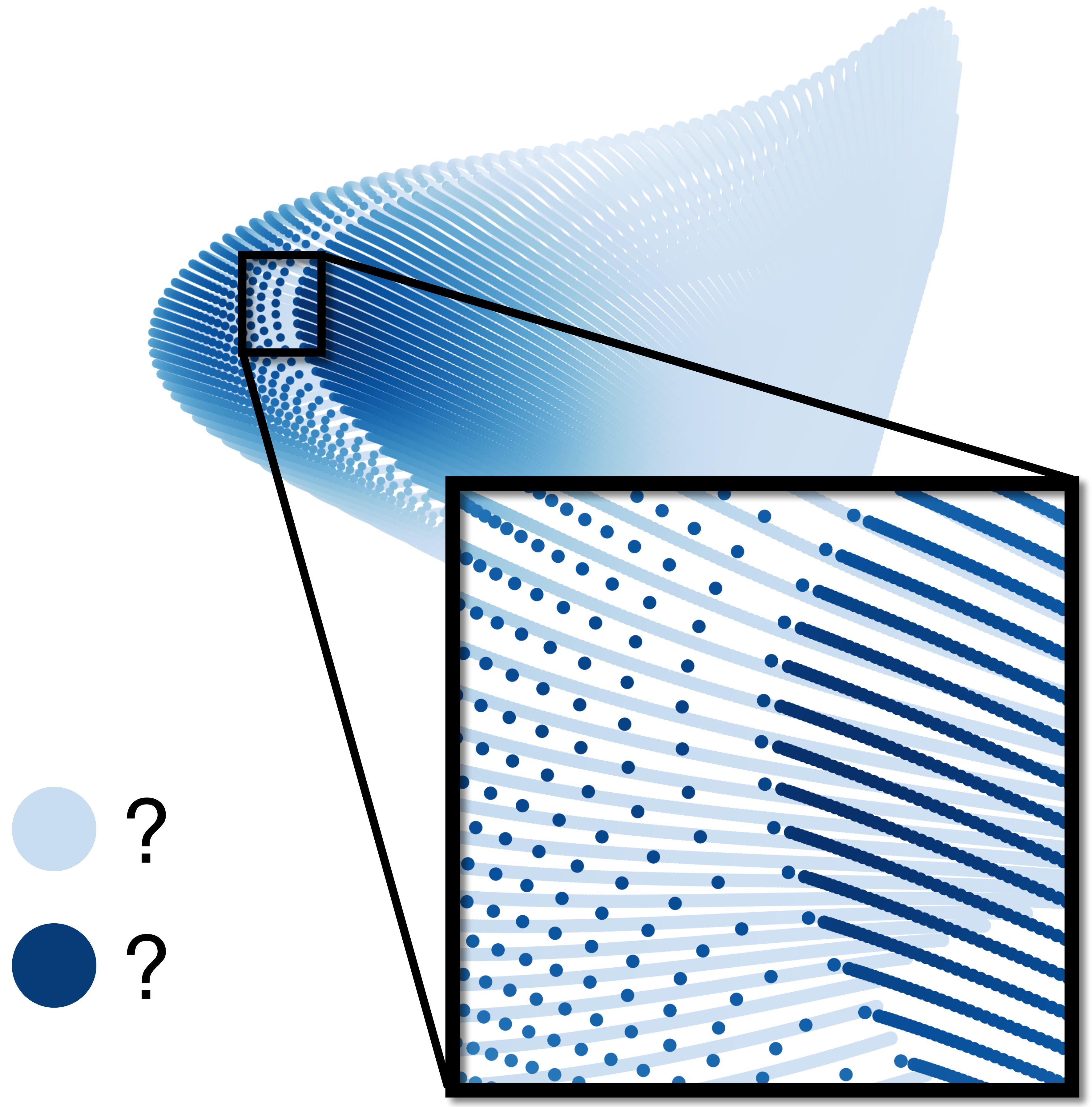


Can we quantify which projection is "**good**"?

nature SCIENTIFIC REPORTS

K. Zdybał, E. Armstrong, J.C. Sutherland, A. Parente
Cost function for low-dimensional manifold topology assessment

We scan the projection at various spatial scales for any variation in a dependent variable values.



$\hat{\mathscr{D}}(\sigma)$

E. Armstrong, J. C. Sutherland, 2021. A technique for characterising feature size and quality of manifolds. *Combustion Theory and Modelling*, *25*(4), pp.646-668.

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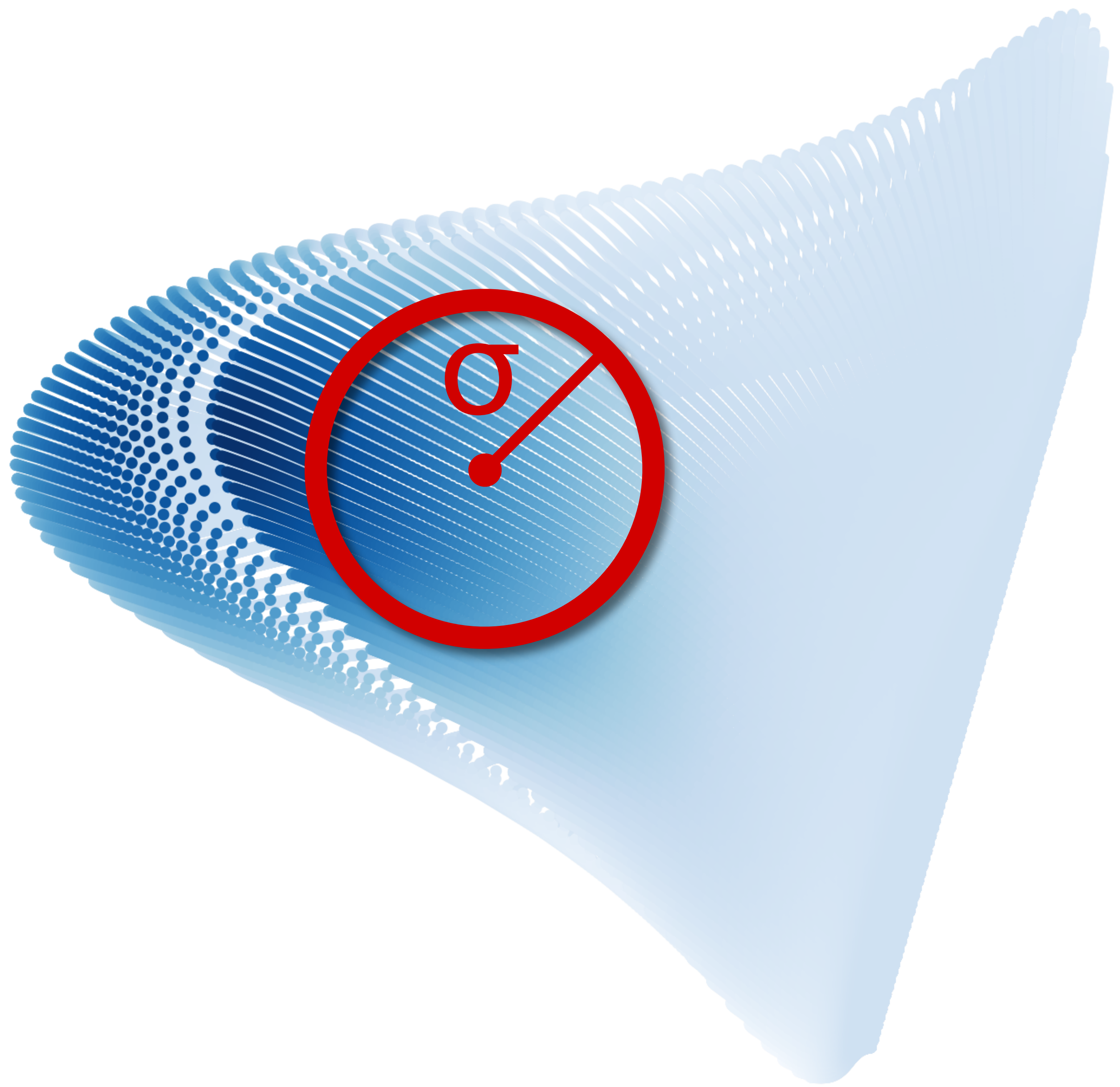

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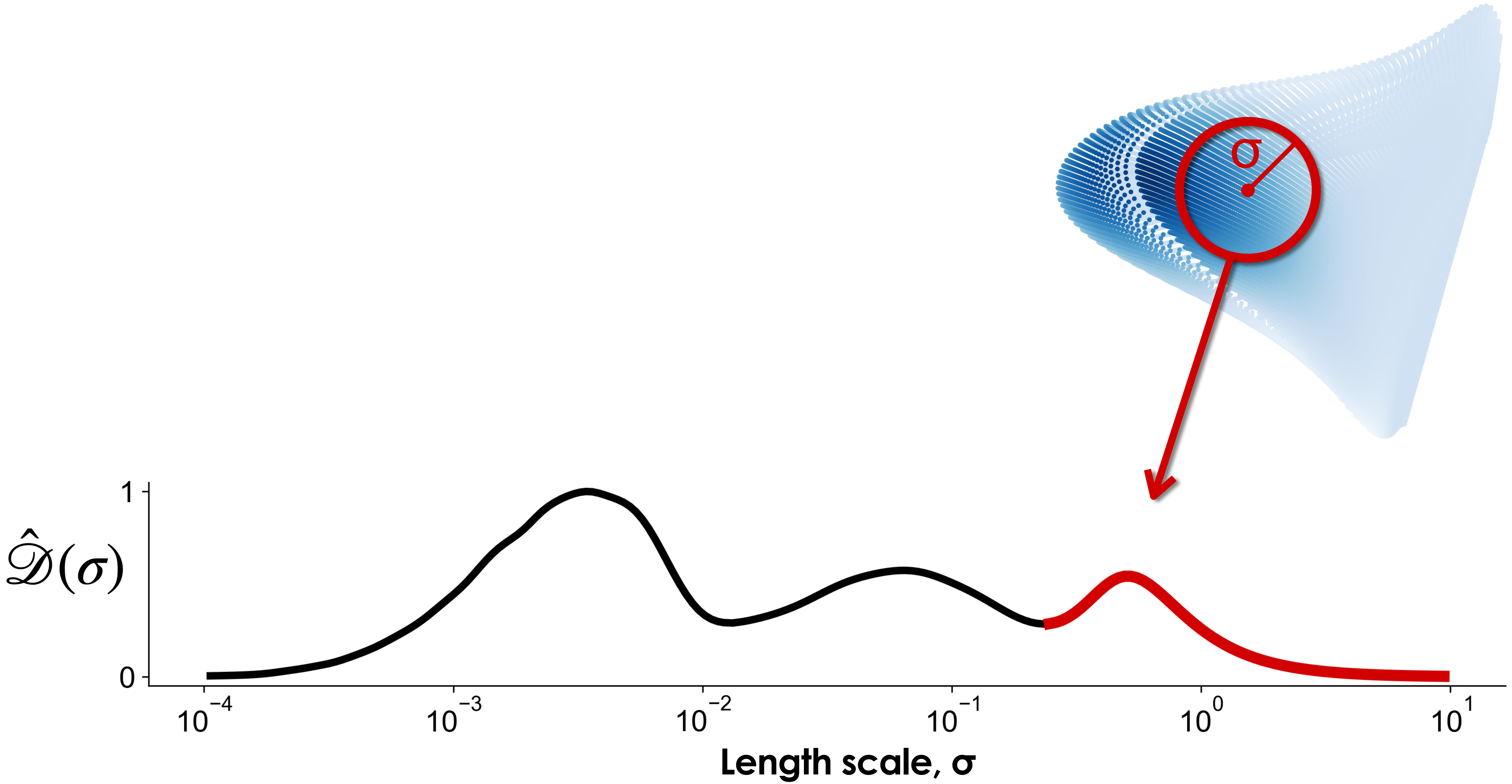
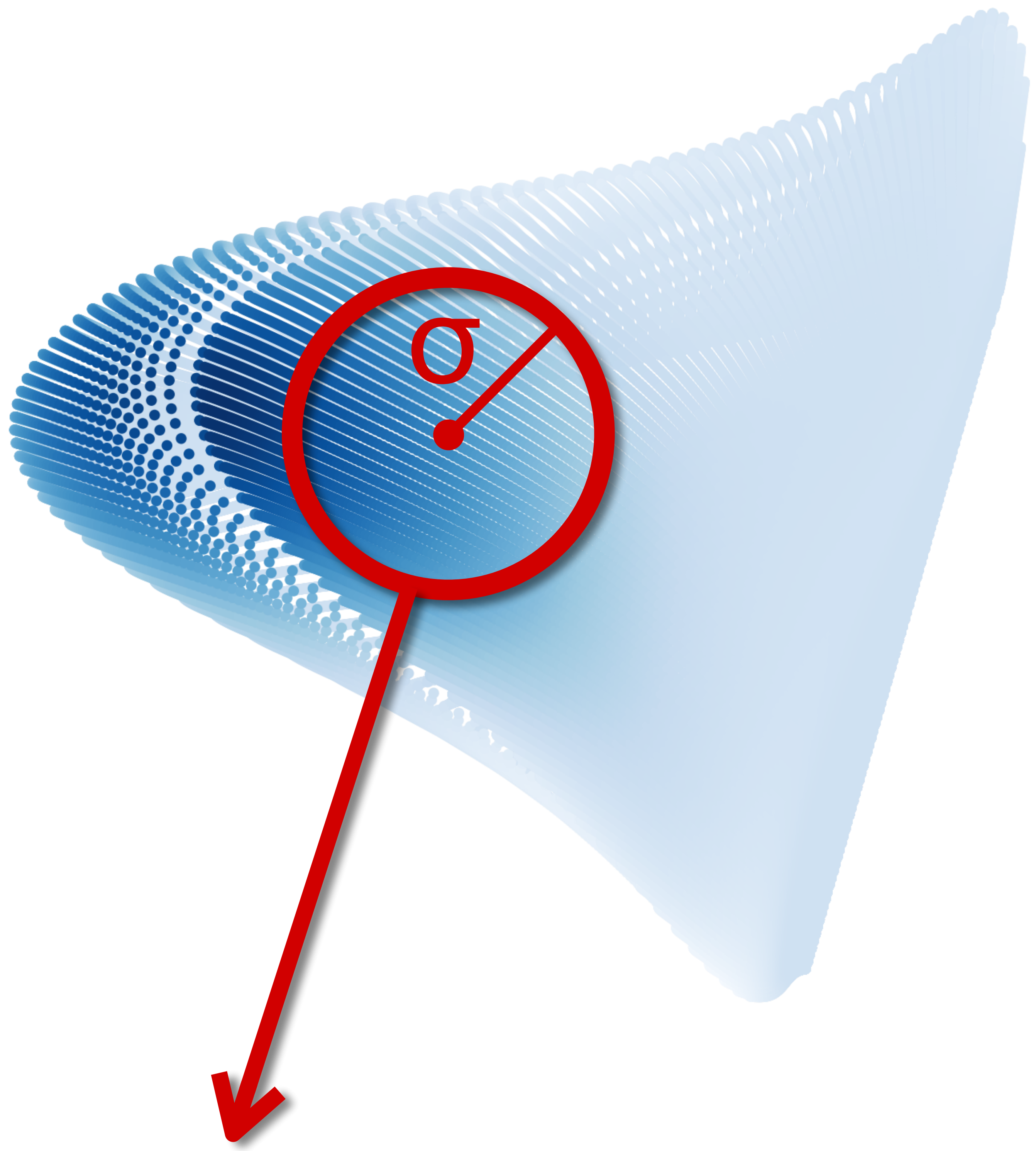
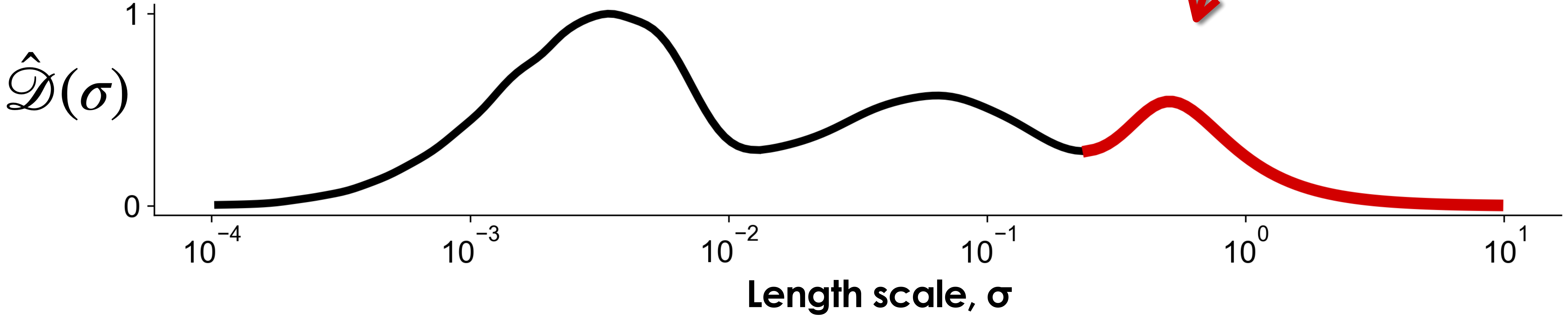


