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Bayesian calibration for summary statistics with applications to a cluster dynamics model

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Acknowledgements

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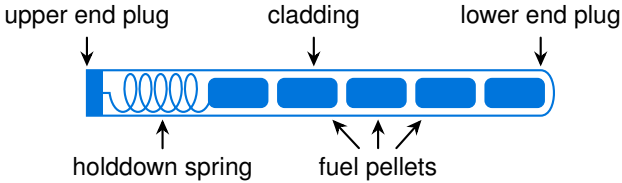
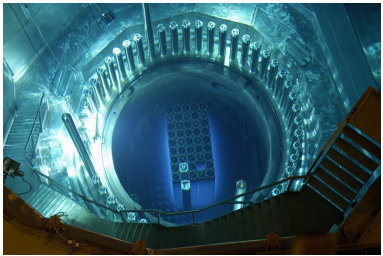
UO_2 nuclear fuel rods

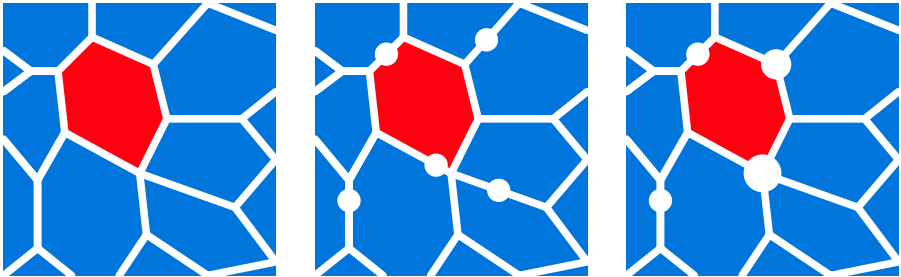
- Nuclear fuel assembly consists of an array of fuel rods filled with fuel pellets





