Solving PDE-Based Bayesian Inverse Problems Using

CUQIpy

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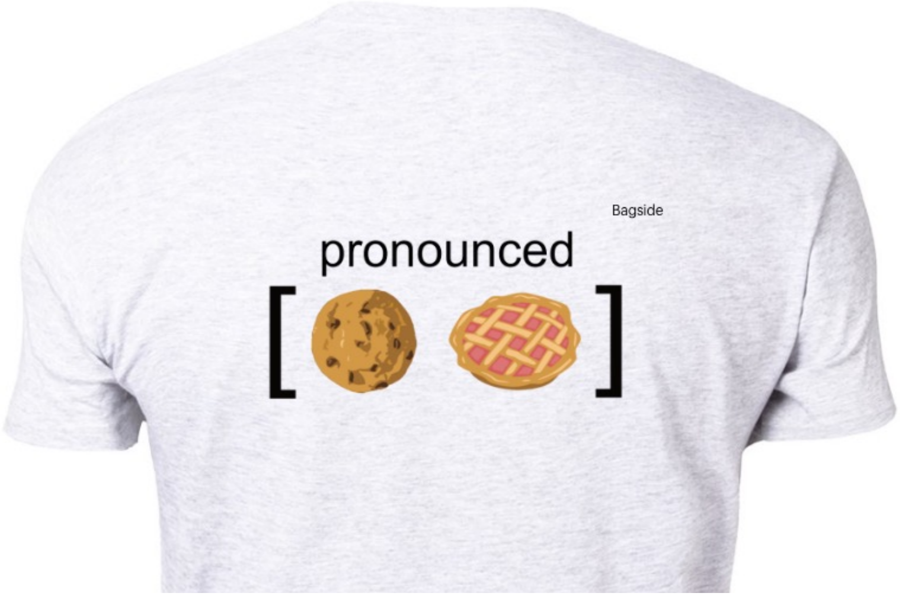
28 Feb 2024



VILLUM FONDEN

The CUQI team




Nov. 2021

- Computational Uncertainty Quantification for Inverse problems
- **2019 – 2025**
- PI: Per Christian Hansen
- https://sites.dtu.dk/cuqi

CUQIpy core-developers

Jakob **Nicolai** **Amal** **Charlie**

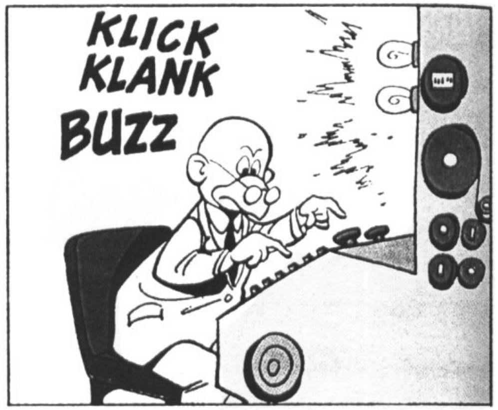
+ CUQI team valuable contribution

CUQIpy in a Nutshell

Vision

Build a <u>software package</u> that uses uncertainty quantification (UQ) to access and quantify uncertainties in solutions to inverse problems.

- **Simplify** the mathematics, statistics and code for the non-expert user.
- Provide **full control** for expert users.
- Allow users to focus on **modeling aspects**.



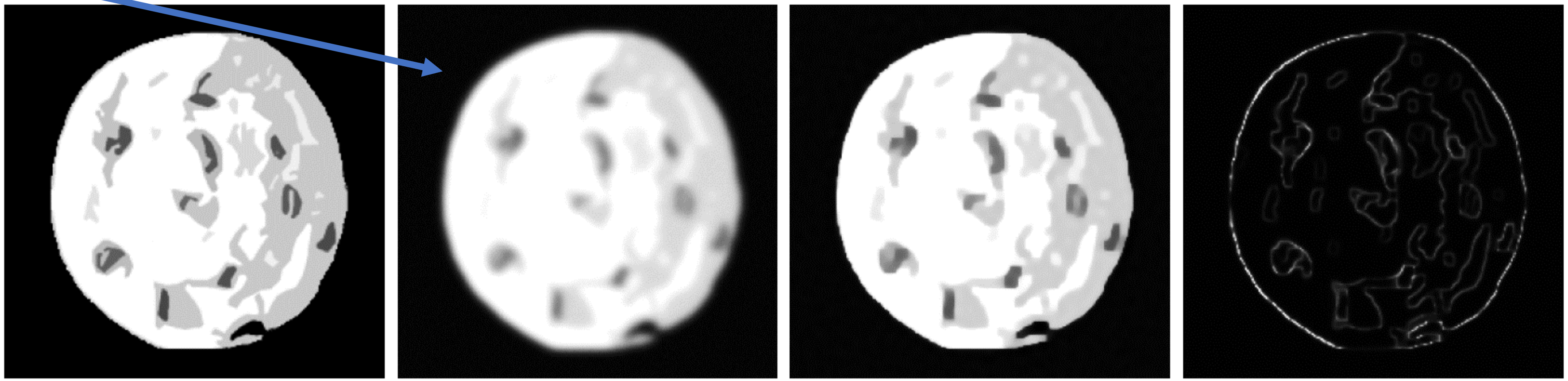
Features

- Easy access to **state-of-the-art** tools in one framework (including 3rd party libraries).
    - Modeling
    - Solving
    - Visualization and statistics
- A suite of **test problems** to allow users to get started.
- Allow users to provide **custom code** for models, distributions, samplers etc.
- Exploit structure to support **large-scale** problems.