We scan the projection at various spatial scales for any variation in a dependent variable values.

Variance under filter width:

$$\frac{\sum_{i=1}^{n}(\phi_i - \mathscr{K}(\sigma))^2}{\sum_{i=1}^{n}(\phi_i - \bar{\phi}_i)^2}$$





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Variance under filter width:

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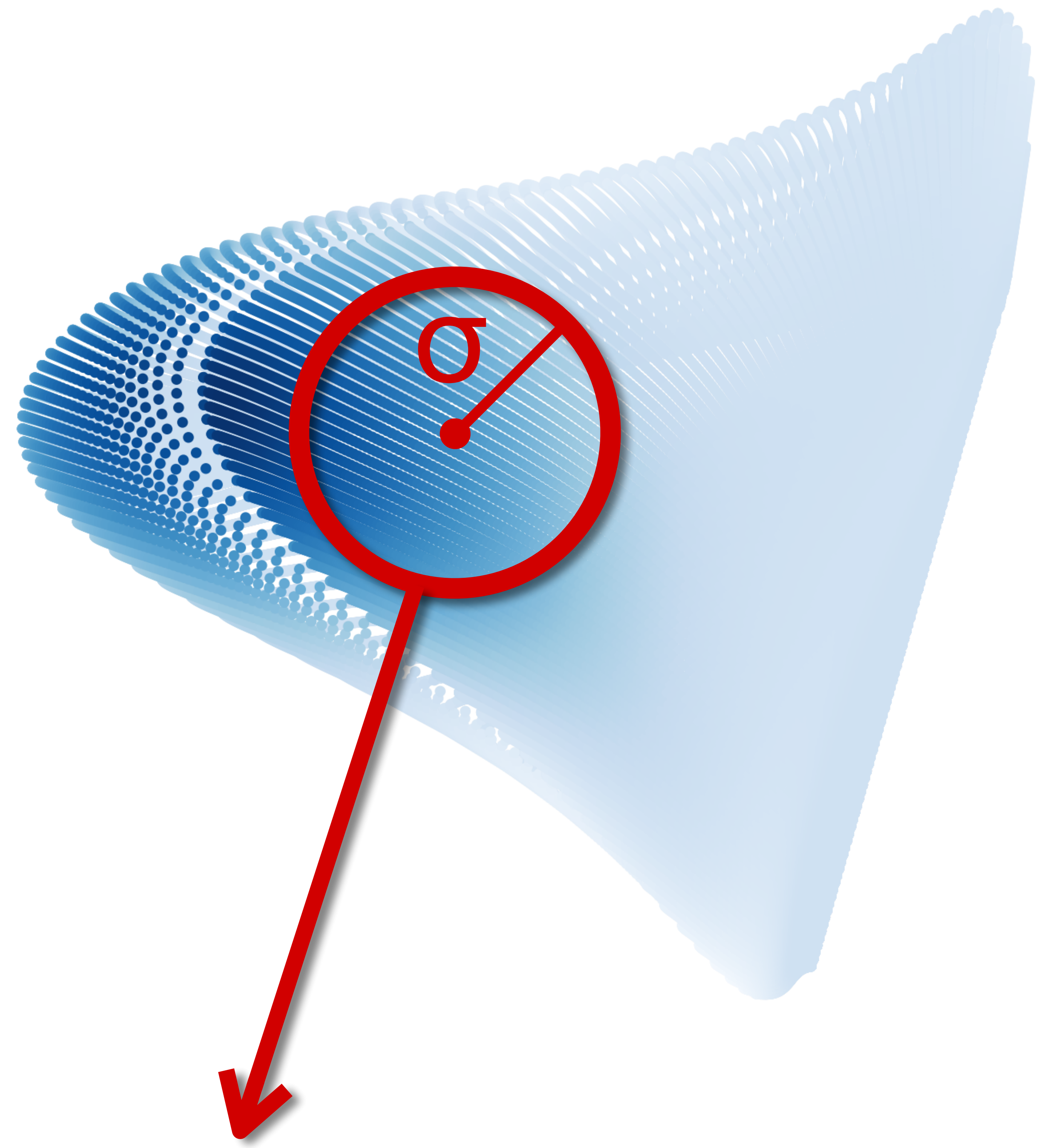

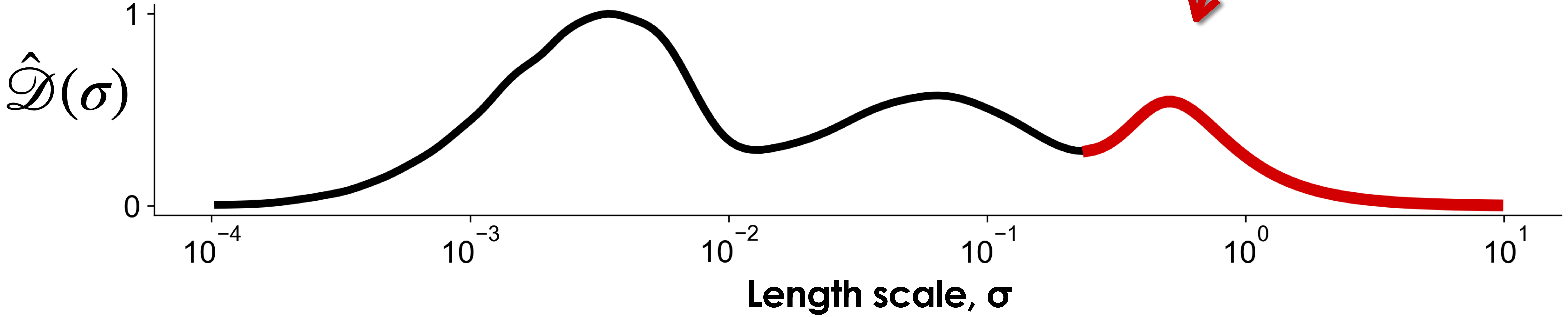

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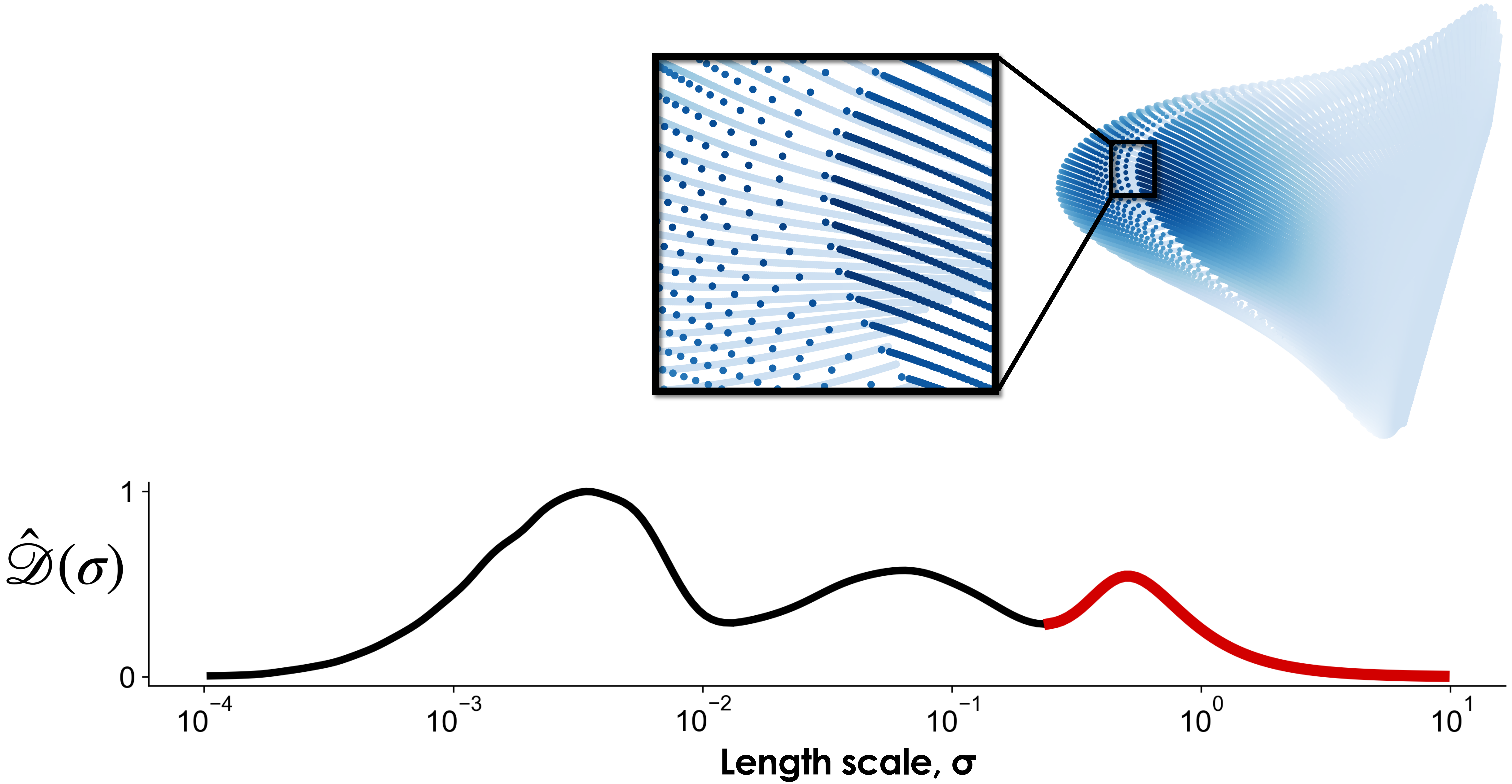

