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Bayesian calibration of a cluster dynamics model

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Acknowledgements



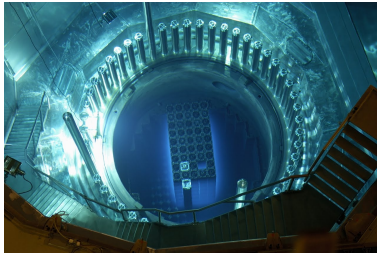
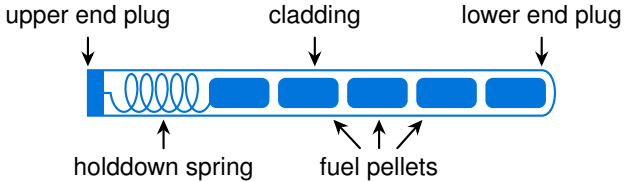
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UO₂ nuclear fuel rods



- Nuclear fuel assembly consists of an array of fuel rods filled with fuel pellets

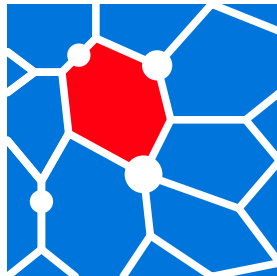
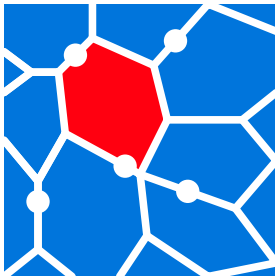
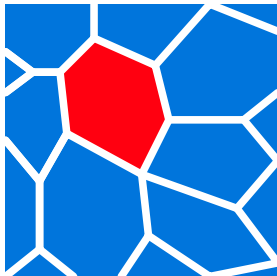


Fission gas release



- Nuclear fuel pellets have a microstructure composed of grains
- Fission gas release happens in three distinct stages: [Andersson et al., 2014]

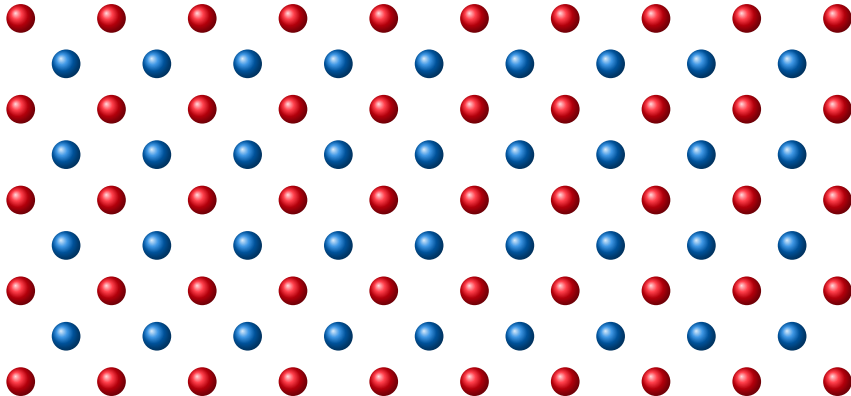
- 1 Nucleation and growth of intra-granular bubbles
- 2 Diffusion to the grain boundaries
- 3 Growth and interconnection of gas bubbles at grain boundaries



Nucleation of intra-granular bubbles



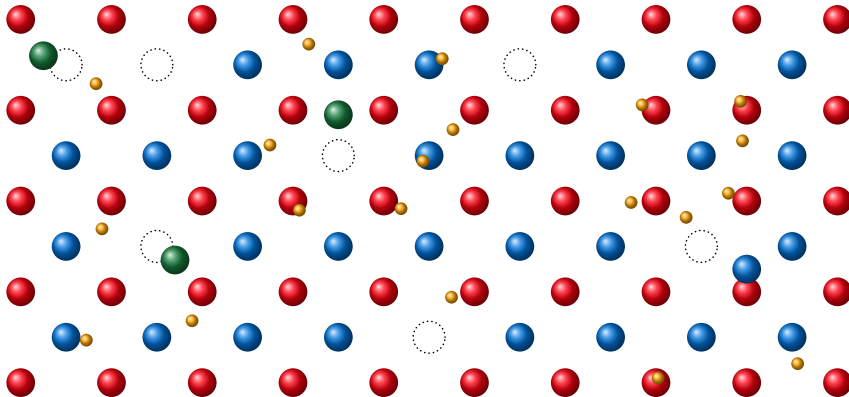
- Uranium (●) and oxygen (●) form a lattice