Cookie deblurring with CUQIpy

$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{y}$

True | Blurred, noisy | Posterior mean | Posterior std



$$d \sim \mathrm{Gamma}(1, 10^{-4})$$

$$s \sim \mathrm{Gamma}(1, 10^{-4})$$

$$\boldsymbol{x} \sim \mathrm{LMRF}(d^{-1}),$$

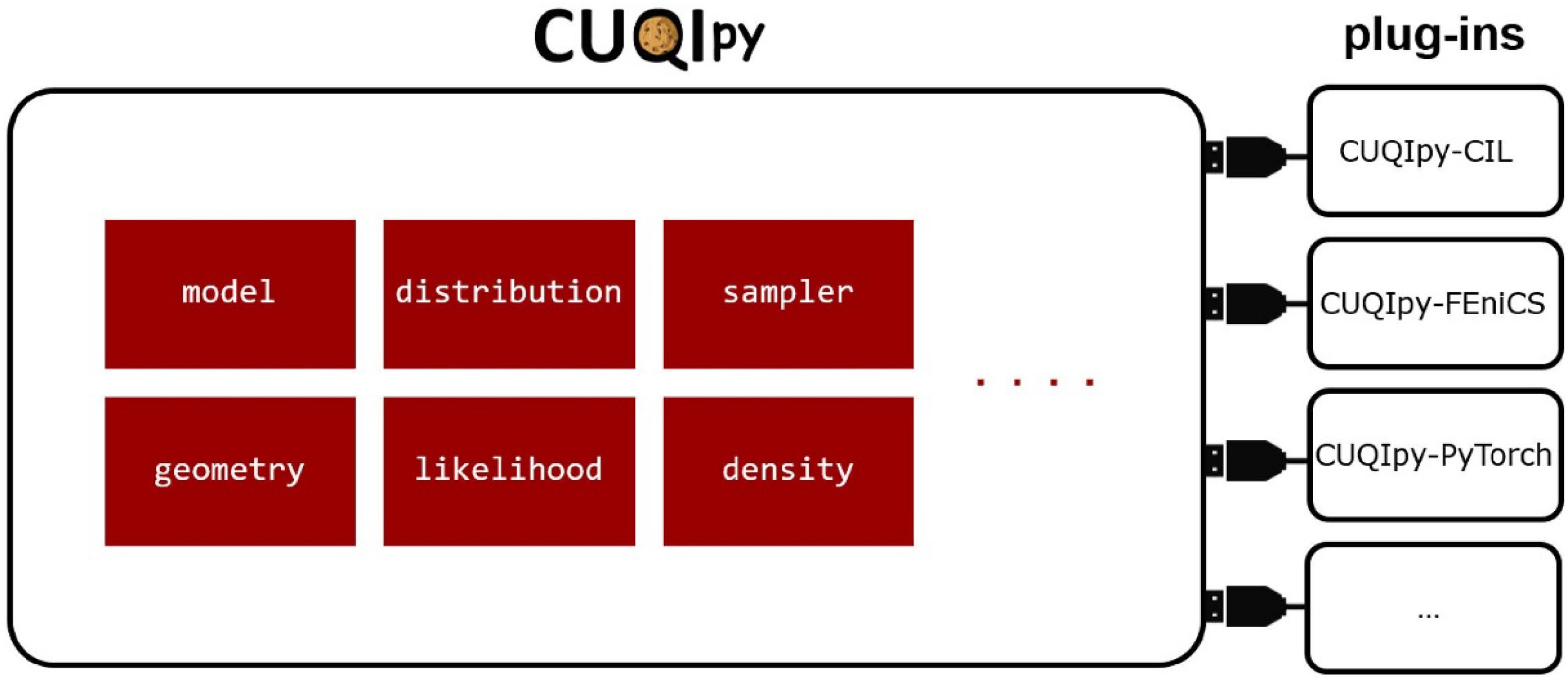
$$\boldsymbol{y} \sim \mathrm{Gaussian}(\boldsymbol{A}\boldsymbol{x}, s^{-1}\boldsymbol{I})$$

```
d = Gamma(1,1e-4), s = Gamma(1,1e-4)
x = LMRF(1/d)
y = Gaussian(A @ x, 1/s)
BP = BayesianProblem(x, y) d, s)
BP.set_data(y=y_obs)
BP.UQ()
```

Automation using BayesianProblem

Riis, Alghamdi, Uribe, et al. “CUQIpy - Part I: computational uncertainty quantification for inverse problems in Python”. (to appear) Inverse Problems
https://github.com/CUQI-DTU/Paper-CUQIpy-1-Core/blob/main/intro/intro.ipynb

CUQIpy modules and plug-ins

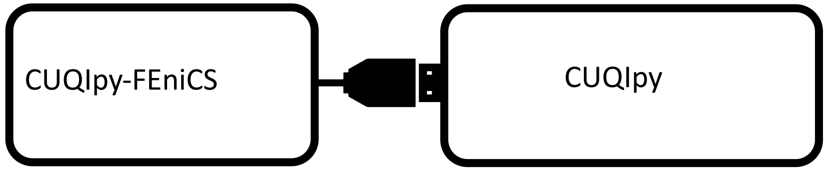


- Plug-in structure modularity / flexible licensing

3 PDE-based Bayesian inverse problems (BIP):

- Case 1: Poisson 2D problem
- Case 2: Electric Impedance Tomography (EIT)
- Case 3: Characterizing ear aqueduct in mice (Diffusion model)