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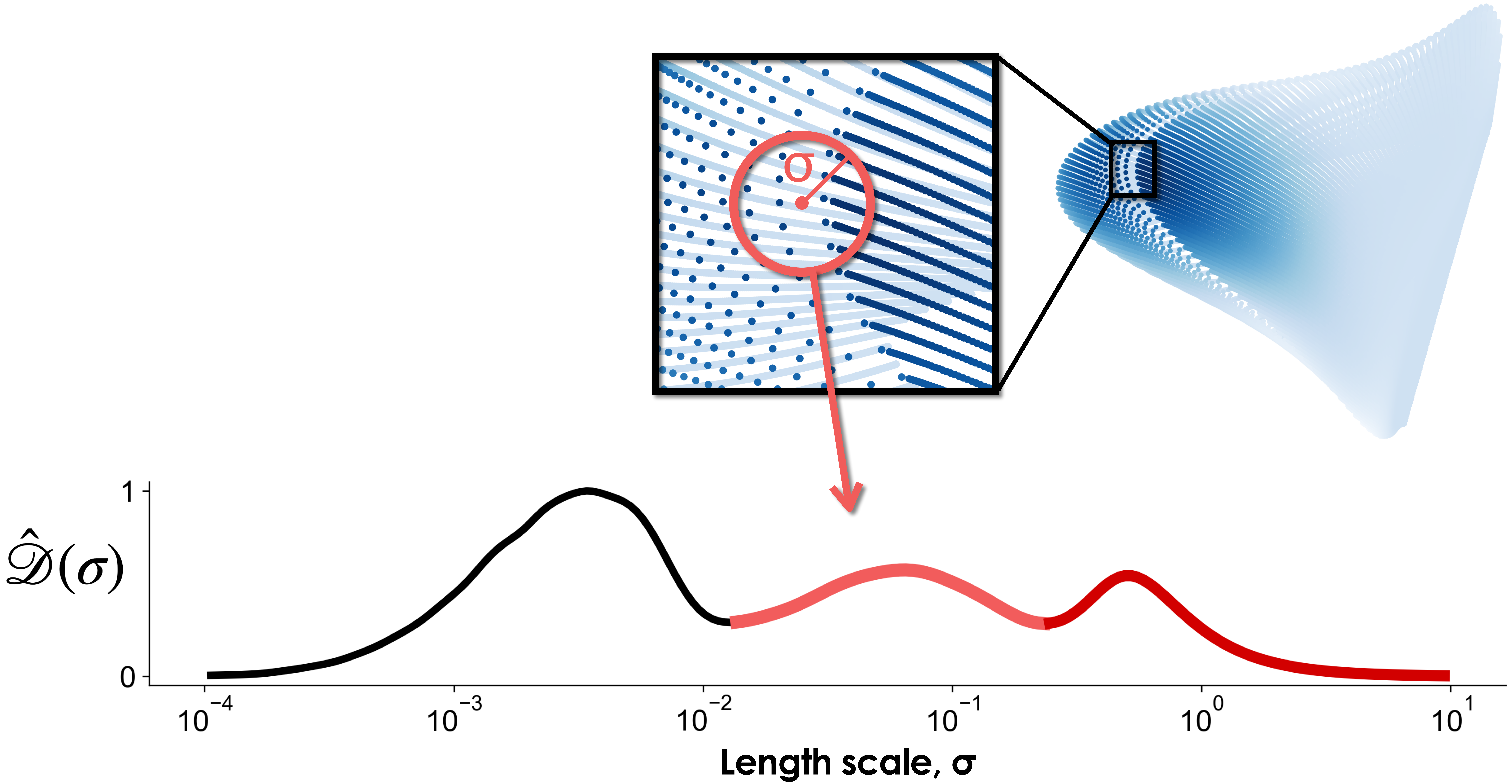

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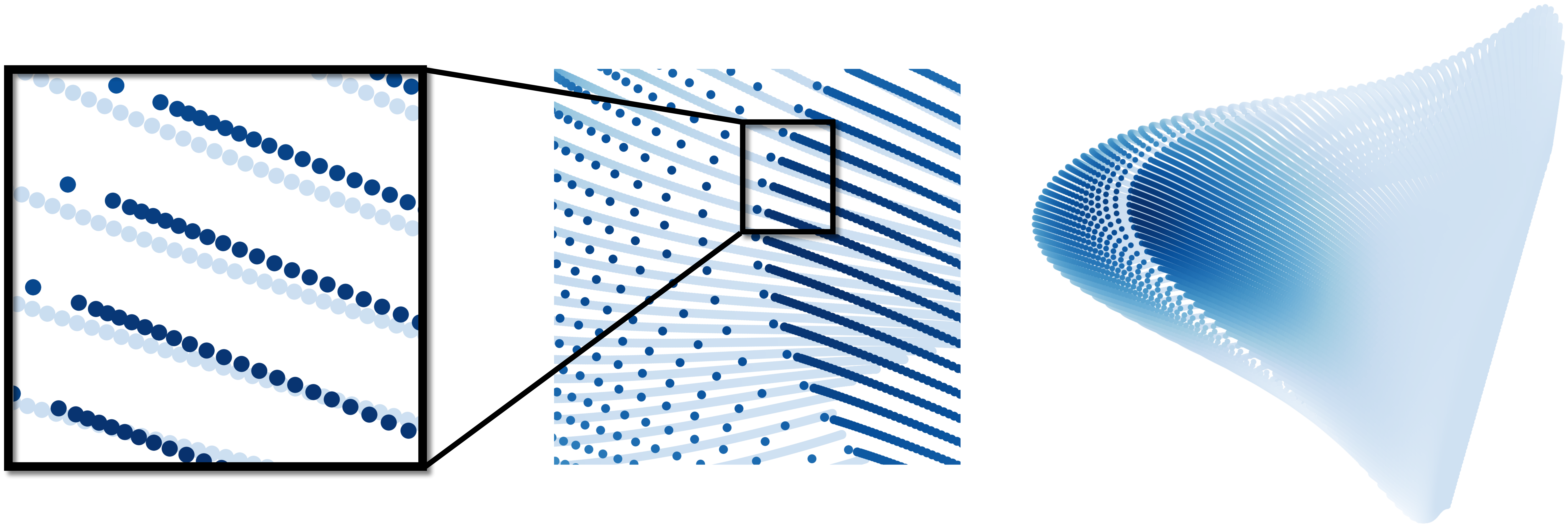

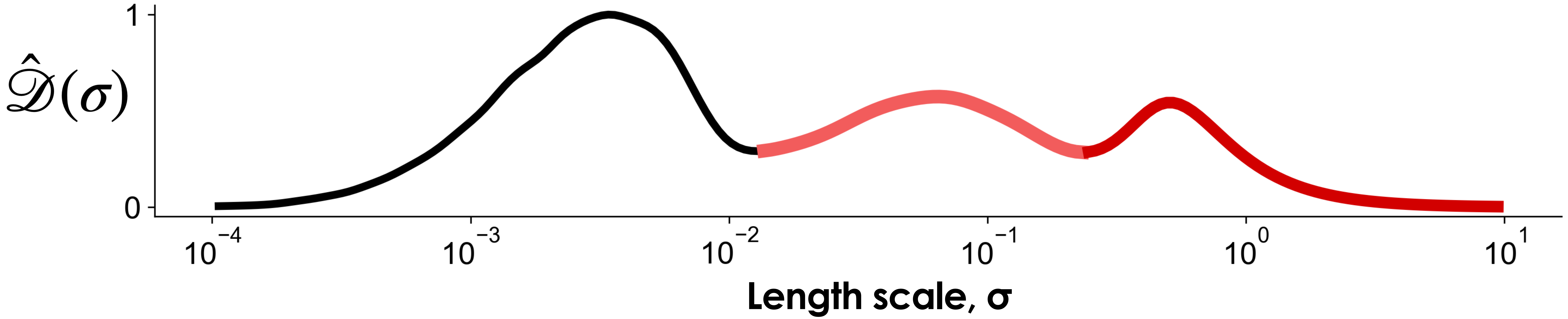

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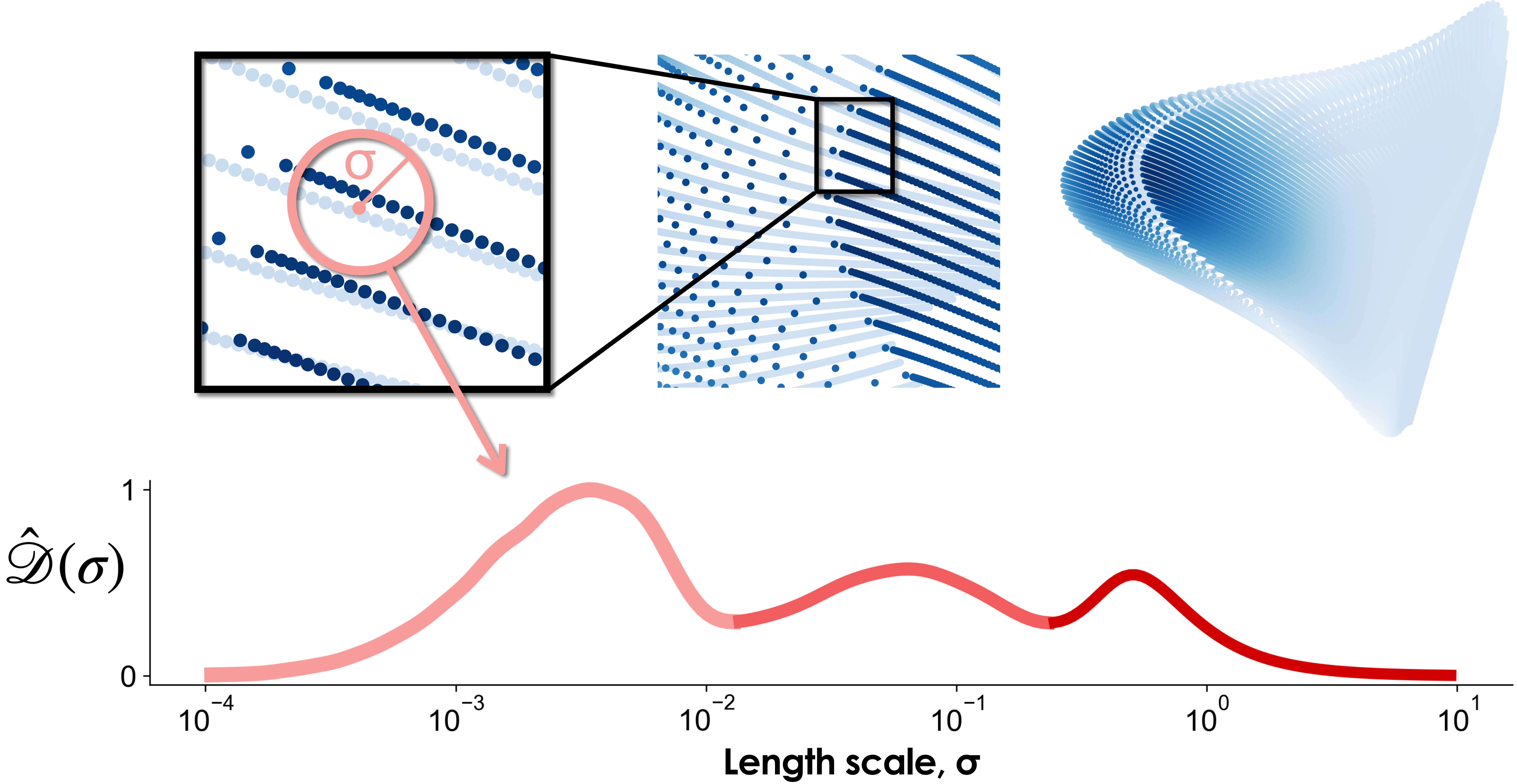
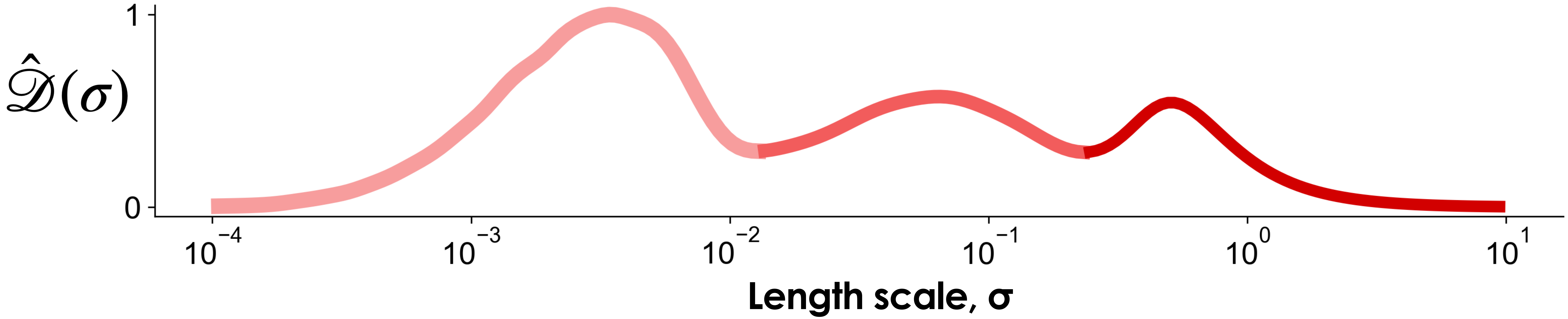
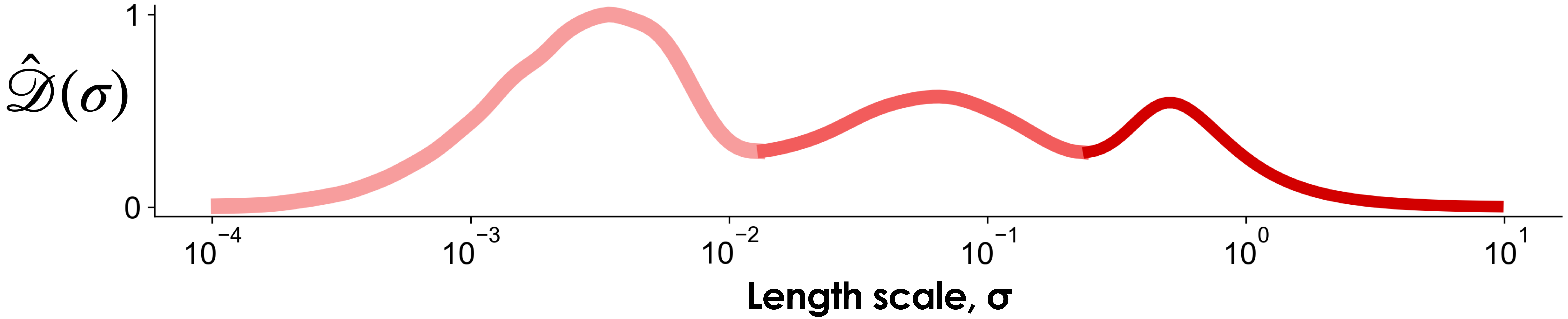