Nucleation of intra-granular bubbles

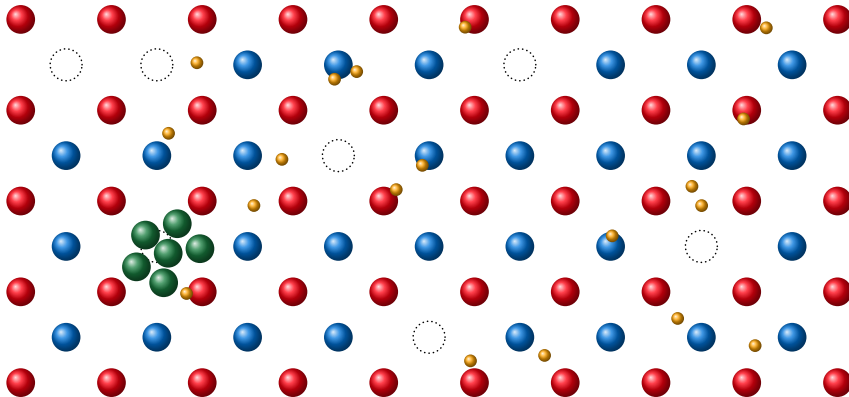
- Uranium (●) and oxygen (●) form a lattice
- Free neutrons (●) initialize the fission process, creating byproducts such as xenon (●)



Nucleation of intra-granular bubbles



- Uranium (●) and oxygen (●) form a lattice
- Free neutrons (●) initialize the fission process, creating byproducts such as xenon (●)
- Xenon gas bubbles get trapped inside the vacancies (○) and migrate to the grain boundary



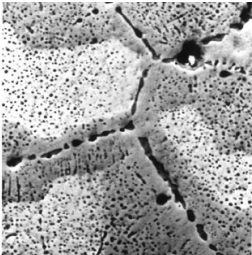


Mechanistic model for intra-granular fission gas evolution

- Evolution equation for the concentration C_n of each cluster with n Xe atoms

$$\frac{\partial C_n}{\partial t} = \underbrace{\dot{F}y_n}_{\text{production of new Xe clusters}} + \underbrace{D_n(T)\nabla C_n}_{\text{diffusion of Xe clusters}} - \underbrace{Q(C_n)}_{\text{interaction between clusters}}$$

- The diffusion coefficient $D_n(T)$ is computed by
 - Density Functional Theory (DFT) under **thermal equilibrium** [Perriot et al., 2019]
 - The Centipede cluster dynamics code under **irradiation** [Matthews et al., 2020]



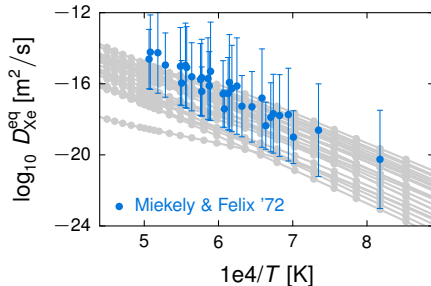
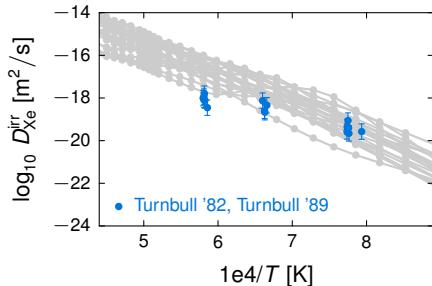
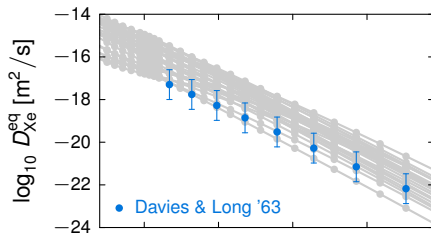
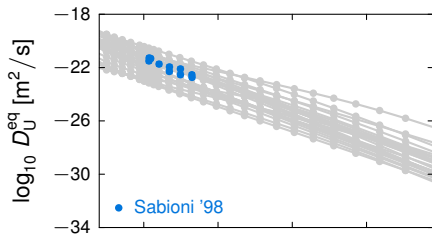
We monitor the following quantities:

- U diffusivity under thermal equilibrium conditions (D_U^{eq})
- Xe diffusivity under thermal equilibrium conditions ($D_{\text{Xe}}^{\text{eq}}$)
- Xe diffusivity under irradiation conditions ($D_{\text{Xe}}^{\text{irr}}$)
- O non-stoichiometry $\text{UO}_{2\pm x}$

Measurements of the diffusivity



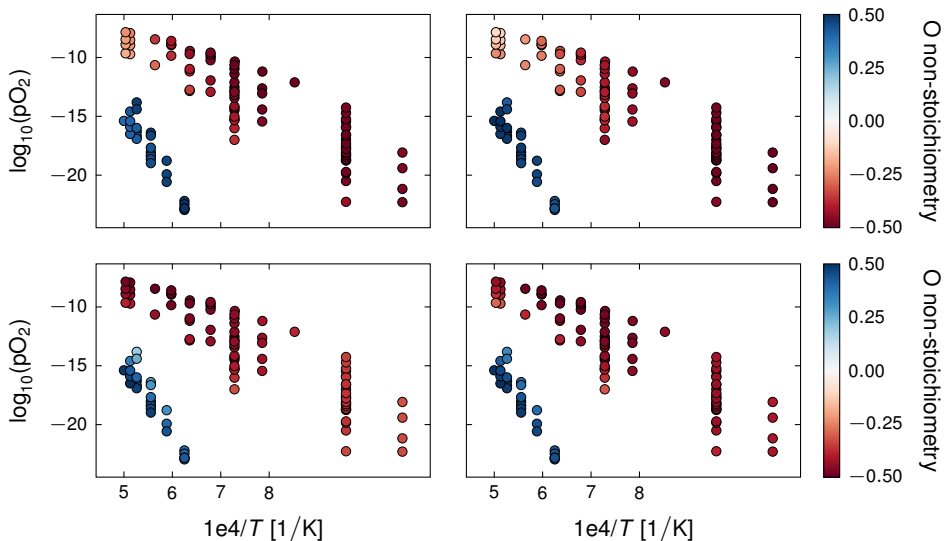
- Centipede predictions of D_U^{eq} , $D_{\text{Xe}}^{\text{eq}}$ and $D_{\text{Xe}}^{\text{irr}}$ with measurements taken from the literature



Measurements of the stoichiometry



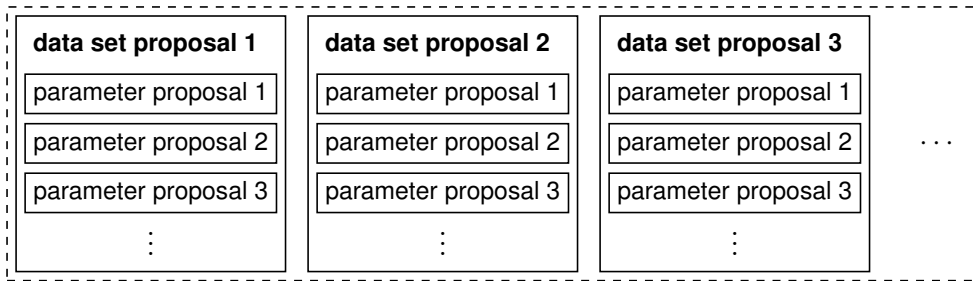
- Centipede predictions of O non-stoichiometry $\text{UO}_{2\pm x}$