PDE-BIP Case 1: 2D Poisson Problem
Bayesian model



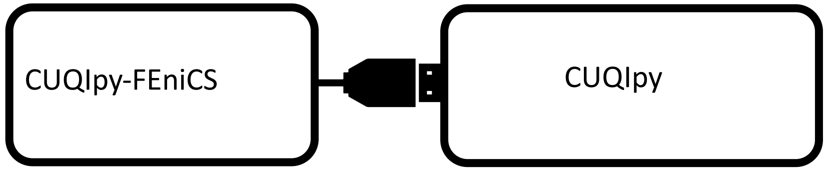
Model

$$\nabla \cdot \left(e^{w(\boldsymbol{\xi})} \nabla u(\boldsymbol{\xi}) \right) = f(\boldsymbol{\xi}) \qquad \text{for} \qquad \boldsymbol{\xi} \in \Gamma = (0,1)^2$$

$$\boldsymbol{w} = \sum_{i=1}^{n_{\mathrm{KL}}} x_i \sqrt{\lambda_i} \boldsymbol{e}_i^{\mathrm{KL}}, \qquad \boldsymbol{x} = [x_1, x_2, \ldots, x_{n_{\mathrm{KL}}}]^{\mathsf{T}}$$

Alghamdi, Riis, Afkham, et al. "CUQIpy - Part II: computational uncertainty quantification for PDE-based inverse problems in Python". (to appear) Inverse Problems
https://github.com/CUQI-DTU/Paper-CUQIpy-2-PDE/blob/main/Poisson/intro_example_Poisson.ipynb

PDE-BIP Case 1: 2D Poisson Problem
Bayesian model



Model

$$\mathbf{y} = \mathbf{A}(\mathbf{x})$$

```
# Step 1: Model
A = FEniCSPoisson2D(dim=(32,32), field_type="KL",
...).model
```

Prior

$$\boldsymbol{x} \sim \text{Gaussian}(\mathbf{0}, \boldsymbol{I})$$

```
# Step 2: Prior
x = Gaussian(np.zeros(n_KL), 1, geometry=G_KL)
```

Data distribution

$$\boldsymbol{y} \sim \text{Gaussian}\left(\boldsymbol{A}(\boldsymbol{x}), s_{\text{noise}}^2 \boldsymbol{I}\right).$$

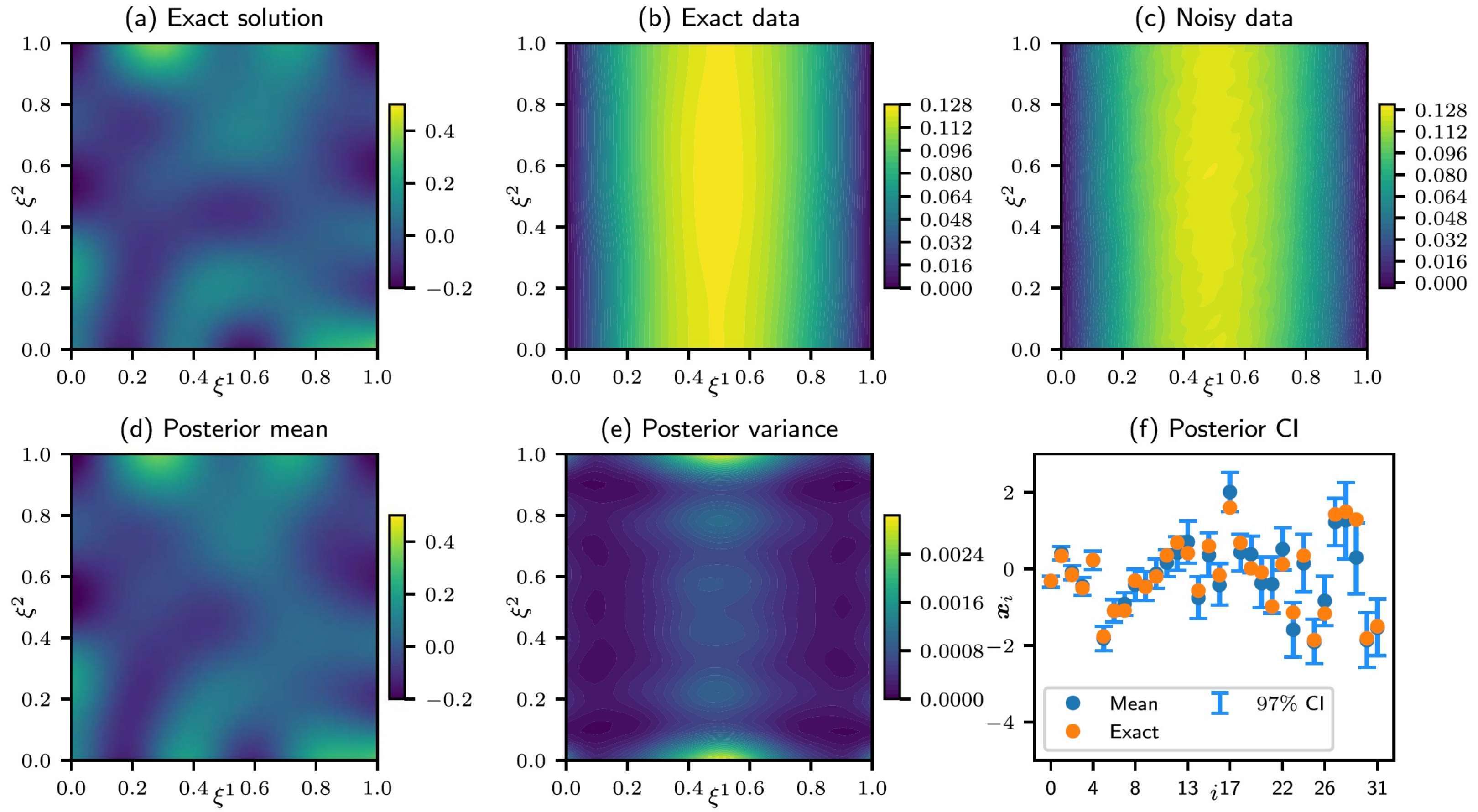
```
# Step 3: Data distribution / Likelihood
y = Gaussian(A(x), s_noise**2, geometry=G_FEM)
```