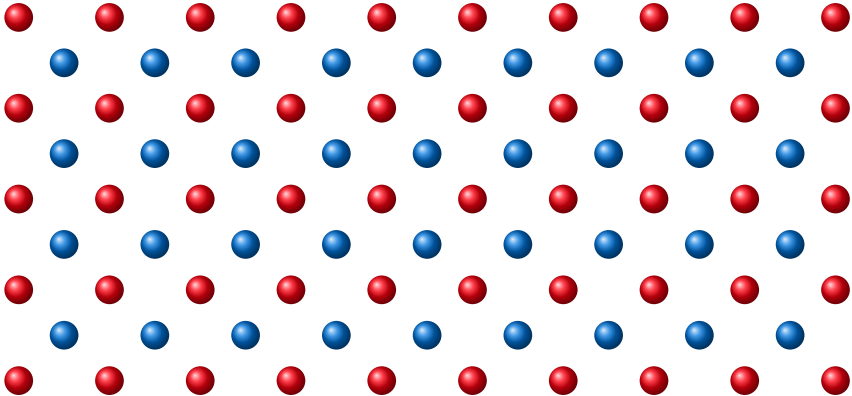
Fission gas release

- 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



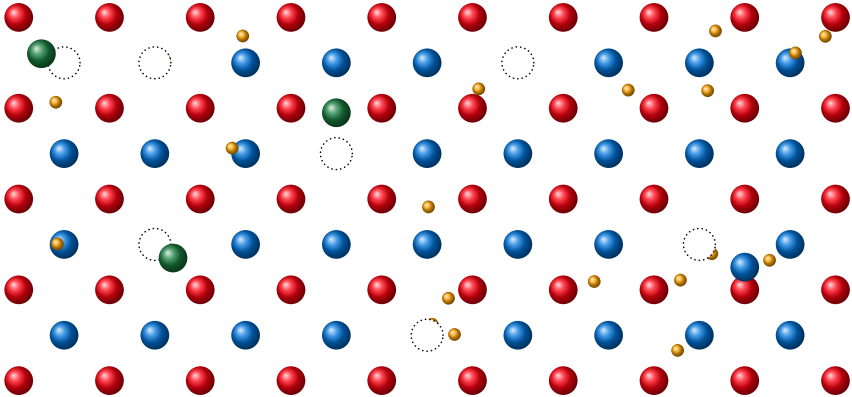
Nucleation of intra-granular bubbles

- Uranium ( ) and oxygen ( ) form a lattice



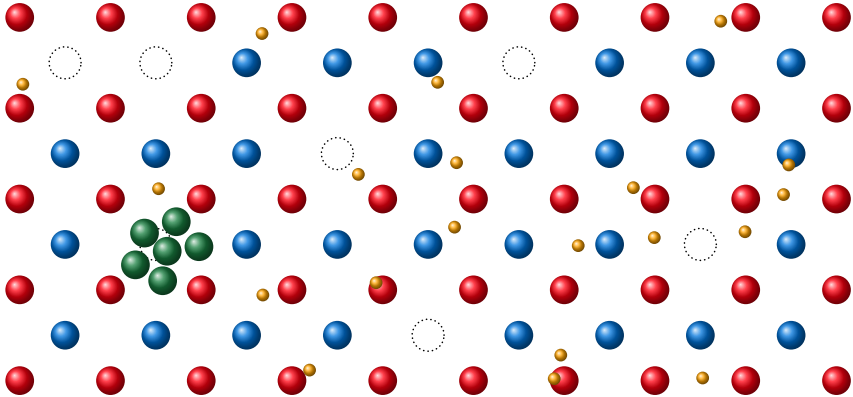
Nucleation of intra-granular bubbles

- 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

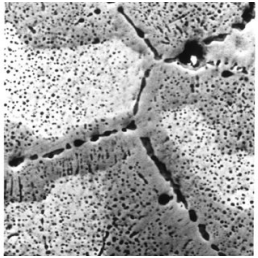


Mechanistic model for intra-granular fission gas evolution

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

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

- 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]

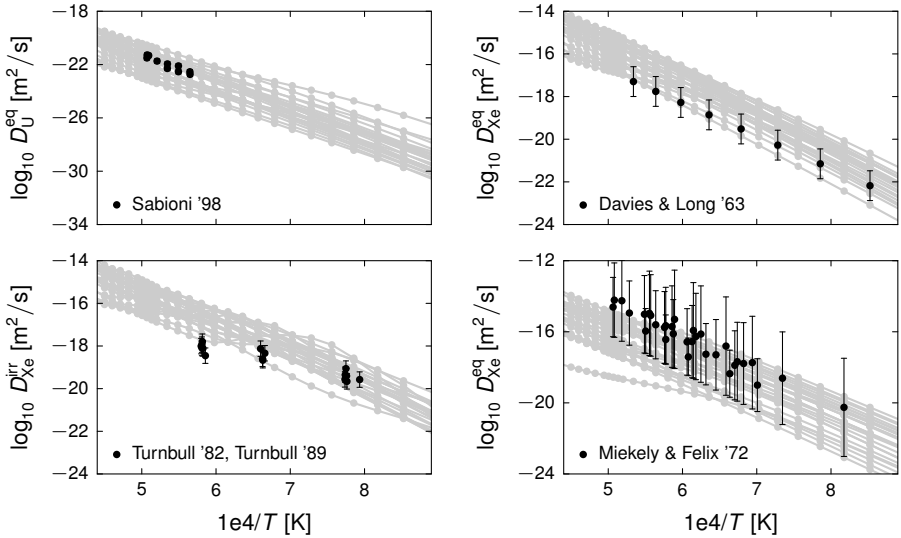


We monitor the following quantities:

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

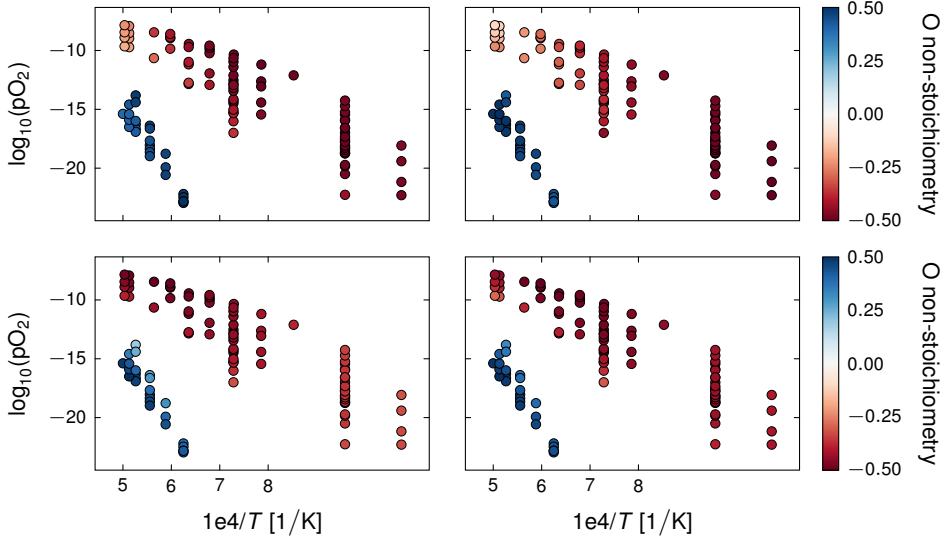
Measurements of the diffusivity

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



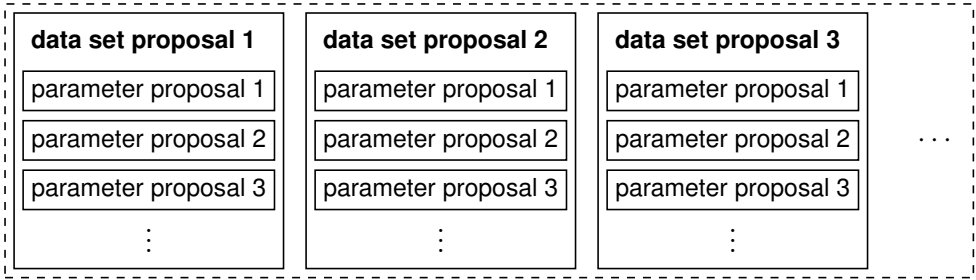
Measurements of the stoichiometry

- `Centipede` predictions of O non-stoichiometry $UO_{2\pm x}$



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]



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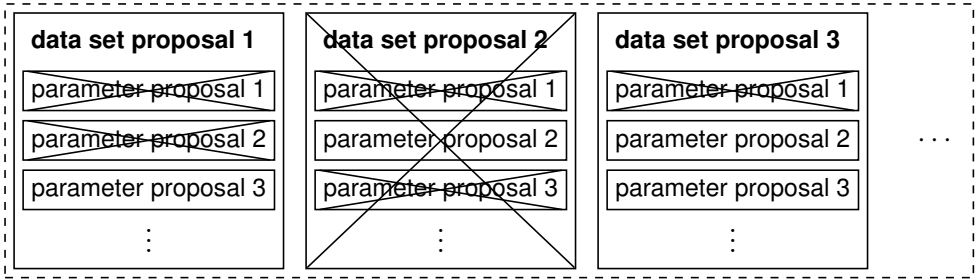


- We want to develop a computationally tractable DFI approach that can deal with multiple experimental data sets of different size

Bayesian calibration

- Given a data set

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

  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

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

  where $\eta \sim \mathcal{N}(0, 1)$ is a standard normal random variable
- This yields a log likelihood of the form

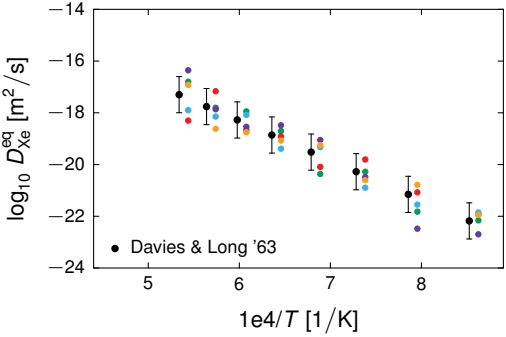
$$\log \mathcal{L}_d(\boldsymbol{\nu}) = -\frac{1}{2}\sum_{n=1}^{N_d}\left[\log(2\pi{\sigma_d^{(n)}}^2) + \frac{\left(z_d^{(n)} - f_d(\boldsymbol{x}_d^{(n)}, \boldsymbol{\nu})\right)^2}{{\sigma_d^{(n)}}^2}\right]$$

  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 $\mathcal{Z}_d^{(k)} := \{z_d^{(n,k)}\}_{n=1}^{N_d}$, $k = 1, 2, \ldots, K_d$, 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

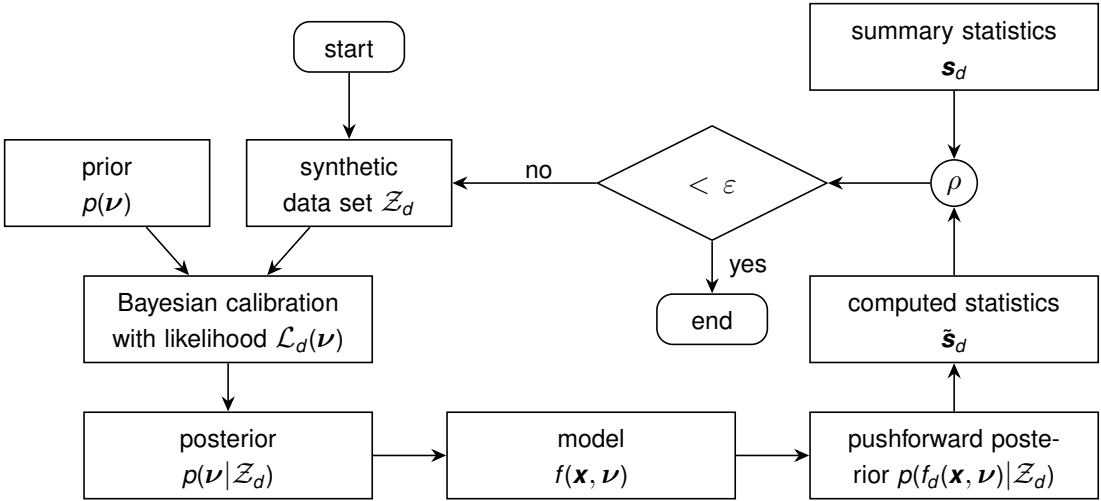
$$\log \mathcal{L}_d(\boldsymbol{\nu}) := -\frac{1}{K_d}\sum_{k=1}^{K_d} \log \mathcal{L}_d^{(k)}(\boldsymbol{\nu})$$