Our cost function penalizes and sums up contributions from all length scales.



Our cost function penalizes and sums up contributions from all length scales.

$$\mathcal{L} = \int_{\widetilde{\sigma}_{min}}^{\widetilde{\sigma}_{max}} \left(\left| \widetilde{\sigma} - \widetilde{\sigma}_{peak} \right|^{r} + b \cdot \frac{\widetilde{\sigma}_{max} - \widetilde{\sigma}_{min}}{\widetilde{\sigma}_{peak} - \widetilde{\sigma}_{min}} \right) \cdot \hat{\mathscr{D}}(\sigma) \mathrm{d}\widetilde{\sigma}$$



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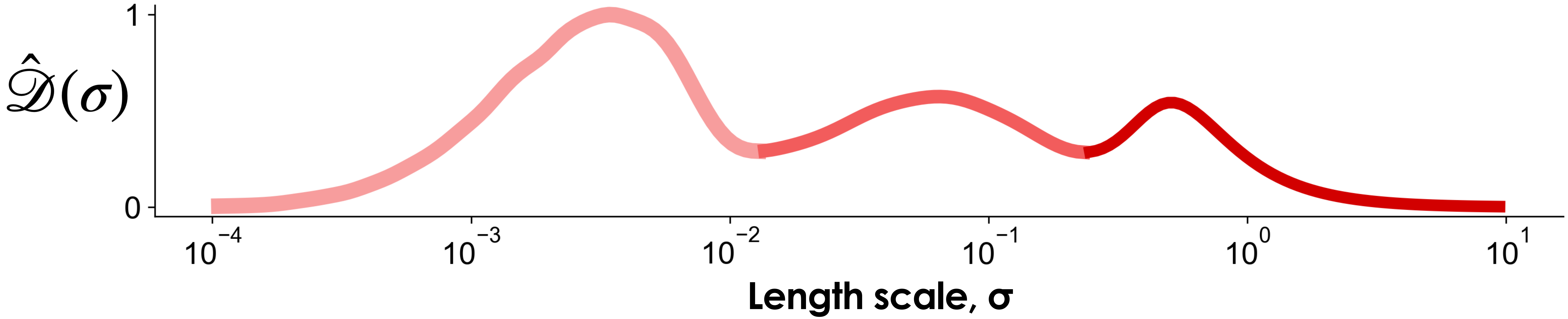

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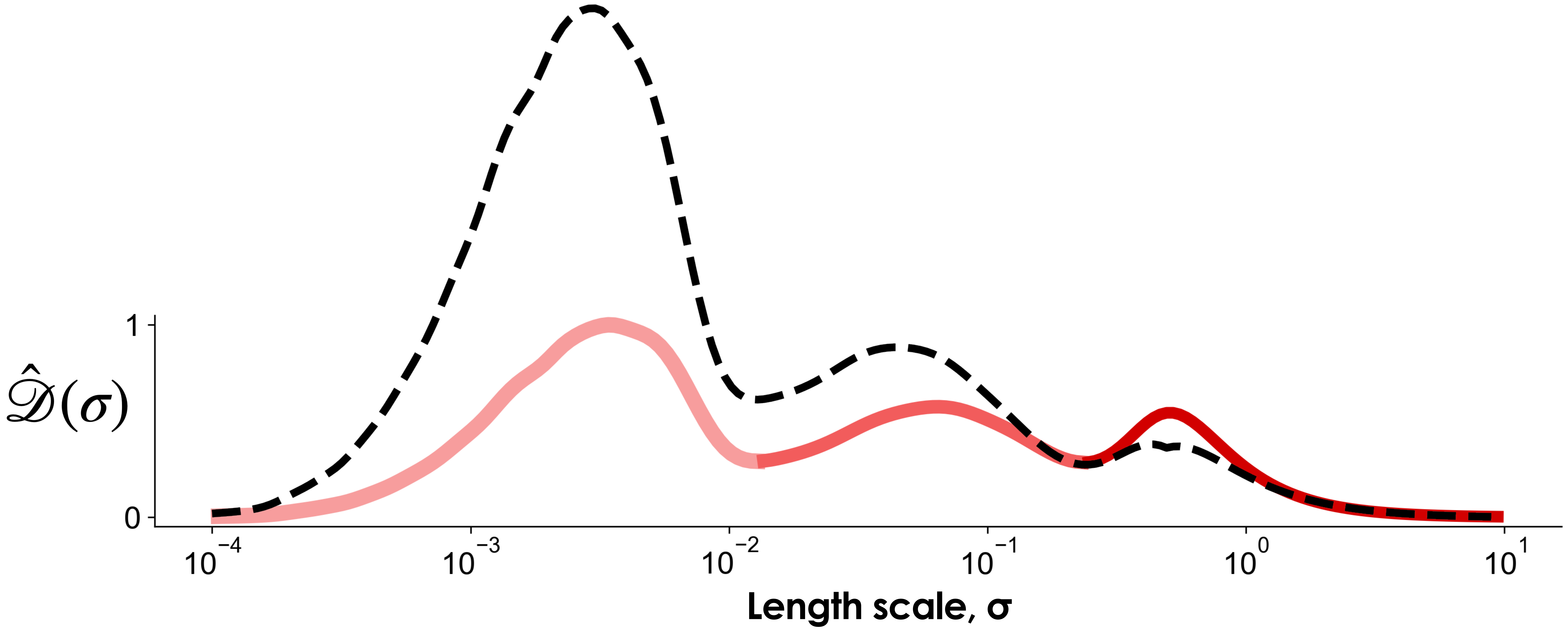

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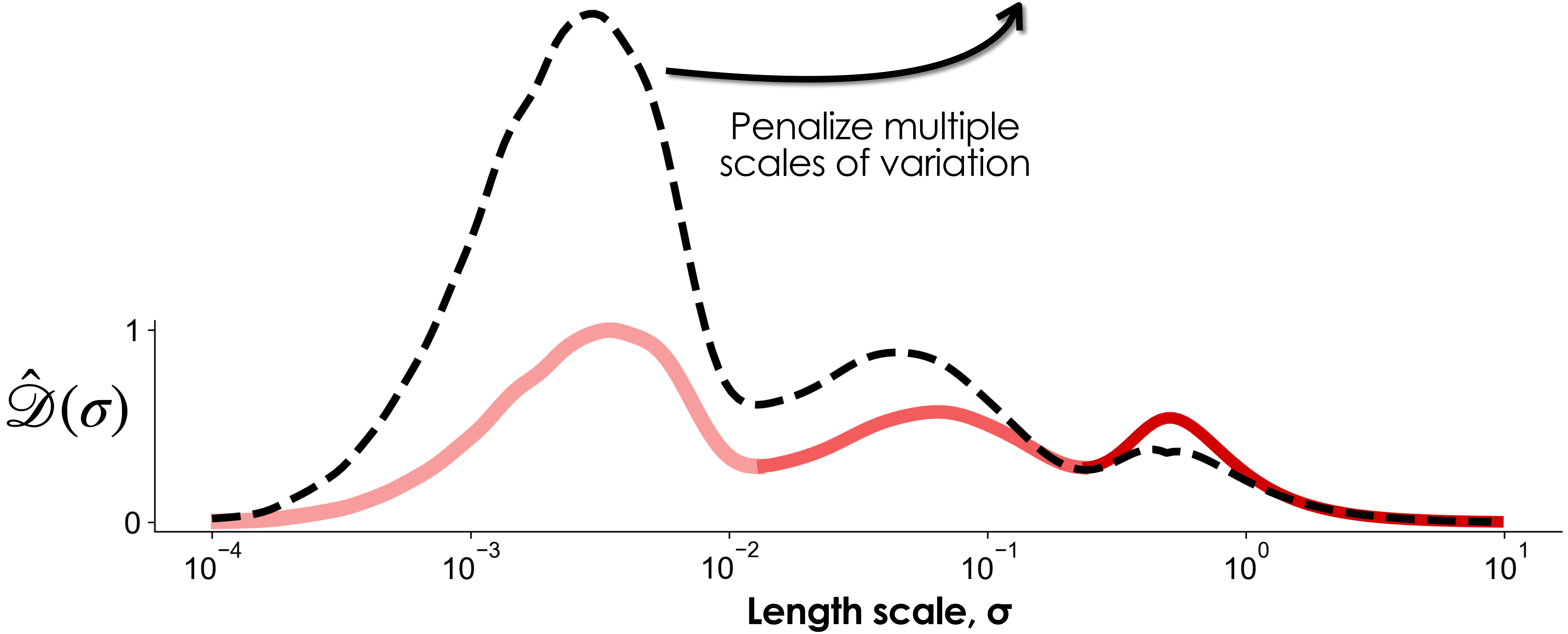
Penalize multiple scales of variation



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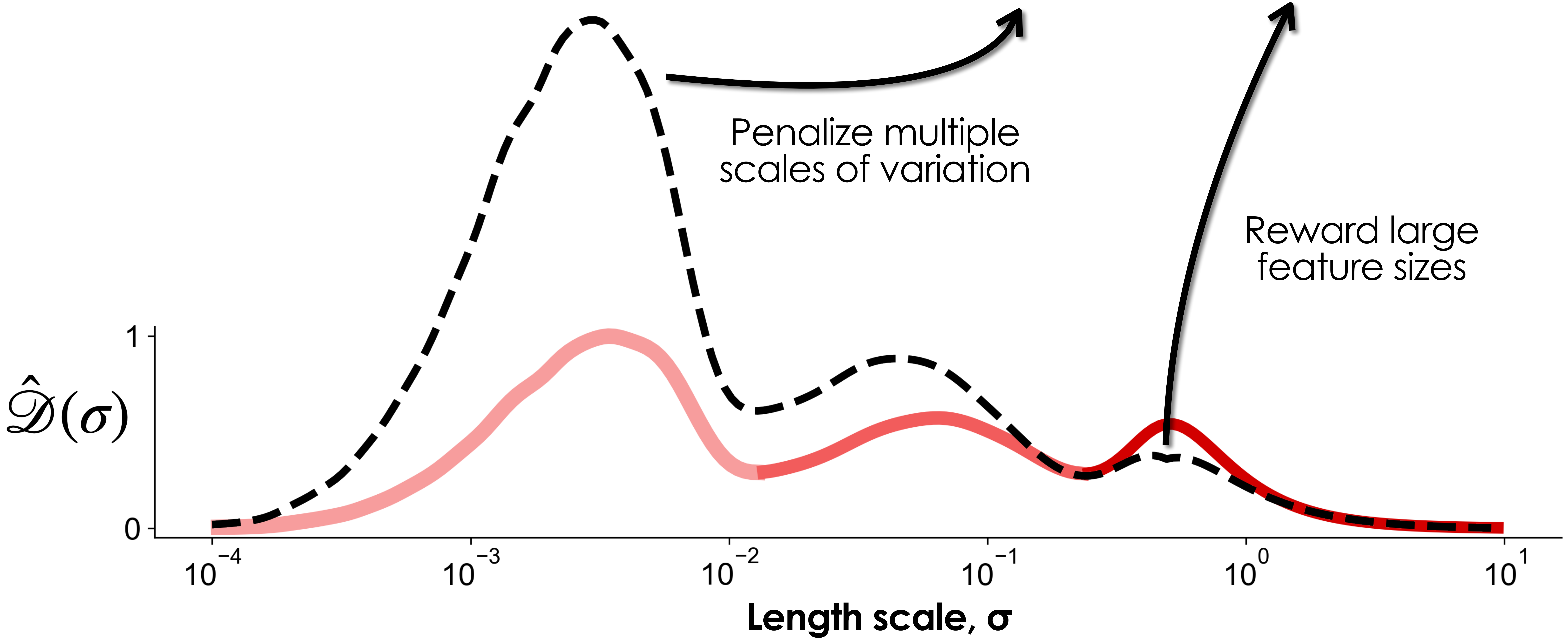