Alghamdi, Riis, Afkham, et al. “CUQIpy - Part II: computational uncertainty quantification for PDE-based inverse problems in Python”. (to appear) Inverse Problems
https://github.com/CUQI-DTU/Paper-CUQIpy-2-PDE/blob/main/Poisson/intro_example_Poisson.ipynb

PDE-BIP Case 1: 2D Poisson Problem
Bayesian model

```
# Sample the prior
x_true = x.sample()
X_true.plot()
```

```
# Sample the data distribution
y_obs = y(x=x_true).sample()
y_obs.plot()
```

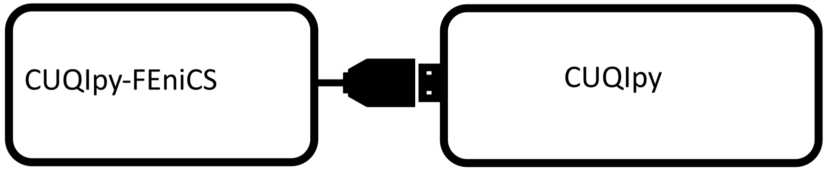


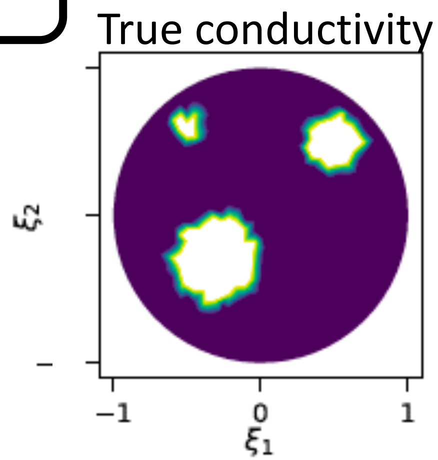

```
# Setting up the Bayesian inverse problem
BP = BayesianProblem(y, x).set_data(y=y_obs)
BP.UQ(..)
```

Automation using BayesianProblem

Alghamdi, Riis, Afkham, et al. “CUQIpy - Part II: computational uncertainty quantification for PDE-based inverse problems in Python”. (to appear) Inverse Problems
https://github.com/CUQI-DTU/Paper-CUQIpy-2-PDE/blob/main/Poisson/intro_example_Poisson.ipynb

PDE-BIP Case 2: EIT
Forward model





EIT problem (medical imaging)

- Infer conductivity
- Measure electric current w on the boundaries
- We impose electrical potential on the boundaries (multiple frequencies $k = 1, 2, 3, 4$)

Forward model

$$-\nabla \cdot (\sigma(\boldsymbol{\xi}) \nabla u_k(\boldsymbol{\xi})) = 0,$$

$$u_k(\boldsymbol{\xi}) = g_k(\boldsymbol{\xi}) = \sin\left(k \arctan\left(\frac{\xi^2}{\xi^1}\right)\right)$$

Observations

$$y_k(\boldsymbol{\xi}) := \frac{\sigma(\boldsymbol{\xi}) \partial u_k(\boldsymbol{\xi})}{\partial \mathbf{n}}$$

```
PDE1 =SteadyStateLinearFEniCSPDE(
    (lhs_form, rhs_form_k1), …,
    observation_operator=obs_map1)

PDE2 = PDE1.with_updated_rhs(rhs_form_k2)
PDE2.observation_operator = obs_map2
```

Similarly for k= 3, 4

EIT Test case by Babak Afkham, with CUQIpy core developer team support

Alghamdi, Riis, Afkham, et al. “CUQIpy - Part II: computational uncertainty quantification for PDE-based inverse problems in Python”. (to appear) Inverse Problems

https://github.com/CUQI-DTU/Paper-CUQIpy-2-PDE/blob/main/EIT/EIT.ipynb

PDE-BIP Case 2: EIT
Prior

Parametrize the conductivity: $\boldsymbol{G}_{\text{Heavi}} \circ \boldsymbol{G}_{\text{KL}}(\boldsymbol{x})$

Finite element function space of

$\sigma_{\text{FEM}}(\boldsymbol{\xi})$

Karhunen-Loève (KL) expansion of Matérn covariance

$$\boldsymbol{r} = \sum_{i=1}^{n_{\text{KL}}} x_i \sqrt{\lambda_i} \boldsymbol{e}_i^{\text{KL}}.$$

Level-Set mapping

$$\boldsymbol{\sigma} = \boldsymbol{G}_{\text{Heavi}}(\boldsymbol{r}) := \frac{1}{2}\left(\sigma^+ (1 - \operatorname{sign}(\boldsymbol{r})) + \sigma^- (1 + \operatorname{sign}(\boldsymbol{r}))\right).$$

```
G_FEM = FEniCSContinuous(Vh)

G_KL = MaternKLExpansion(G_FEM, …)

G_Haevi = FEniCSMappedGeometry(G_KL,
    map=heaviside, …)
```