Objectives

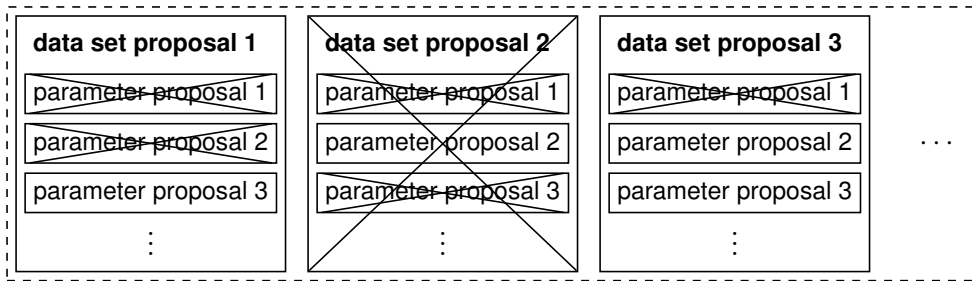
- Our goal is to perform **Bayesian calibration** of the Centipede cluster dynamics code, taking into account that only **summary statistics of the data** (i.e., a measurement value with an associated measurement error) are available
- **Data-free inference** (DFI) involves an outer iteration in the data space and an inner iteration in the parameter space [Berry et al., 2012, Chowdhary and Najm, 2016]



Objectives



- Our goal is to perform **Bayesian calibration** of the Centipede cluster dynamics code, taking into account that only **summary statistics of the data** (i.e., a measurement value with an associated measurement error) are available
- **Data-free inference** (DFI) involves an outer iteration in the data space and an inner iteration in the parameter space [Berry et al., 2012, Chowdhary and Najm, 2016]



- We want to develop a **computationally tractable** DFI approach that can deal with **multiple experimental data sets** of different size

Bayesian calibration

- Given a data set

$$\mathcal{D}_d = \{\mathbf{x}_d^{(n)}, y_d^{(n)}, \mathbf{s}_d^{(n)}\}_{n=1}^{N_d}$$

and a prior $p(\boldsymbol{\nu})$, we want to compute the posterior $p(\boldsymbol{\nu}|\mathcal{D}_d)$

- Prior and posterior are connected through the likelihood function ([Bayes' theorem](#))

$$p(\boldsymbol{\nu}|\mathcal{D}_d) \propto \mathcal{L}_d(\boldsymbol{\nu})p(\boldsymbol{\nu})$$

- Assume model outputs are available as

$$z_d^{(n)} := \underbrace{f_d(\mathbf{x}_d^{(n)}, \boldsymbol{\nu})}_{\text{model}} + \underbrace{\sigma_d^{(n)}\eta}_{\text{additive noise}}$$

where $\eta \sim \mathcal{N}(0, 1)$ is a standard normal random variable

- This yields a log likelihood of the form

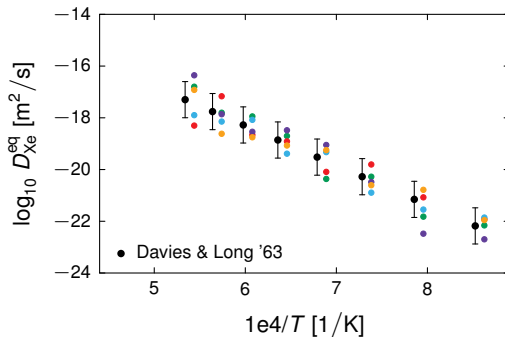
$$\log \mathcal{L}_d(\boldsymbol{\nu}) = -\frac{1}{2} \sum_{n=1}^{N_d} \left[\log(2\pi\sigma_d^{(n)2}) + \frac{\left(z_d^{(n)} - f_d(\mathbf{x}_d^{(n)}, \boldsymbol{\nu})\right)^2}{\sigma_d^{(n)2}} \right]$$

and samples of the posterior can be obtained using an [accept-reject scheme](#)

