Bayesian inference with partial differential equations using Stan

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Proposed interface to external PDE libraries in Stan

```
functions {
  real[,] solve_with_sensitivity(real[] theta);
  real[,] solve(real[] theta);
  real[,] pde_model(real[] theta, int need_sens, real[] x_r, int[]
   ↪  x_i){
    if(need_sens)
      return solve_with_sensitivity(theta);
    else
      return solve(theta);}}
/* ... */
QoI = forward_pde(pde_model, k, x_r, x_i);
```

- `solve_with_sensitivity`: user function that maps PDE parameter θ to *quantity of interest* (QoI) $\widetilde{\mathcal{J}}(\theta) = \mathcal{J}(u;\theta)$ and $d\widetilde{\mathcal{J}}/d\theta$.

Example 1: Laplace equation

- LibMesh [KPSC06]: QUAD9 elements with AMR.
- Sensitivity solution: discrete adjoint method

$$\nabla^2[(\theta_1 + 2\theta_2)u] = 0, \quad \forall x \in \Omega_0 \subset \mathbb{R}^2. \quad \to \mathcal{R}(u, v; \theta) = 0, \forall v \in V \quad (1)$$

$$\tilde{\mathcal{J}}(\theta) = \mathcal{J}(u(\theta)) = \int_\Omega u(x;\theta), \quad \hat{\mathcal{J}} = \tilde{\mathcal{J}}(\theta) + \mathcal{N}(0, \sigma). \quad (2)$$

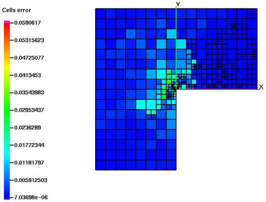


Figure: u error

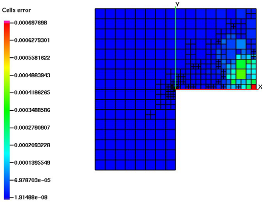
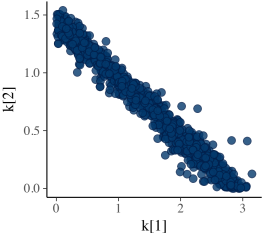


Figure: u^* error



Example 2: Darcy's flow

- MFEM [mfe]: Raviart-Thomas for $\vec{u}$ and P_0 for p.
- Sensitivity solution: finite difference method

$$\begin{bmatrix} {\color{red}k} & \nabla \\ \nabla\cdot & 0 \end{bmatrix} \begin{bmatrix} \vec{u} \\ p \end{bmatrix} = \begin{bmatrix} \vec{f} \\ g \end{bmatrix} \longrightarrow \begin{bmatrix} A(k) & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{p} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{bmatrix}. \tag{3}$$

$$\widetilde{\mathcal{J}}(\theta) = \mathcal{J}(u(\theta)) = \|u_h - u_0\|_2, \qquad \hat{\mathcal{J}} = \widetilde{\mathcal{J}}(\theta) + \mathcal{N}(0, 0.01). \tag{4}$$

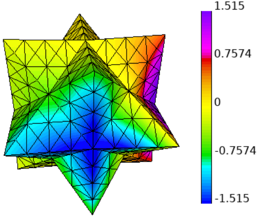


Figure: p

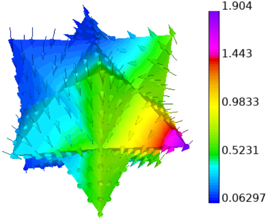
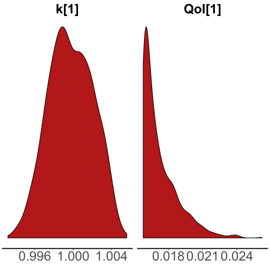


Figure: $\vec{u}$

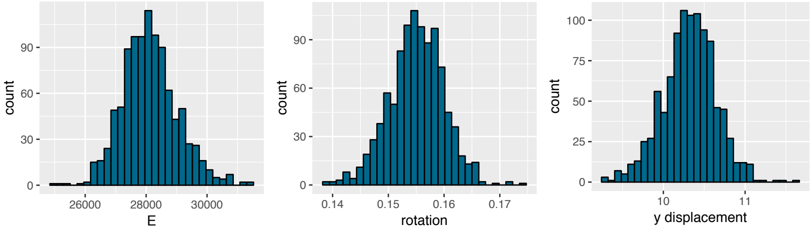


Example 3: nonlinear beam

- OpenSees [MSF10]: Displacement-Based Beam-Column Element + corrotational transformation
- Sensitivity solution: direct differentiation method(DDM) [CVM03]

$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \rightarrow \begin{bmatrix} \epsilon_a(x) \\ \kappa(x) \end{bmatrix} = Bv \rightarrow \{\epsilon_i\} \rightarrow \sigma_i = \sigma_i(\epsilon_i; E) \rightarrow p = \begin{bmatrix} N \\ M \end{bmatrix} \rightarrow \int_0^L B^t p dx$$

- Inference of Young's modulus E from rotation v_3 of a cantilever beam.
- Use E to predict the y displacement v_2 of another beam.



Thank you

What's next?

- Inverse problem using GP emulation [CMMY91] /ROM [ZY18].
- Biomedical applications such as tumor growth [XVG16].

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