PDE-BIP Case 2: EIT

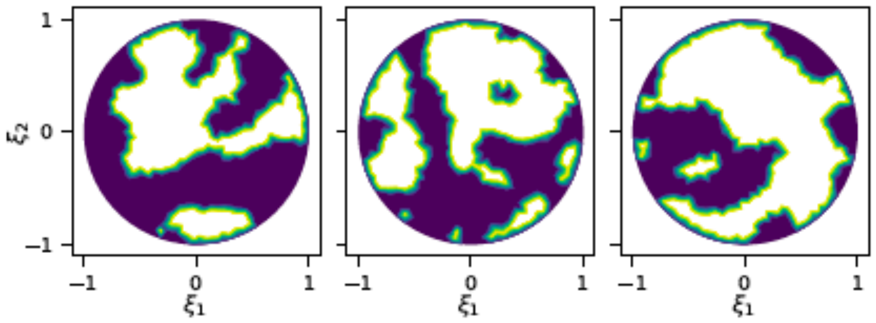
Prior

Parametrize the conductivity: $G_{\text{Heavi}} \circ G_{\text{KL}}(\boldsymbol{x})$

$$\boldsymbol{x} \sim \text{Gaussian}(\boldsymbol{0}, \boldsymbol{I}_{n_{\text{KL}}})$$

```
x = Gaussian(0, 1, geometry=G_Haevi)
```

```
prior_sample = x.sample(5)
prior_sample.plot()
```



PDE-BIP Case 2: EIT
Multiple likelihood posterior

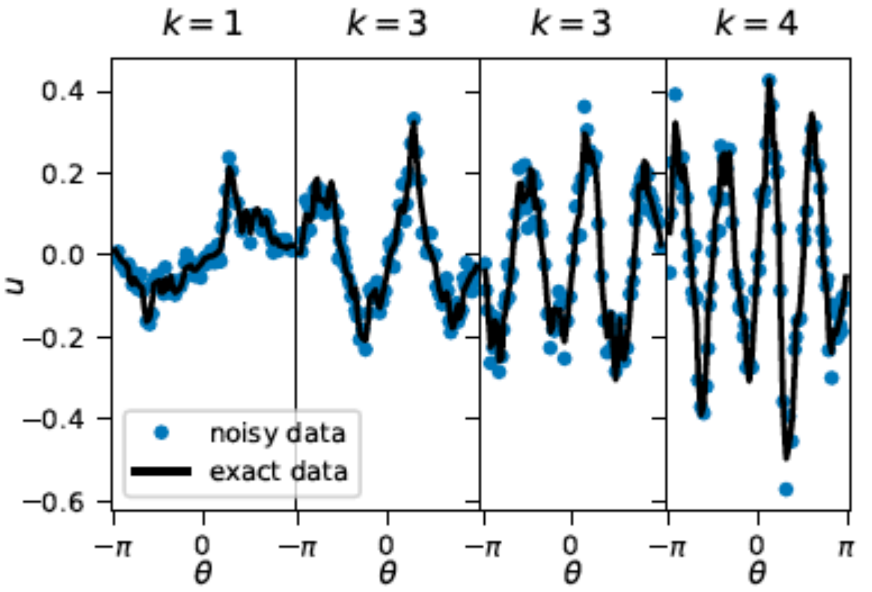
Data distribution

$$\boldsymbol{y}_k \sim \text{Gaussian}\left(\boldsymbol{A}_k\left(\boldsymbol{x}\right), s_{\text{noise}}^2 \boldsymbol{I}_m\right)$$

$$k = 1, 2, 3, 4.$$

```
y1 = Gaussian(A1(x),
     s_noise**2,
     geometry=G_cont)
```

Similarly for k= 2, 3, 4



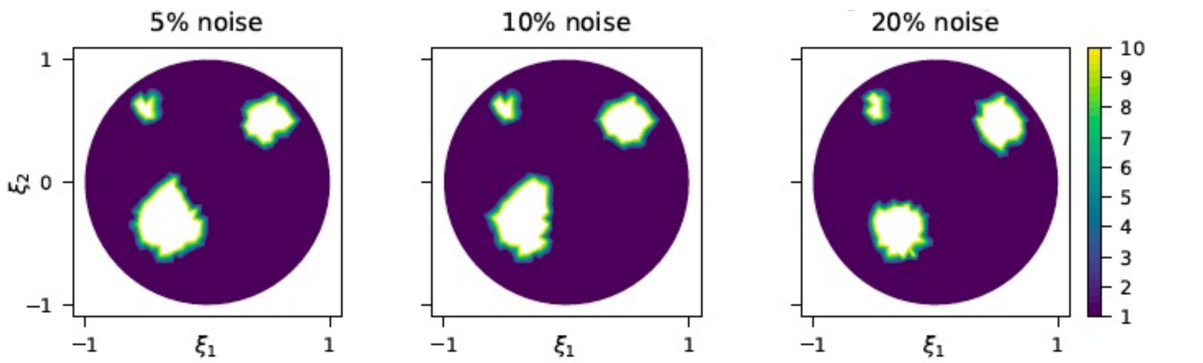
Posterior

$$p(\mathbf{x}|\mathbf{y}_1, \ldots, \mathbf{y}_k) \propto p(\mathbf{y}_1, \ldots, \mathbf{y}_k|\mathbf{x})p(\mathbf{x}) = p(\mathbf{y}_1|\mathbf{x}) \ldots p(\mathbf{y}_k|\mathbf{x})p(\mathbf{x})$$