Bayesian calibration

- DFI approach defines consistent data sets using a metric based on [maximum entropy](#)
- We will formulate an [alternative metric for consistency](#) that avoids the outer loop over the data space altogether
- Define a collection of K_d synthetic data sets $\mathcal{Z}_d^{(k)} := \{z_d^{(n,k)}\}_{n=1}^{N_d}$, $k = 1, 2, \dots, K_d$, where

$$z_d^{(n,k)} \sim \mathcal{N}\left(y_d^{(n)}, \beta_d s_d^{(n)^2}\right)$$



Consistent data sets

- Each synthetic data set represents an opinion on the posterior $p(\boldsymbol{\nu}|\mathcal{D}_d)$ that can be combined using **logarithmic pooling**

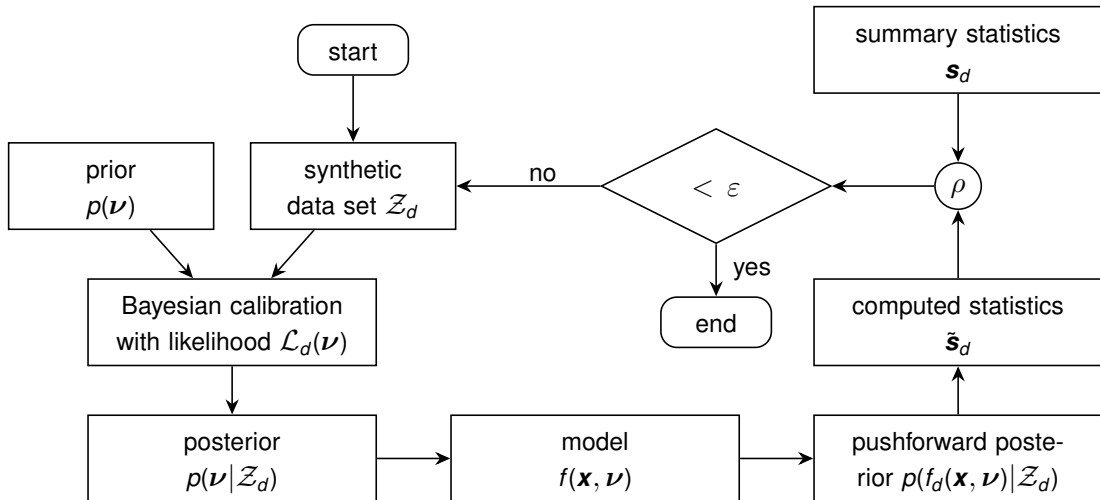
$$\log \mathcal{L}_d(\boldsymbol{\nu}) := -\frac{1}{K_d} \sum_{k=1}^{K_d} \log \mathcal{L}_d^{(k)}(\boldsymbol{\nu})$$

- The pooled posterior can be propagated through the model to obtain the pushforward posterior $p(f_d(\mathbf{x}, \boldsymbol{\nu})|\mathcal{Z}_d)$
- A data set is consistent if summary statistics $\tilde{\mathbf{s}}_d = \{\tilde{s}_d^{(n)}\}_{n=1}^{N_d}$ extracted from the pushforward posterior agree with the reported summary statistics $\mathbf{s}_d = \{s_d^{(n)}\}_{n=1}^{N_d}$, i.e.,

$$\rho(\mathbf{s}_d, \tilde{\mathbf{s}}_d) < \varepsilon$$

where ρ is a distance metric, and the condition can be satisfied by choosing **an appropriate data scaling parameter** β_d

Framework for obtaining consistent data sets





Full likelihood construction

- A final likelihood can be constructed by combining the information from different data sources

$$\log \mathcal{L}(\boldsymbol{\nu}) := \sum_{d=1}^D \alpha_d \log \mathcal{L}_d(\boldsymbol{\nu})$$

where $\alpha = (\alpha_d)_{d=1}^D$ are positive **weights** that allow us to express our confidence in the respective experimental data sets