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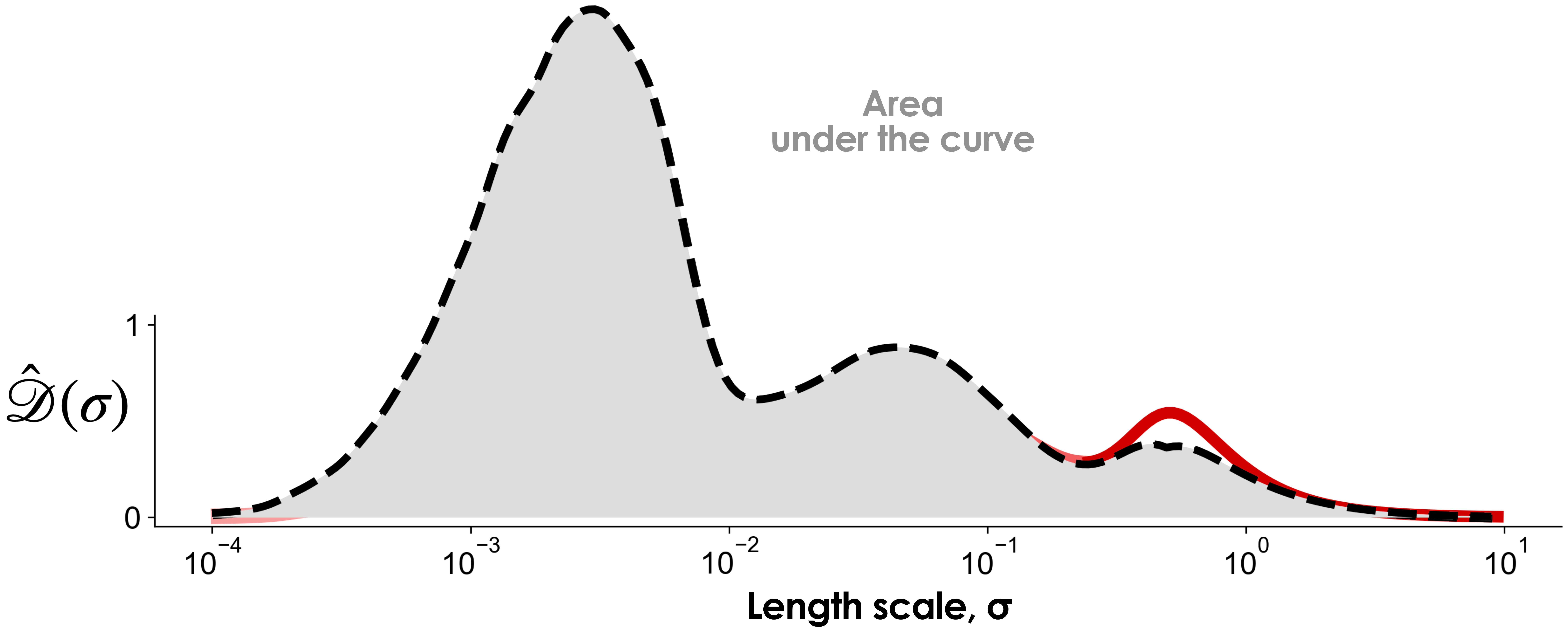

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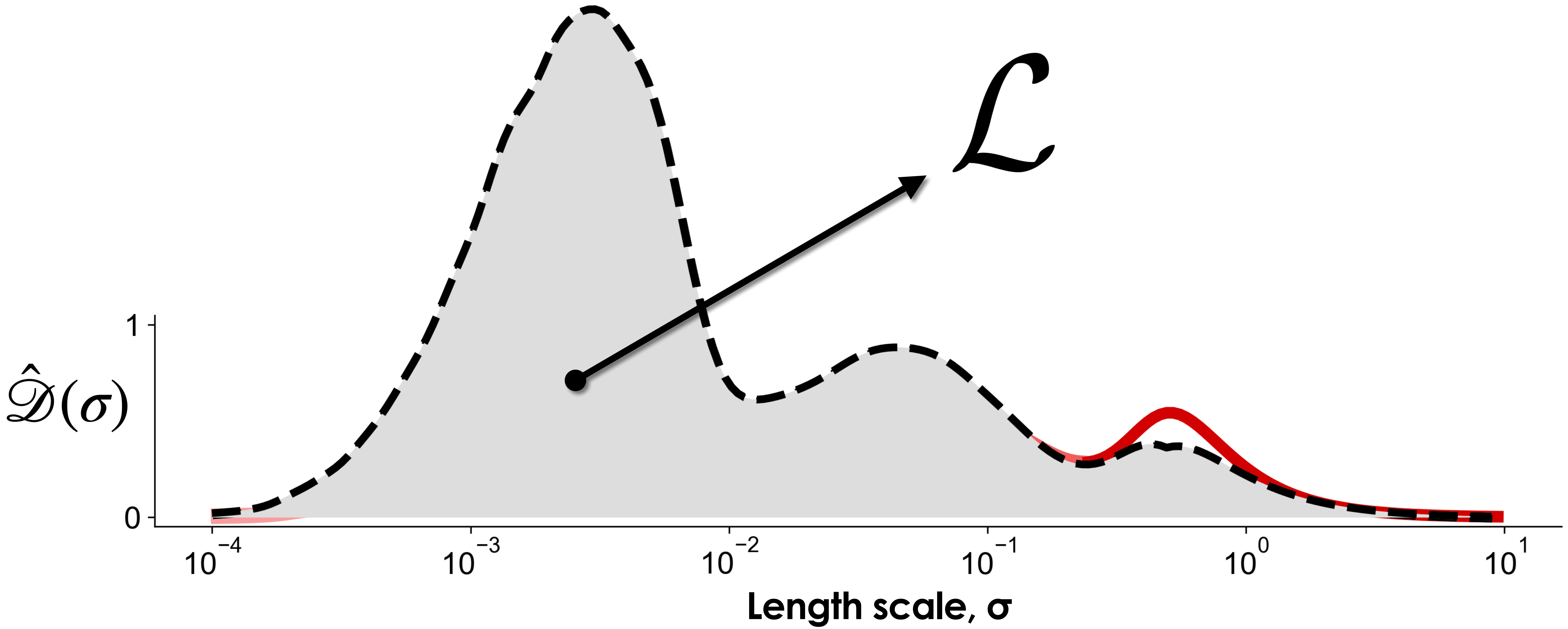
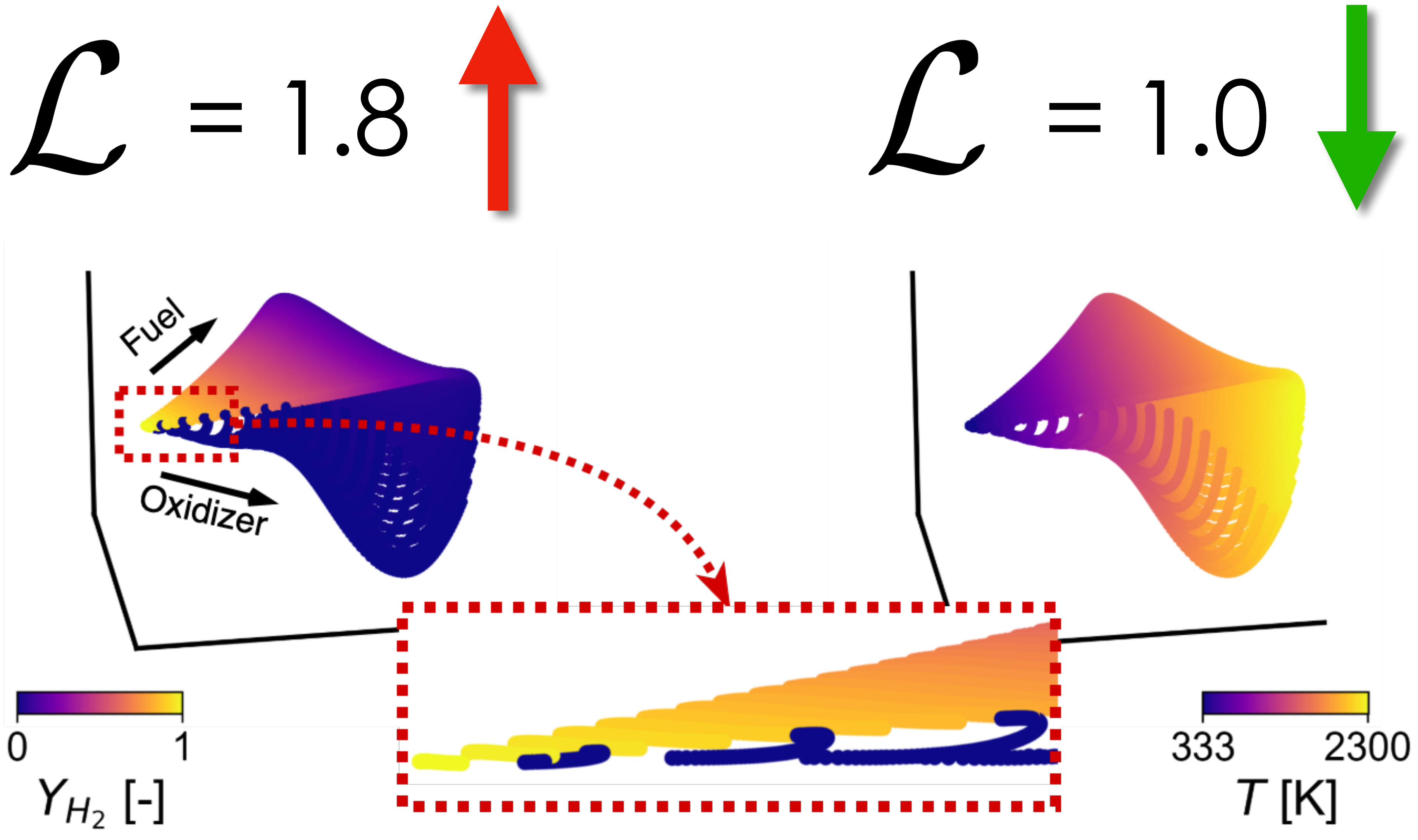
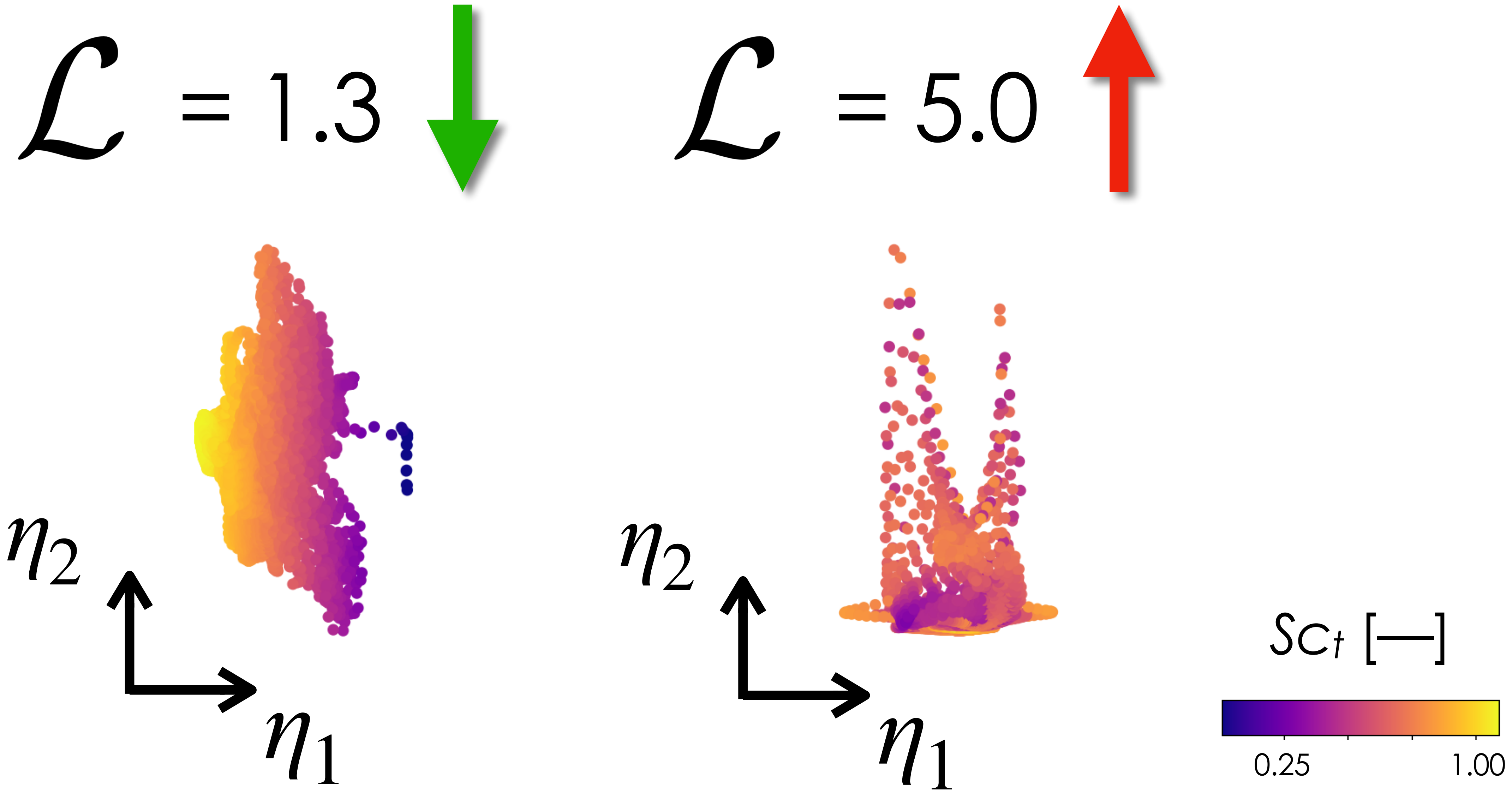