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

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

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 $\boldsymbol{\alpha} = (\alpha_d)_{d=1}^{D}$ 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

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

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

Polynomial chaos expansion surrogates

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

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

where the multi-index $\boldsymbol{u}$ is part of the index set $\mathcal{I} \subseteq \mathbb{N}_0^d$, $c_{\boldsymbol{u}}$ is an unknown coefficient, and $\phi_{\boldsymbol{u}}$ is a multivariate orthogonal polynomial expressed in terms of the i.i.d. random variables $\boldsymbol{\xi} := (\xi_1, \xi_2, \ldots, \xi_d)$

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

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

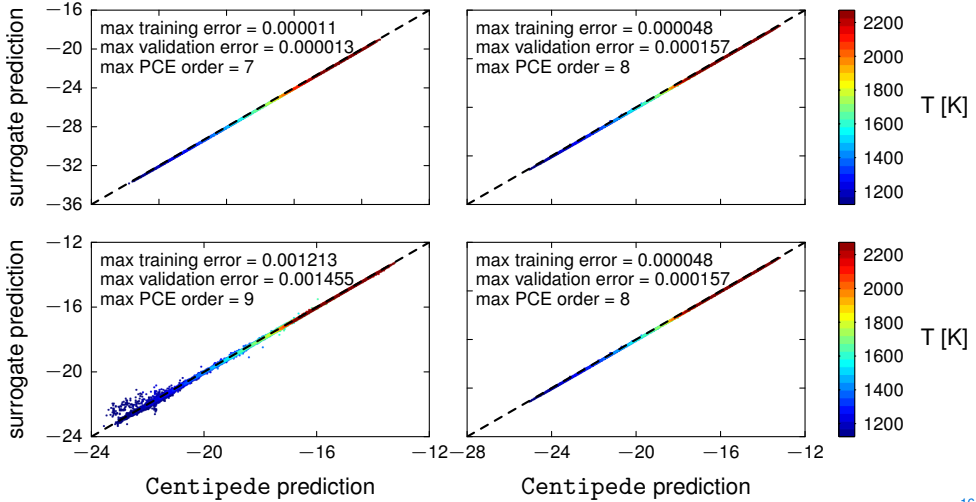
Numerical experiments

- `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 pressure

  are allowed to vary separately for each data set (for a total of $7 - 2 + 4 \times 2 =$ 15 parameters to calibrate)