- To account for the different number of measurement locations N_d in each data set, choose

$$\alpha_d := \frac{DN_d^{-1}}{\sum_{d=1}^D N_d^{-1}}$$

d	experimental data set	measured quantity	N_d	T0 [K]	Hf_p02
1	Sabioni	D_U^{eq}	10	1973	5.10
2	Davies & Long	$D_{\text{Xe}}^{\text{eq}}$	8	1973	5.10
3	Turnbull	$D_{\text{Xe}}^{\text{irr}}$	16	1973	5.10
4	Miekely & Felix	$D_{\text{Xe}}^{\text{eq}}$	32	1973	6.11
5	stoichiometry	$\text{UO}_{2\pm x}$	104	-	-

Polynomial chaos expansion surrogates

- Using the Centipede predictions $f_d(\mathbf{x}_d^{(n)}, \boldsymbol{\nu})$ directly in the log-likelihood is too expensive
- We propose to replace the model predictions by a **polynomial surrogate model**, i.e.,

$$f_d(\mathbf{x}_d^{(n)}, \boldsymbol{\nu}) \approx \mathcal{P}_d^{(n)}(\boldsymbol{\nu}) := \sum_{\mathbf{u} \in \mathcal{I}} c_{\mathbf{u}} \phi_{\mathbf{u}}(\boldsymbol{\xi}(\boldsymbol{\nu}))$$

where the multi-index $\mathbf{u}$ is part of the index set $\mathcal{I} \subseteq \mathbb{N}_0^d$, $c_{\mathbf{u}}$ is an unknown coefficient, and $\phi_{\mathbf{u}}$ is a multivariate orthogonal polynomial expressed in terms of the i.i.d. random variables

$$\boldsymbol{\xi} := (\xi_1, \xi_2, \dots, \xi_d)$$

$$\phi_{\mathbf{u}}(\boldsymbol{\xi}) := \prod_{j=1}^s \phi_{u_j}(\xi_j)$$

- We use weighted iterative **Bayesian compressive sensing** [Sargsyan et al., 2014] to compute the index set $\mathcal{I}$ and the coefficients $c_{\mathbf{u}}$, $\mathbf{u} \in \mathcal{I}$