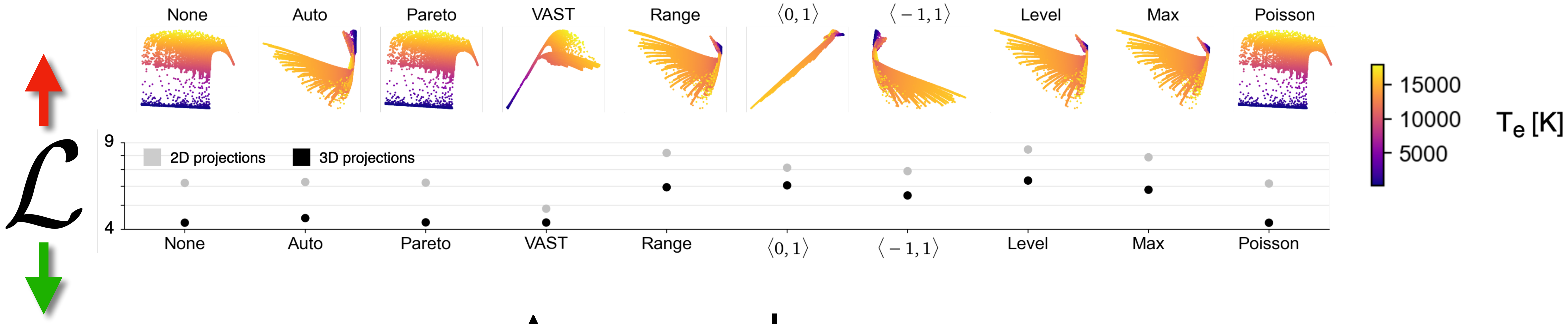
We demonstrated the application of the cost function to various datasets.



Numerical and experimental combustion



Atmospheric pollutant dispersion



Argon plasma

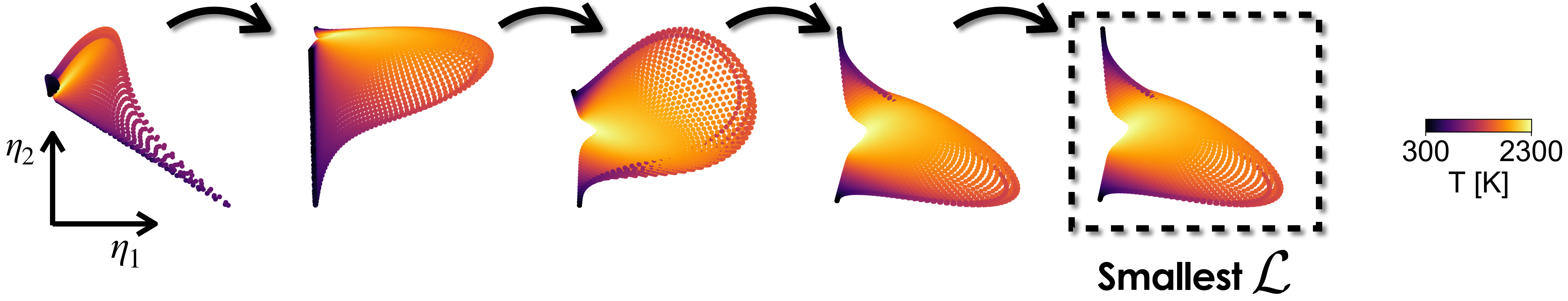
We propose a manifold-informed state variable selection strategy.

PROCEEDINGS OF
THE COMBUSTION INSTITUTE

K. Zdybał, J.C. Sutherland, A. Parente
Manifold-informed state vector subset for reduced-order modeling
Distinguished Paper Award from The Combustion Institute

Our variable selection is optimized with respect to the cost function.

$$\mathbf{X} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X_1 & X_2 & X_3 & X_4 & X_5 & X_6 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix} \xrightarrow{\mathcal{L}} \mathbf{X} = \begin{bmatrix} \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ X_1 & X_2 & X_3 & X_4 & X_5 & X_6 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$



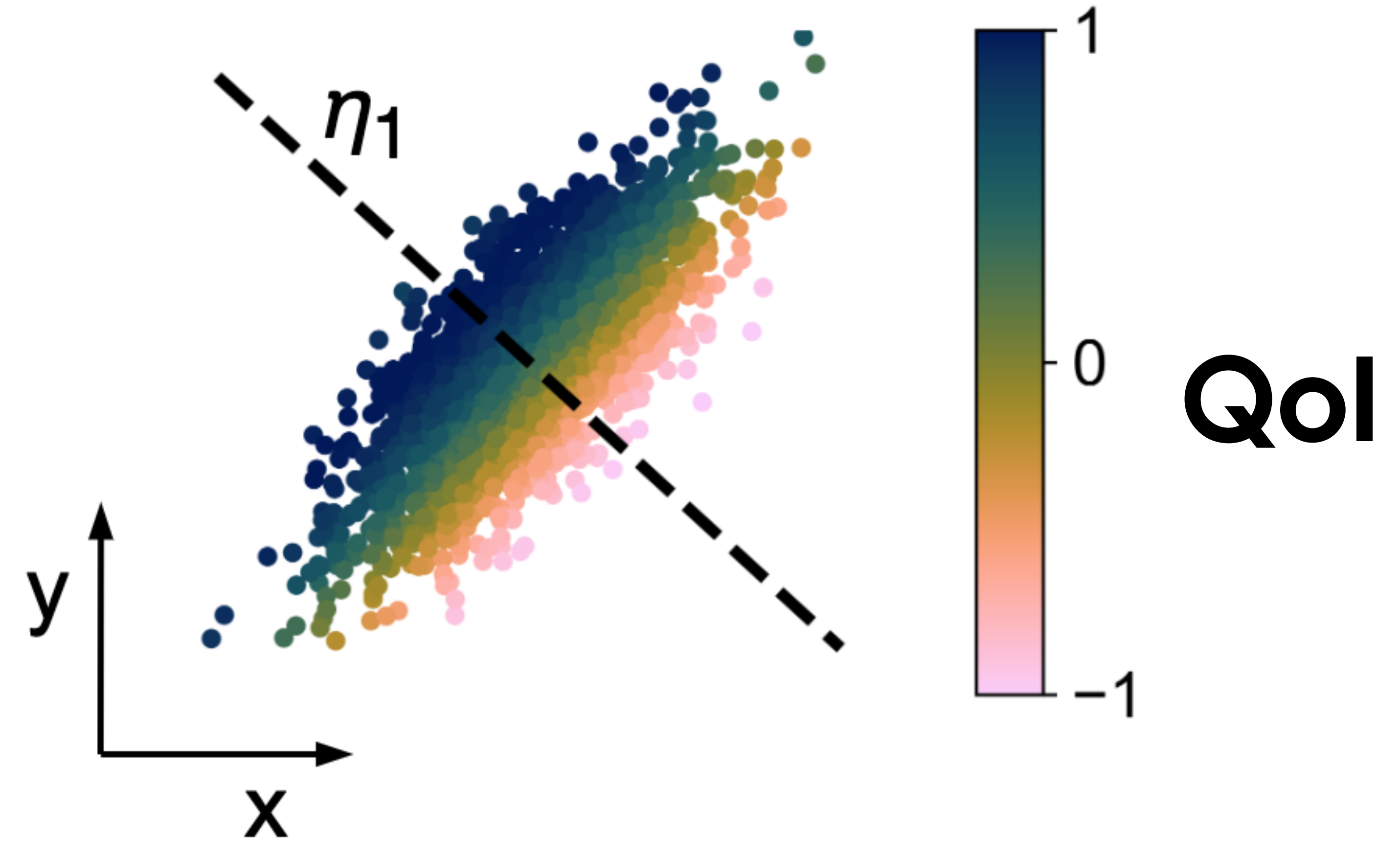
$\mathbf{X}$ = [T, H_2, O_2, O, OH, H_2O, H, HO_2, CO, CO_2, HCO]

We propose a QoI-informed dimensionality reduction strategy.

CellPress Patterns

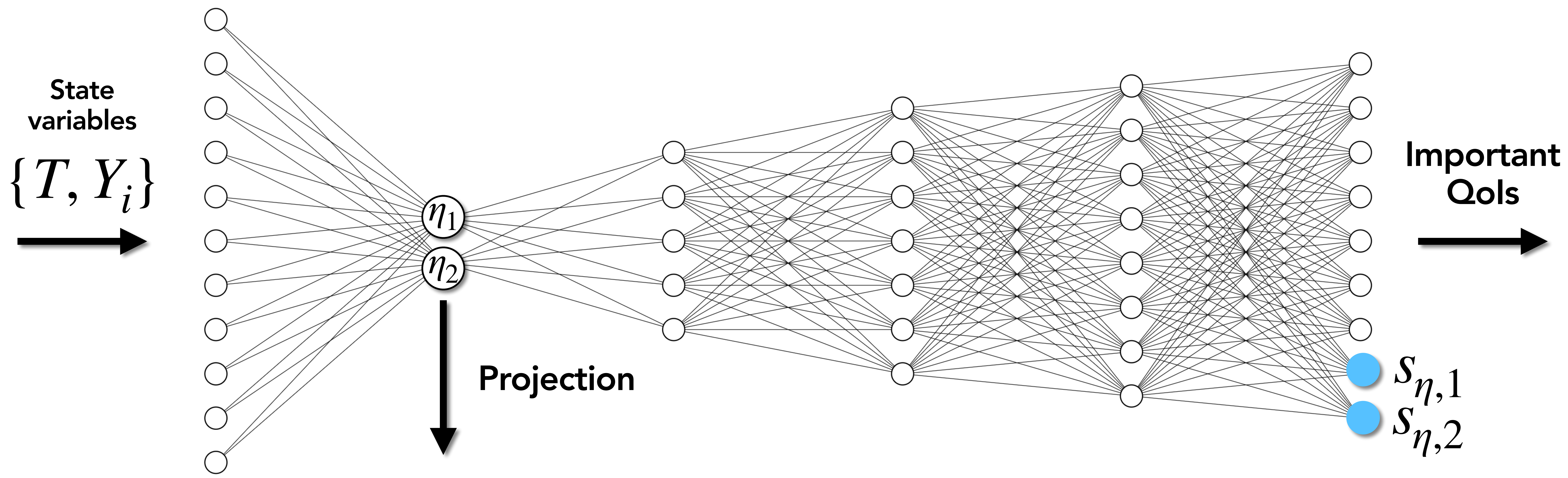
K. Zdybał, A. Parente, J.C. Sutherland
Improving reduced-order models through nonlinear decoding of projection-dependent outputs

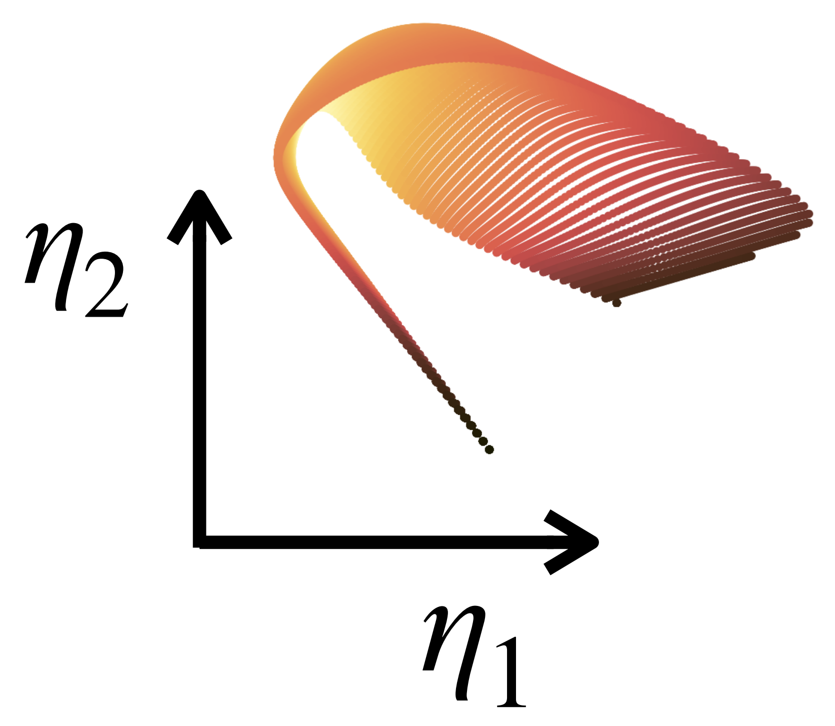
We compute data representations informed by important **quantities of interest (QoIs)**.



$$\frac{\partial \boldsymbol{\eta}}{\partial t} = \underbrace{-\nabla \cdot \mathbf{C}_{\boldsymbol{\eta}}}_{\text{Convection}} \underbrace{- \nabla \cdot \mathbf{D}_{\boldsymbol{\eta}}}_{\text{Diffusion}} + \underbrace{\boxed{\mathbf{S}_{\boldsymbol{\eta}}}}_{\text{Source}}$$

We compute data representations informed by important quantities of interest.