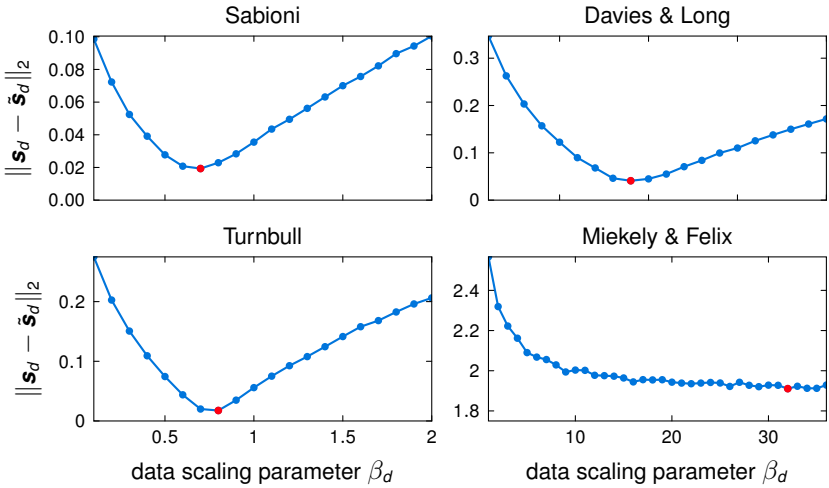
PCE surrogate model construction

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



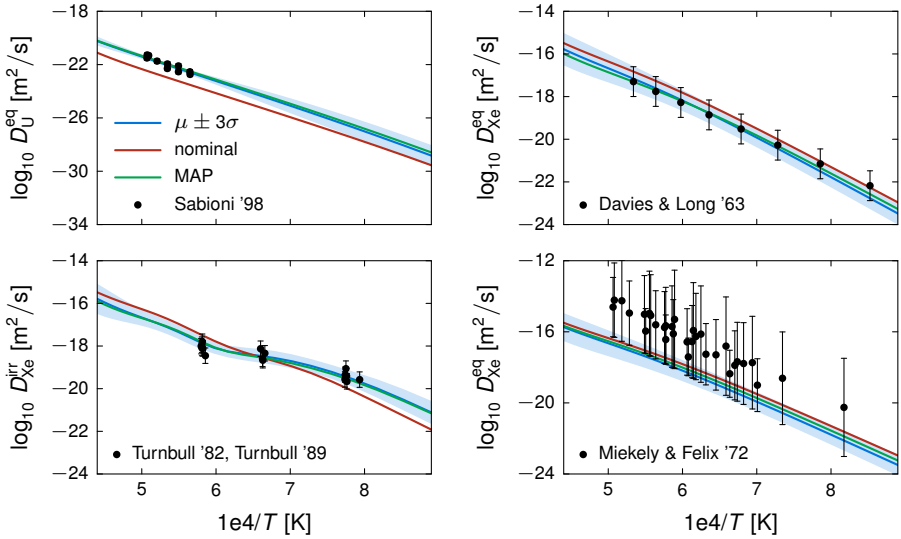
Generating consistent data sets

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



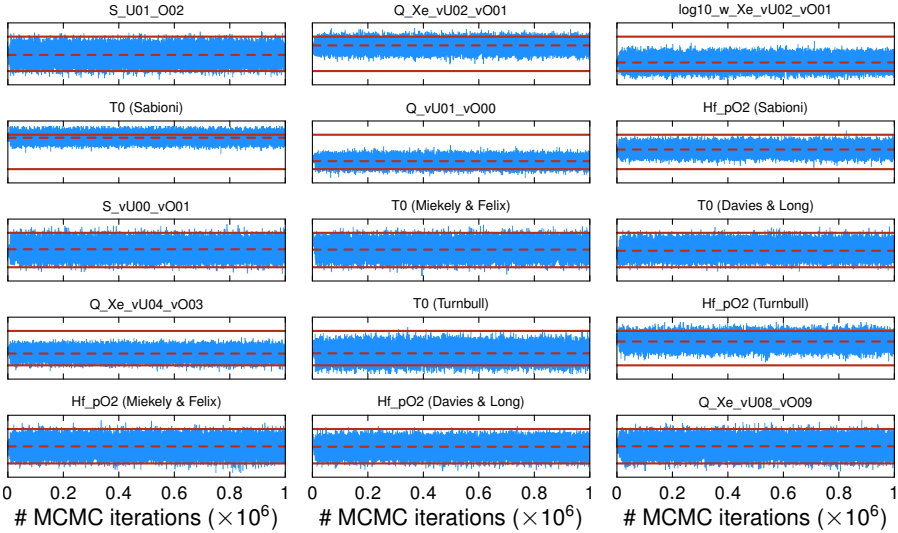
Pushforward posterior

- Calibrated pushforward posterior diffusivities show good match to the data



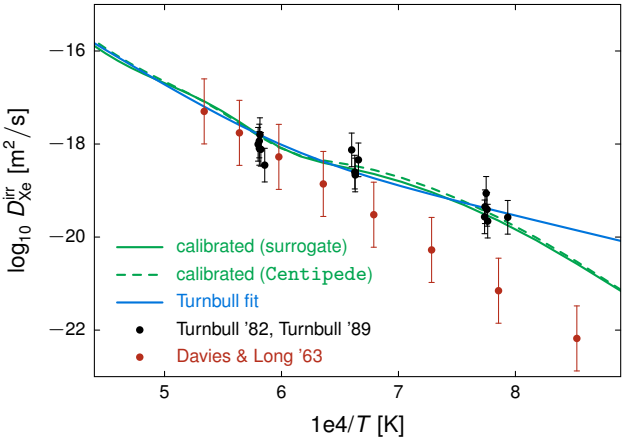
MCMC chains

- 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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