Numerical experiments

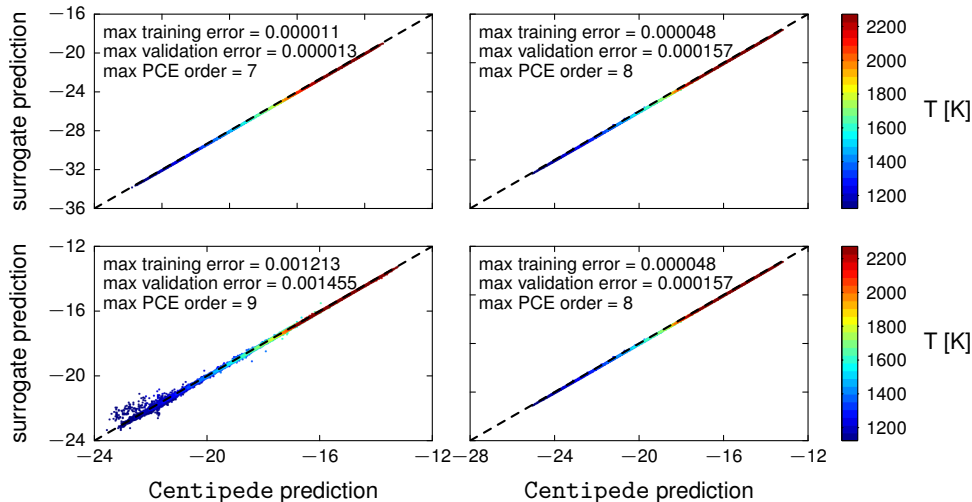


- Centipede is implemented within the phase-field code MARMOT [Tonks et al., 2012] using the MOOSE framework [Permann et al., 2016]
- MOOSE provides easy access to the C++ Finite Element code libMesh [Kirk et al., 2006] and the scalable nonlinear PDE solver PETSc [Balay et al., 2022]
- Polynomial surrogates are constructed using UQTK [Debusschere, 2017]
- DFI approach implemented in C++ and linked to UQTK libraries
- Used global sensitivity analysis (GSA) to identify a subset of 9 important parameters (initially 183 parameters)
- Additionally, two operating conditions
 - T0: temperature at which UO_2 is perfectly stoichiometric
 - Hf_pO2: the temperature of the oxygen partial pressureare allowed to vary separately for each data set (for a total of $7 - 2 + 4 \times 2 = 15$ parameters to calibrate)

PCE surrogate model construction

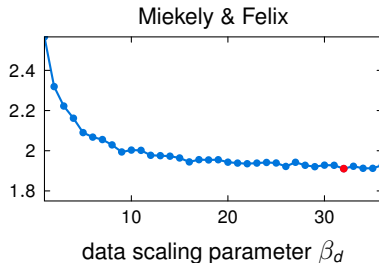
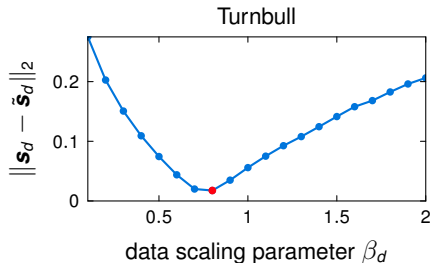
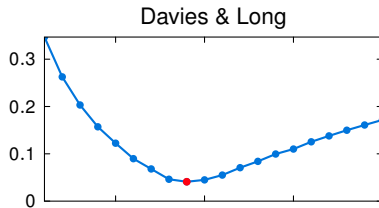
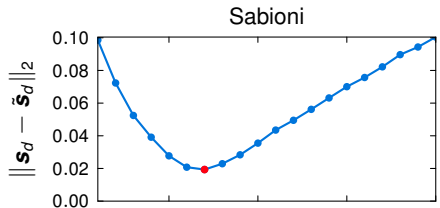


- PCE surrogates constructed using 10,000 training points and 1,000 validation points
- PCE basis constructed using BCS shows good surrogate accuracy



Generating consistent data sets

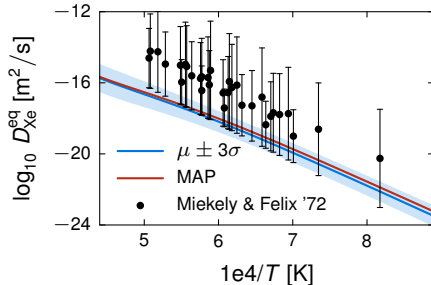
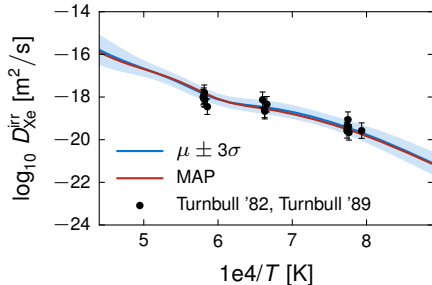
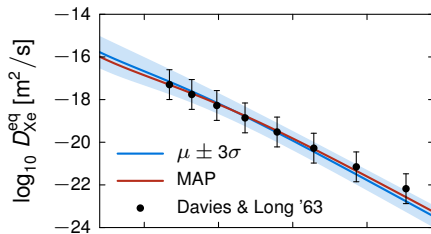
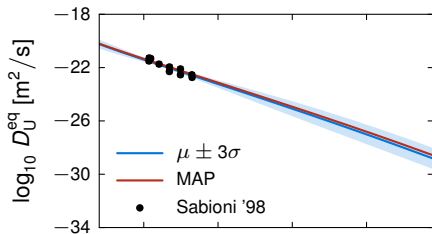
- Performed a grid search over the standard deviation scaling factors β_d , $d = 1, 2, \dots, D$ to find consistent data sets where the distance metric $\rho(\mathbf{s}_d, \tilde{\mathbf{s}}_d) := \|\mathbf{s}_d - \tilde{\mathbf{s}}_d\|_2$