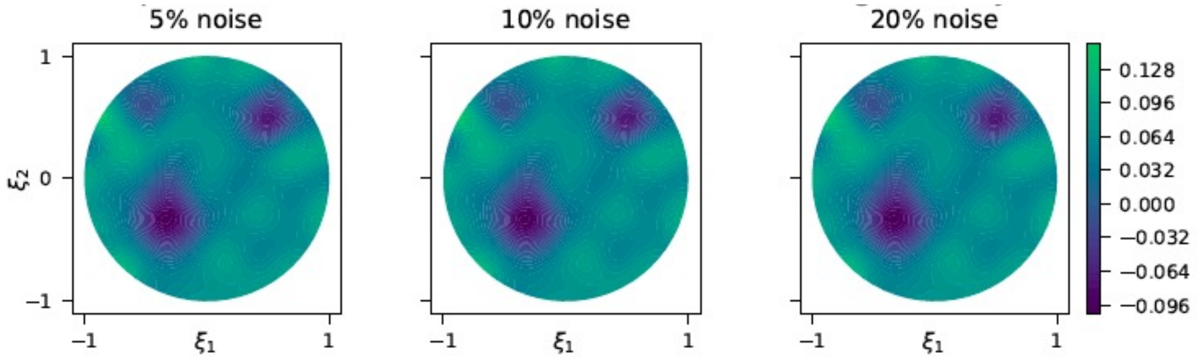
```
post = JointDistribution(x, y1, y2, y3, y4)(y1=y1_data, y2=y2_data, y3=y3_data, y4=y4_data)
```

PDE-BIP Case 2: EIT Results

```python
# Plot mean
posterior_samples.plot_mean()
```

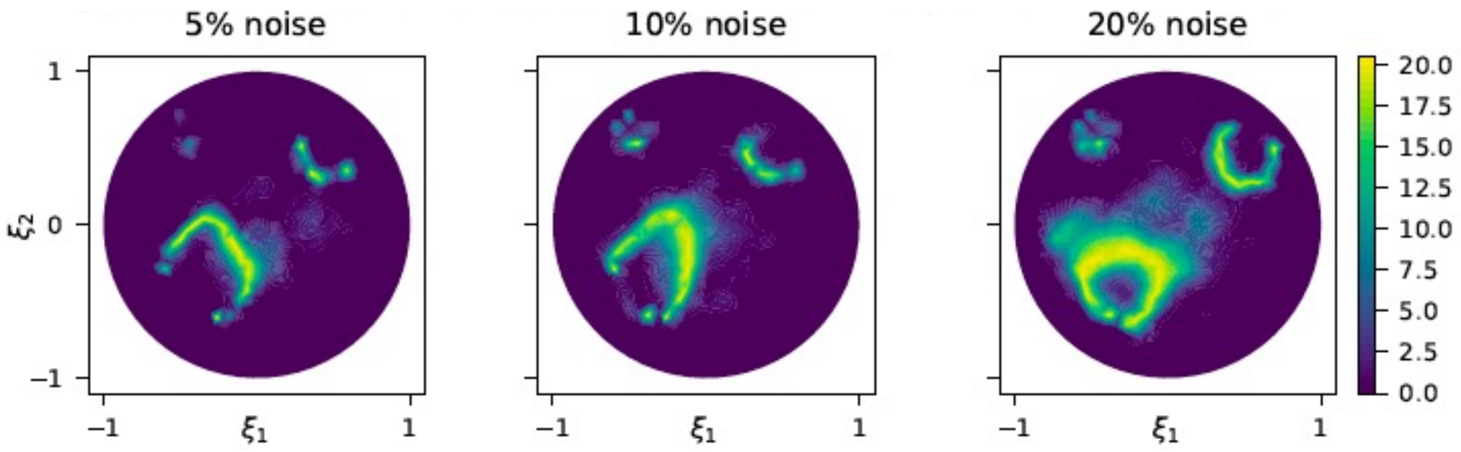



```python
# Plot mean
posterior_samples.geometry = G_KL
posterior_samples.plot_mean()
```

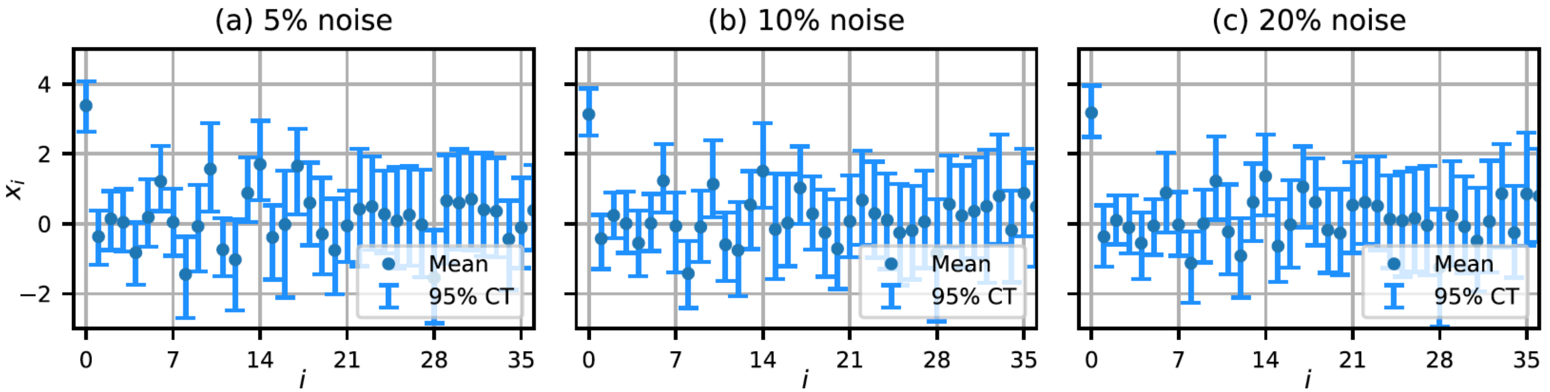


PDE-BIP Case 2: EIT
Results

```python
# Plot variance
posterior_samples.funvals.vector.plot_variance()
```




```python
# Plot credibility intervals
posterior_samples.plot_ci(95, plot_par=True)
```