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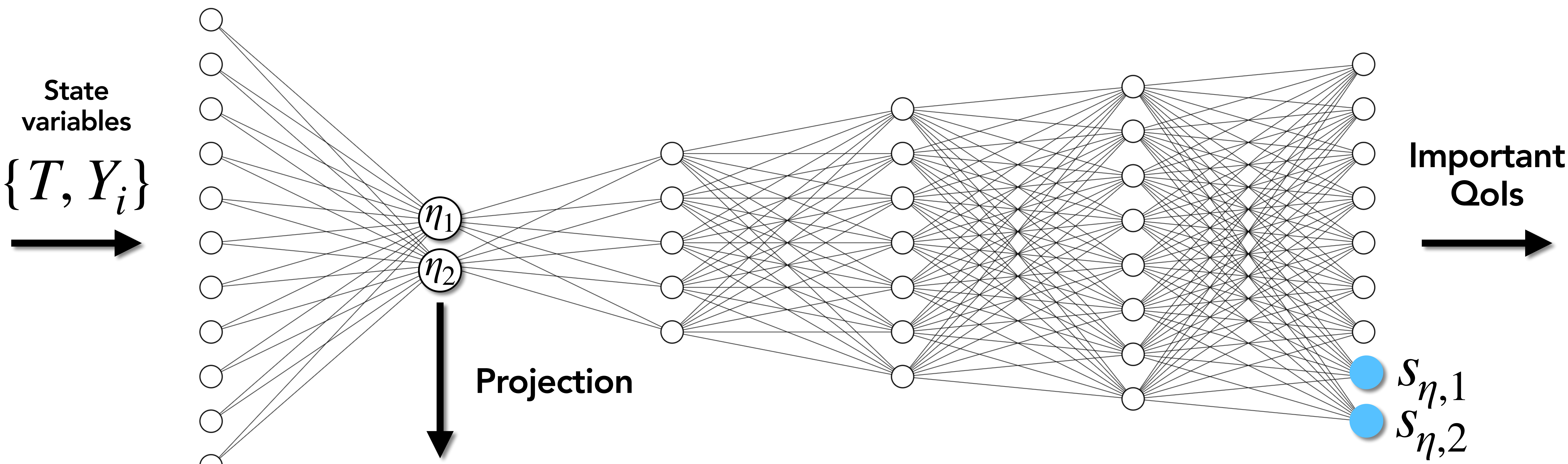

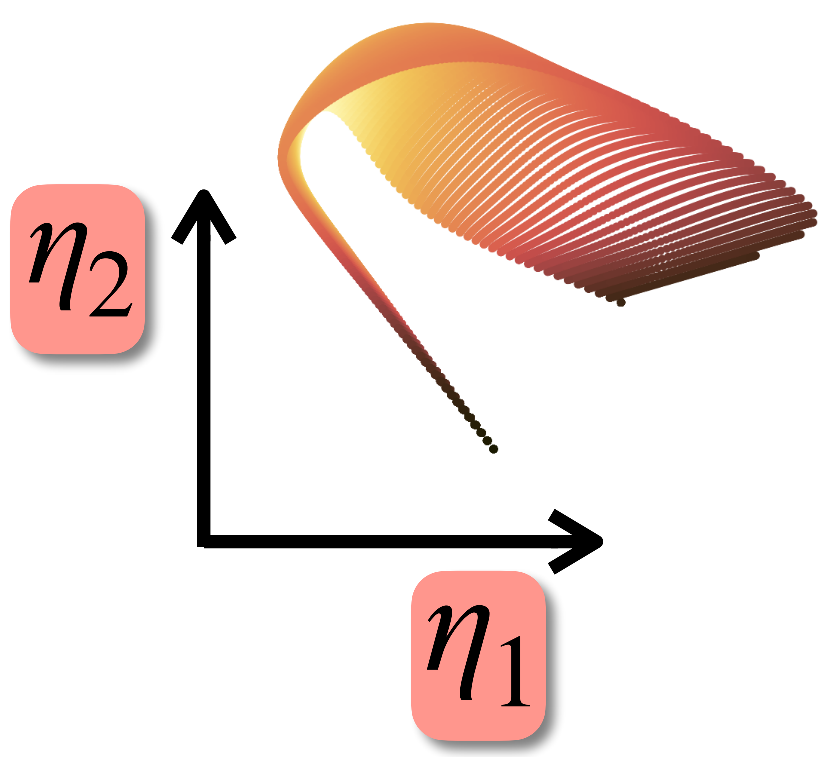

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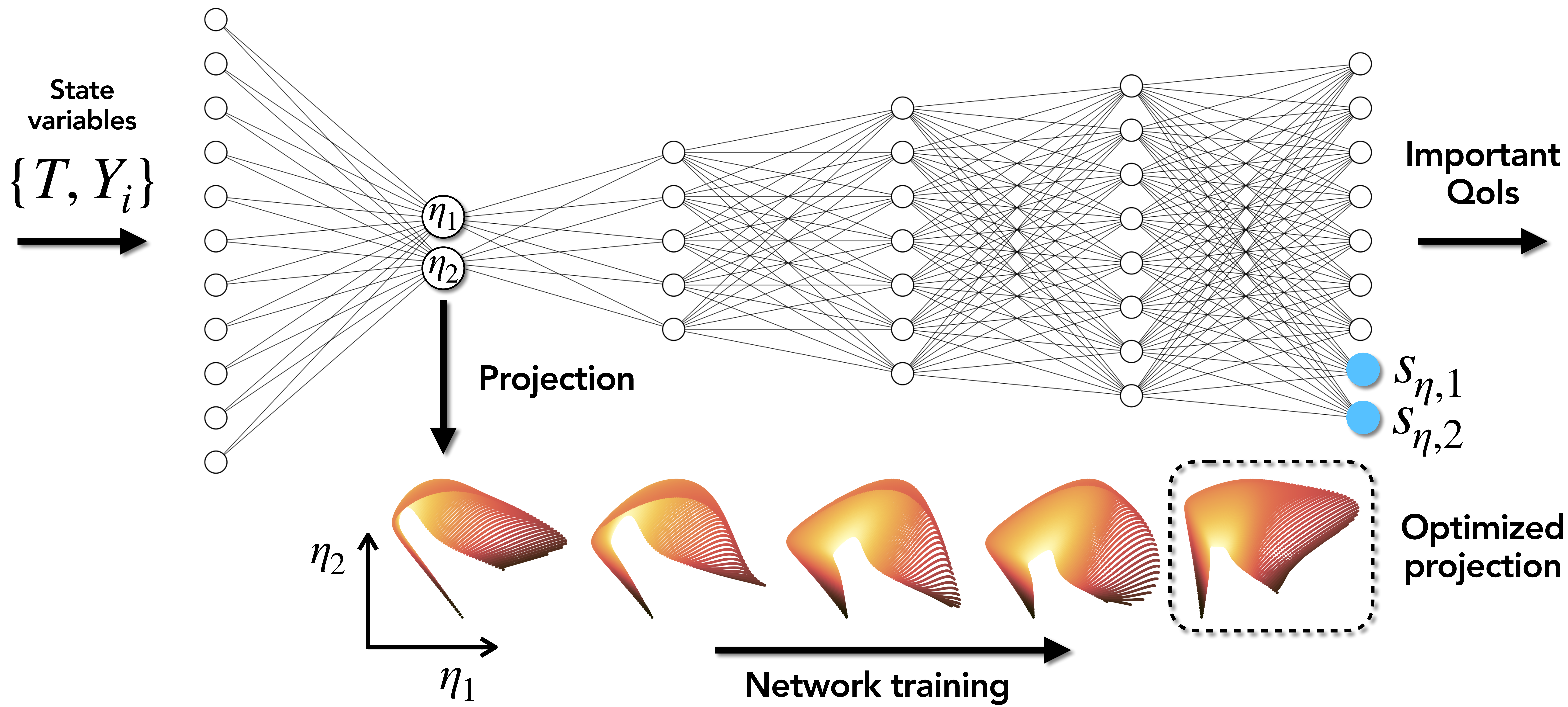
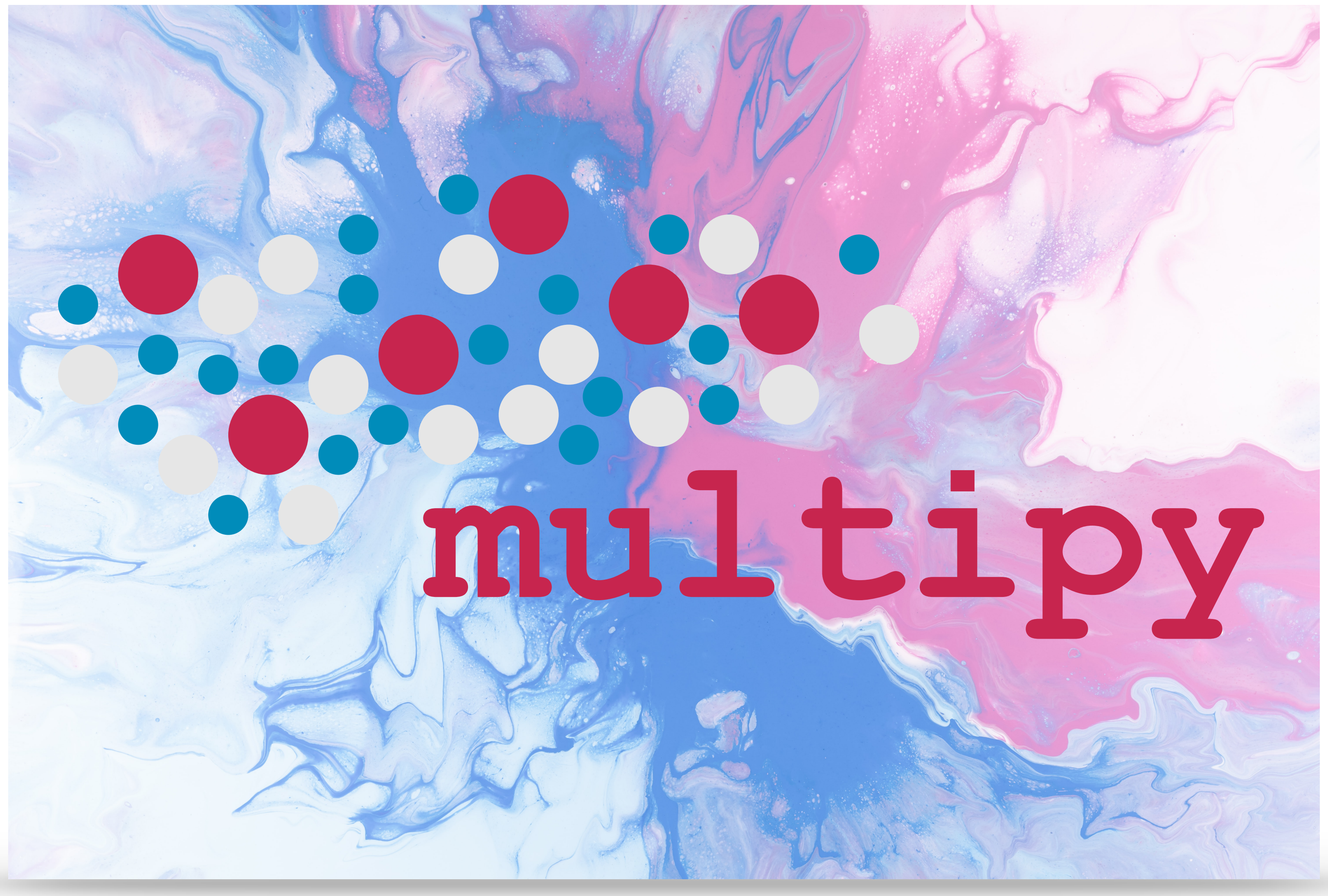


We’ve built tools to help improve

reduced-order models.