Pushforward posterior



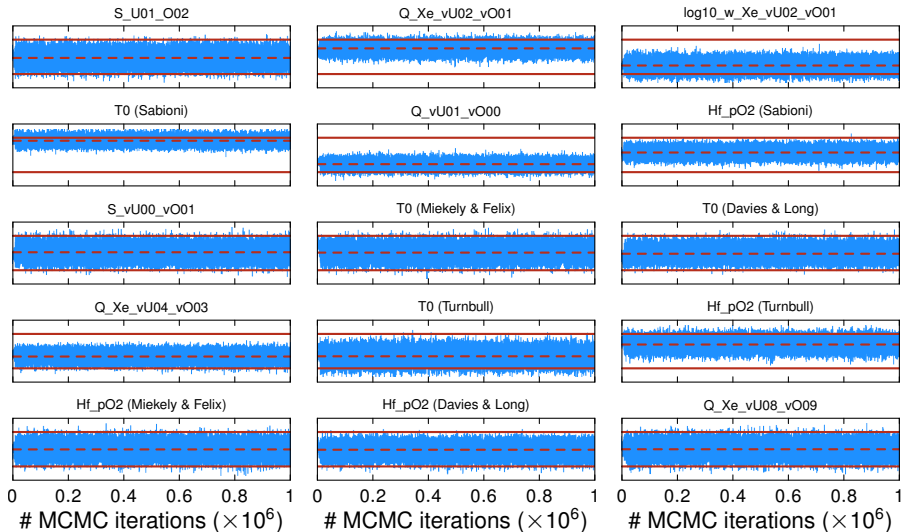
- Calibrated pushforward posterior diffusivities show good match to the data



MCMC chains

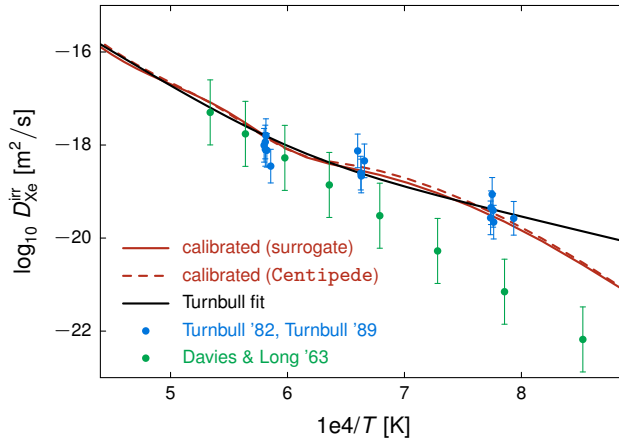


- Good mixing of MCMC chains



Turnbull correlation

- Comparison of the pushforward MAP prediction for Xe irradiation computed with surrogate model and actual Centipede code shows good agreement
- Comparison to Turnbull fit (best available experimental fit from literature)





Conclusion and future work

- We devised a **Bayesian inference strategy** to estimate the parameters in the cluster dynamics code Centipede, where the reported data on UO_2 diffusivity and stoichiometry is available as mean values with an associated measurement error
- Our calibration strategy involves **synthetic data sets** that are consistent in the sense that the statistics computed from the pushforward posterior agree with the reported summary statistics
- We used our Bayesian inference strategy to calibrate 9 Centipede parameters against 5 different experimental data sets with 208 measurements in total
- The predicted pushforward posterior is in **good agreement** with the experimental data
- In future efforts, we will work on improving the surrogate accuracy to be able to include more parameters in the study (original model consists of 183 parameters)



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Thank you



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