PDE-BIP Case 3: Characterize flow of brain-injected tracer in mice inner ear

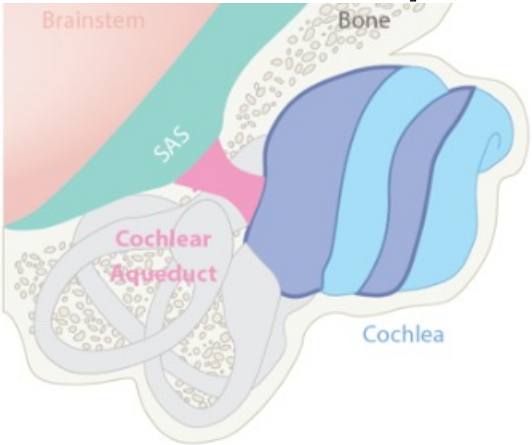
CUQIpy

- Joint work with Barbara K. Mathiesen and Peter A. R. Bork, Center for Translational Neuromedicine, University of Copenhagen

Motivation and implications:

- Understand tracer/particle/therapeutics flow from brain to inner ear.
- Can we identify existence of a membrane in the inner ear?
- Implications on e.g., delivery of therapeutics to inner ear (to rescue hearing)

Figures credit [Mathiesen, Barbara K., et al., 2023]



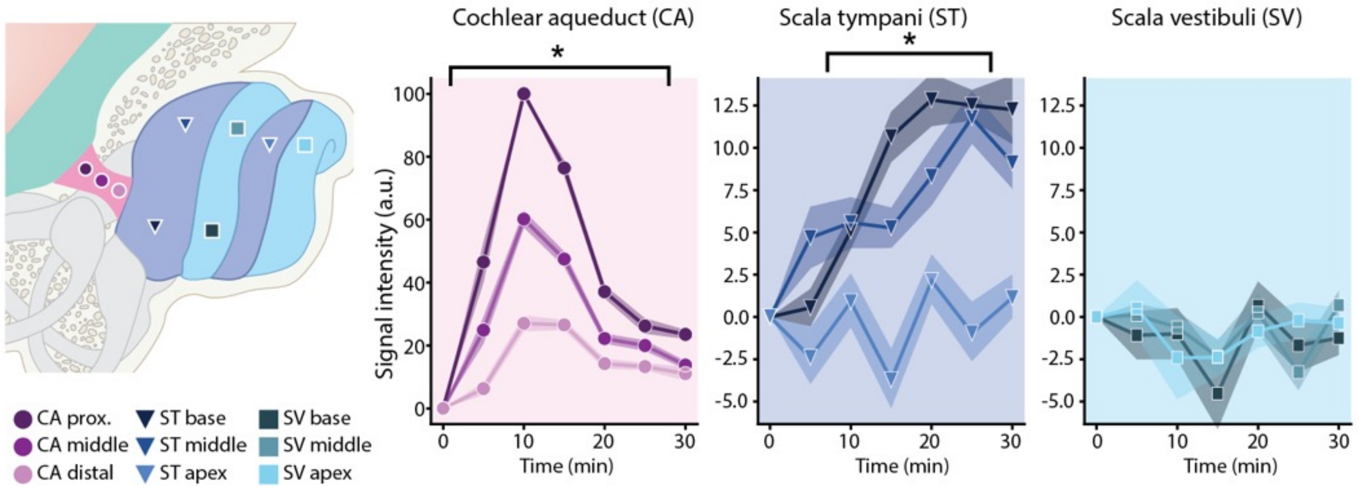
Mathiesen et al. (2023). Delivery of gene therapy through a cerebrospinal fluid conduit to rescue hearing in adult mice. *Science Translational Medicine*, *15*(702), eabq3916

PDE-BIP Case 3: Characterize flow of brain-injected tracer in mice inner ear

CUQIpy

Approach

- Bayesian inversion framework in CUQIpy
  - Advection-diffusion model
  - Gaussian Markov Random Field
- CT/X-ray tracer data



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PDE-BIP Case 3: Characterize flow of brain-injected tracer in mice inner ear