I have developed two open-source python libraries:



Background photo by Pawel Czerwinski on Unsplash

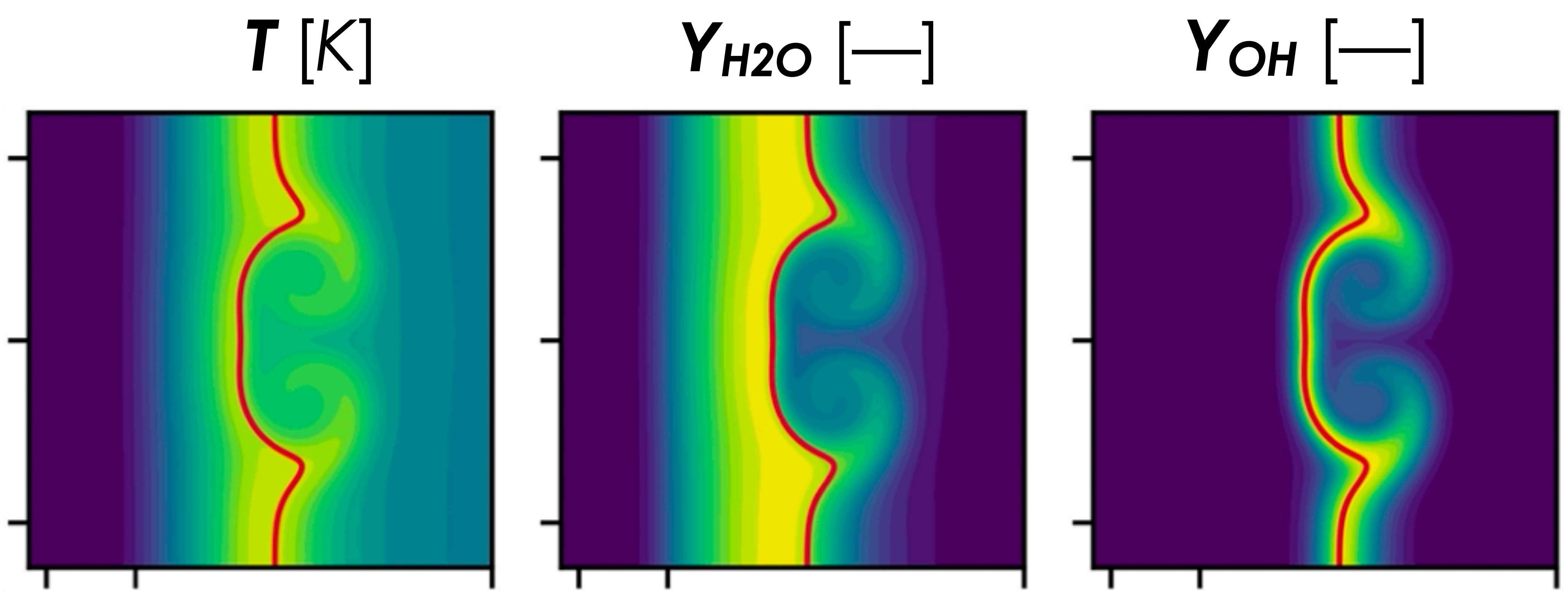
PCAfold: *Tools and algorithms for low-dimensional manifold assessment and optimization*

GitHub.com/kamilazdybal/PCAfold

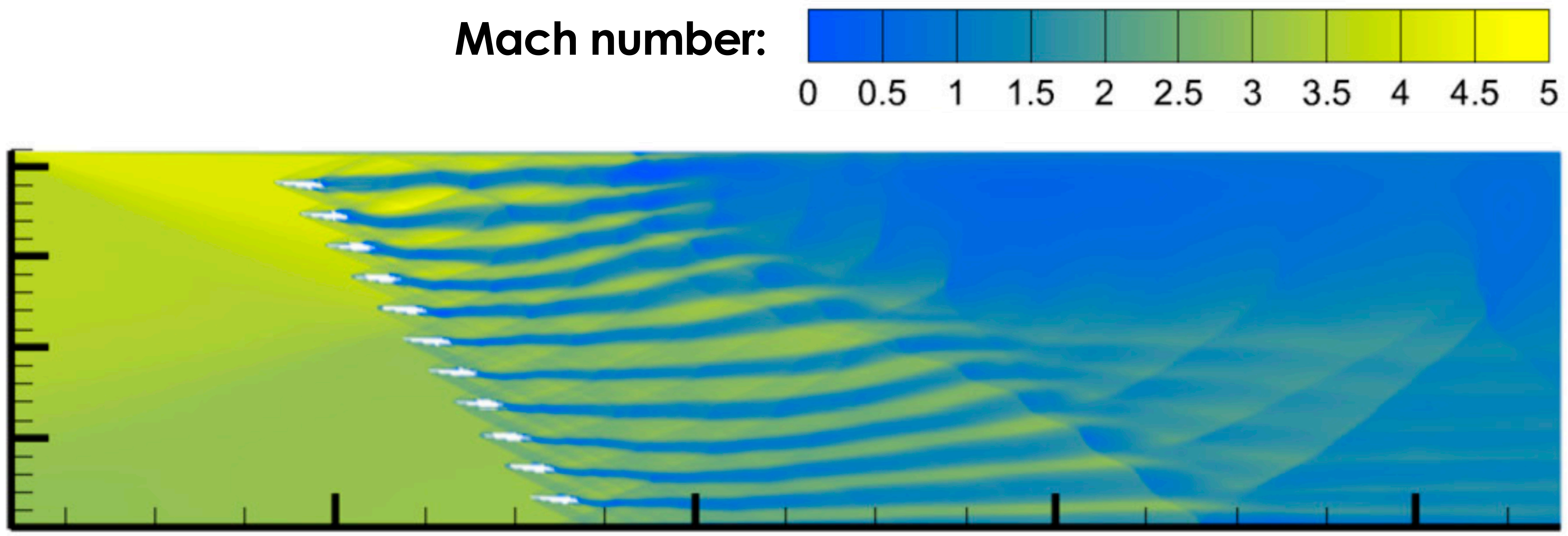
multipy: *An educational Python library for **multi**component mass transfer*

GitHub.com/kamilazdybal/multipy

The tools and algorithms from my thesis have been used by others.



E. Armstrong, J.C. Sutherland
Reduced-order modeling with reconstruction-informed projections
***Combustion and Flame**, 2023*



A.C. Ispir, B.H. Saracoglu, T. Magin, A. Coussement
A methodology for estimating hypersonic engine performance by coupling supersonic reactive flow simulations with machine learning techniques
***Acta Astronautica**, 2023*

Our Python library PCAfold is used by students and researchers from various institutions.

K. Zdybał, E. Armstrong, A. Parente, J.C. Sutherland
PCAfold: Python software to generate, analyze and improve PCA-derived low-dimensional manifolds

K. Zdybał, J.C. Sutherland, A. Parente
Manifold-informed state vector subset for reduced-order modeling

K. Zdybał, E. Armstrong, J.C. Sutherland, A. Parente
Cost function for low-dimensional manifold topology assessment

A.C. Ispir, **K. Zdybał**, B.H. Saracoglu, T. Magin, A. Parente, A. Coussement
Reduced-order modeling of super-sonic fuel-air mixing in a multi-strut injection scramjet engine using machine learning techniques

K. Zdybał, G. D'Alessio, A. Attili, A. Coussement, J.C. Sutherland, A. Parente
Local manifold learning and its link to domain-based physics knowledge

K. Zdybał, E. Armstrong, A. Parente, J.C. Sutherland
PCAfold 2.0—Novel tools and algorithms for low-dimensional manifold assessment and optimization

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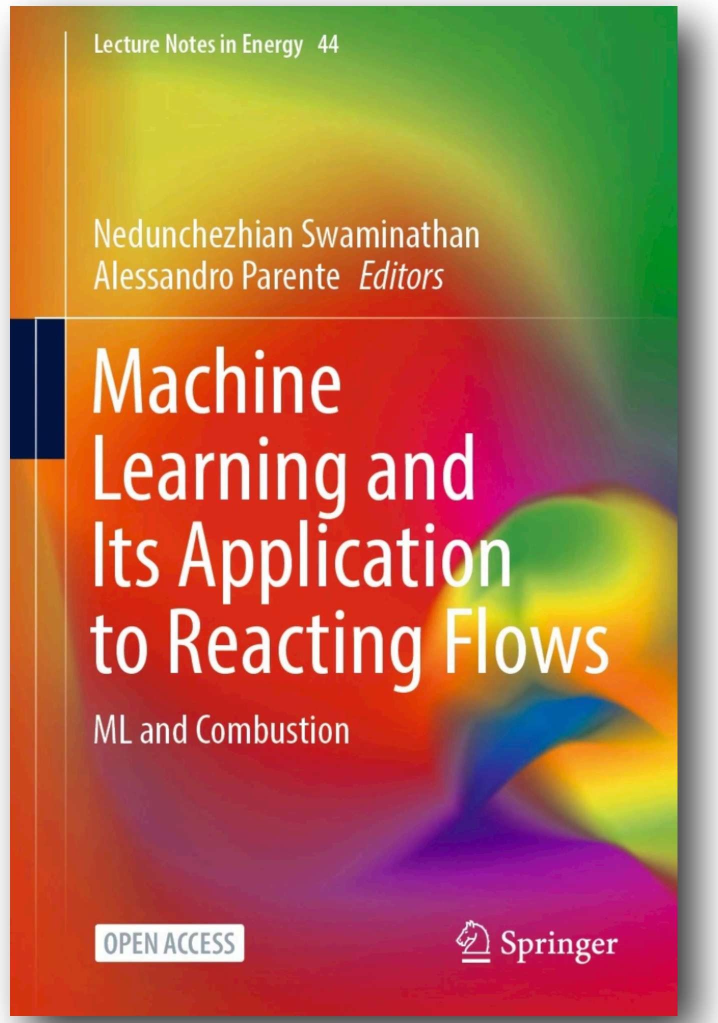
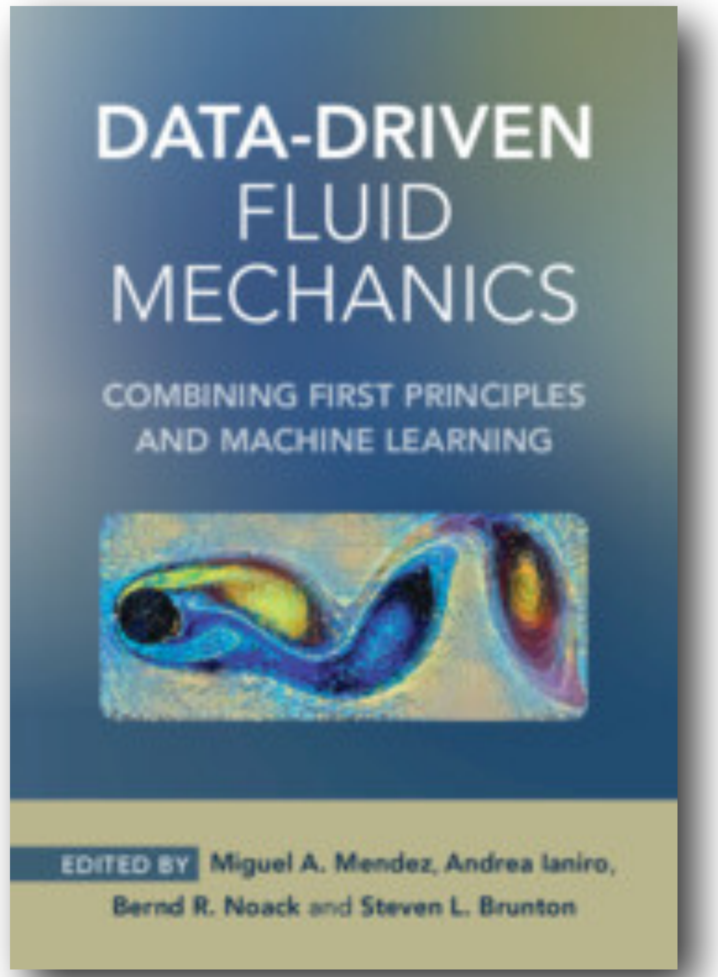
Improving reduced-order models through nonlinear decoding of projection-dependent outputs



Springer

K. Zdybał, M. R. Malik, A. Coussement, J. C. Sutherland, A. Parente
Reduced-order modeling of reactive flows using data-driven approaches



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K. Zdybał, G. D'Alessio, G. Aversano, M. R. Malik,
A. Coussement, J. C. Sutherland, A. Parente
Advancing reactive flow simulations with data-driven models

Selected conference talks:

- 18th International Conference on Numerical Combustion
- 39th International Symposium on Combustion

- Mathematics of Data Science, 2022
- Computational Science and Engineering, 2023

Invited talks:

Upcoming!

Award number 1953350

Reduced-order modeling of turbulent reacting flows using data-driven approaches

Kamila Zdybał

Supervisors: Prof. Alessandro Parente, Prof. James C. Sutherland

12 October 2023
18th ERCOFTAC Autumn Festival, Liège