The forward model

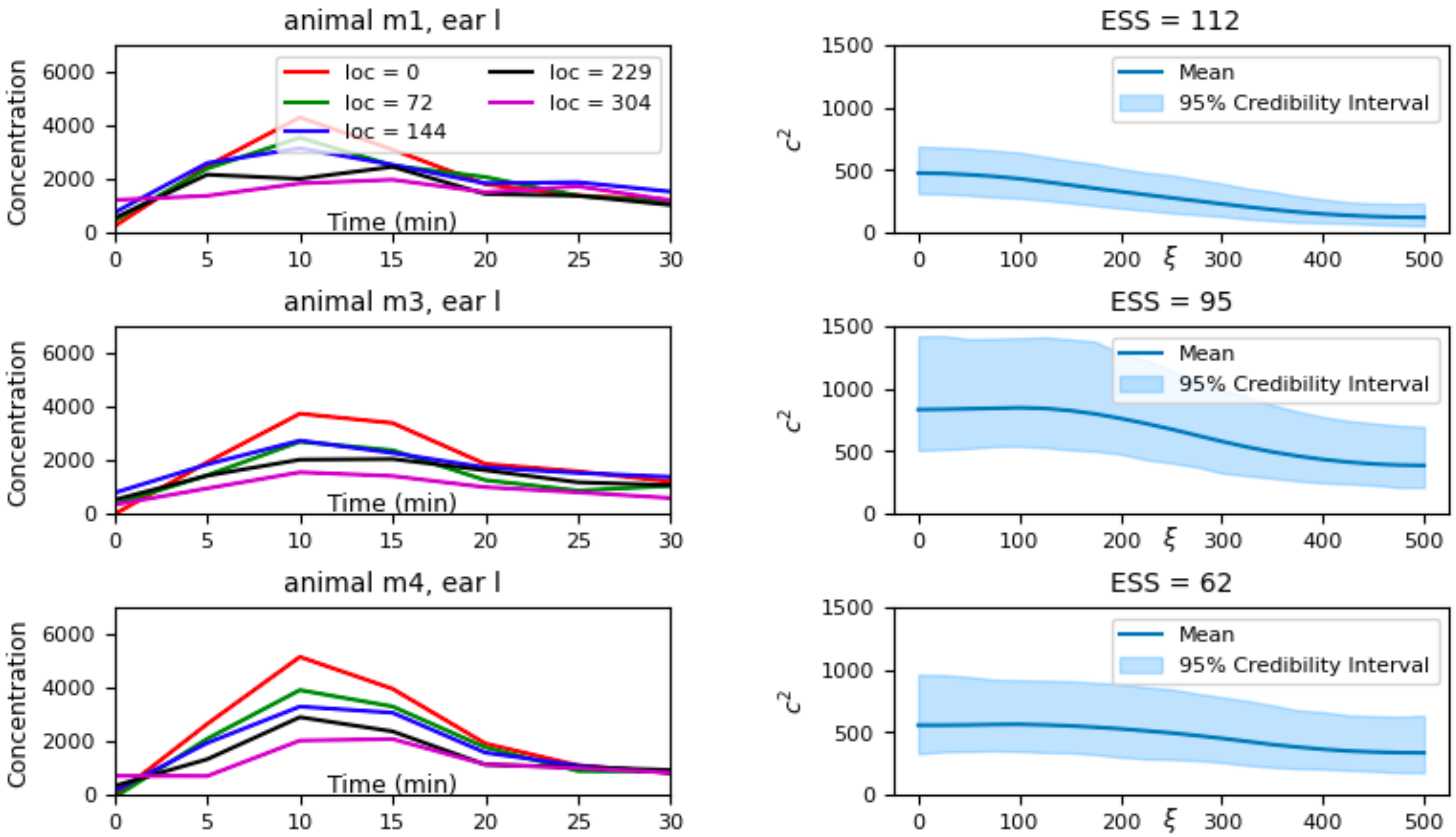
$$y^{\text{obs}} = A(x) + \epsilon$$

- x is the unknown parameters representing $c^2(\xi)$, the varying in space diffusivity
- ϵ is the measurement noise
- y^{obs} is the noisy concentrations at the given times and locations
- A is the forward map from x to the non-noisy measurement y (involves solving the time-dependent diffusion equation)

Preliminary results show identification of low diffusivity area towards the ear

We are interested in advection-diffusion model characterization estimation

Results from different animals



Future directions

- Increate parameterization/prior support
- Increase automatic/symbolic differentiation support
  - FEniCS derivatives [hIPPYlib]
  - FEniCS-adjoint?
  - Sundials?
  - pyTorch?
- Large-scale
- Other applications and methods
  - e.g. delayed acceptance
  - Photoacoustic tomography

Upcoming event

Workshop: UQ for Inverse Problems and Imaging (UQIPI24)

- September 16-20, 2024 @ ICMS, Bayes Centre, Edinburgh
- Organizers: Per Christian Hansen, Marcelo Pereyra, and Yiqiu Dong.
- Workshop homepage: https://www.icms.org.uk/UQIPI24

Programme

	Monday	Tuesday	Wednesday	Thursday	Friday
Morning	UQ tutorial	CUQIpy course	Workshop	Workshop	Workshop
After-noon	CUQIpy course	Workshop	Workshop	Workshop	Social event
Evening	CUQIpy course for the nerds	Reception		Guided tour & workshop dinner	

Plenary Speakers

- Yoann Altmann, Heriot-Watt University
- Tatiana Bubba, University of Bath
- Per Christian Hansen, Technical University of Denmark
- Aku Seppänen, University of Eastern Finland
- Julián Tachella, CNRS and ENS de Lyon
- Faouzi Triki, Grenoble-Alpes University

CUQIpy resources

- **Main repository:** https://github.com/CUQI-DTU/CUQIpy
- **Training notebooks:** https://github.com/CUQI-DTU/CUQIpy-demos
- **Documentation:** https://cuqi-dtu.github.io/CUQIpy/
- **Plugins:**
    - CUQIpy_CIL: https://github.com/CUQI-DTU/CUQIpy-CIL
    - CUQIpy_FEniCS: https://github.com/CUQI-DTU/CUQIpy-FEniCS
    - CUQIpy_PyTorch: https://github.com/CUQI-DTU/CUQIpy-PyTorch
    - CUQIpy_Umbridge: https://github.com/CUQI-DTU/CUQIpy-UMBridge
- **User showcase** https://github.com/CUQI-DTU/CUQIpy-User-Showcase
- **Publications:** Part I: https://iopscience.iop.org/article/10.1088/1361-6420/ad22e7
  https://github.com/CUQI-DTU/Paper-CUQIpy-1-Core
  Part II: https://iopscience.iop.org/article/10.1088/1361-6420/ad22e8
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