SAND2020-2253PE

Hyper-differential sensitivity analysis of PDE-constrained inverse problems

Isaac Sunseri[1,2], Joseph Hart[1], Bart van Bloemen Waanders[1], and Alen Alexanderian[2]
[1] Sandia National Laboratories, [2]NC State University

Goals

- Learn how uncertainty in model parameters (besides inversion parameters) and data affect the solution of an inverse problem
- Compare the relative importance of accurately measuring different model parameters and data sources
- Augment experimental design techniques

Model Problem - Subsurface Flow

We define

- Auxiliary parameters (θ_a): uncertain model parameters
- Experimental parameters (θ_e): experimental conditions/data

and consider a deterministic inverse problem:

$$m^\star = \underset{m\in\mathcal{M}}{\operatorname{argmin}} J(m,\theta_e,\theta_a) := \frac{1}{2}\|\mathcal{Q}_p p(m,\theta_a) - \boldsymbol{y}_p(\theta_e)\|^2_{\mathbf{W}_p} + \frac{1}{2}\|\mathcal{Q}_c c(m,\theta_a) - \boldsymbol{y}_c(\theta_e)\|^2_{\mathbf{W}_c} + \alpha\mathcal{R}(m)$$

where c and p solve

$$\begin{aligned}
-\nabla\cdot(e^m\nabla p) &= 0 && \text{in } \Omega\\
c_t - \nabla\cdot\left(\epsilon\nabla c\right) - \nabla\cdot(e^m\nabla p\, c) &= g && \text{in } [0,T]\times\Omega\\
p &= p_1 && \text{on } \Gamma_1\\
p &= p_2 && \text{on } \Gamma_3\\
\nabla p\cdot n &= 0 && \text{on } \Gamma_0\cup\Gamma_2\\
\nabla c\cdot n &= 0 && \text{on } [0,T]\times\Gamma\\
c(0,x) &= 0 && \text{in } \Omega
\end{aligned}$$

HDSA

Hyper-differential sensitivity analysis (HDSA) [1,2] computes the sensitivity of the solution of an optimization problem with respect to the combination of auxiliary and experimental parameters.

The **sensitivity operator** $\mathcal{D}$ is found by applying the Implicit Function Theorem [3] to J_m (the Fréchet derivative of J w.r.t. m).

$$\mathcal{D} = -\mathcal{H}^{-1}\mathcal{B}$$

- $\mathcal{H} := J_{m,m}(m^\star,\theta^\star)$ - Hessian of J w.r.t m
- $\mathcal{B} := J_{m,\theta}(m^\star,\theta^\star)$ - Fréchet derivative of J_m w.r.t. θ
- $\theta^\star$ - nominal parameter values
- Adjoint-based gradient and Hessian computation

Pointwise sensitivity indicies measure the change in the solution w.r.t a perturbation of the i^{th} element of the k^{th} parameter.

$$S_i^k = \frac{\|\mathcal{D}e_i^k\|_{\mathcal{M}}}{\|e_i^k\|_{\Theta}}$$

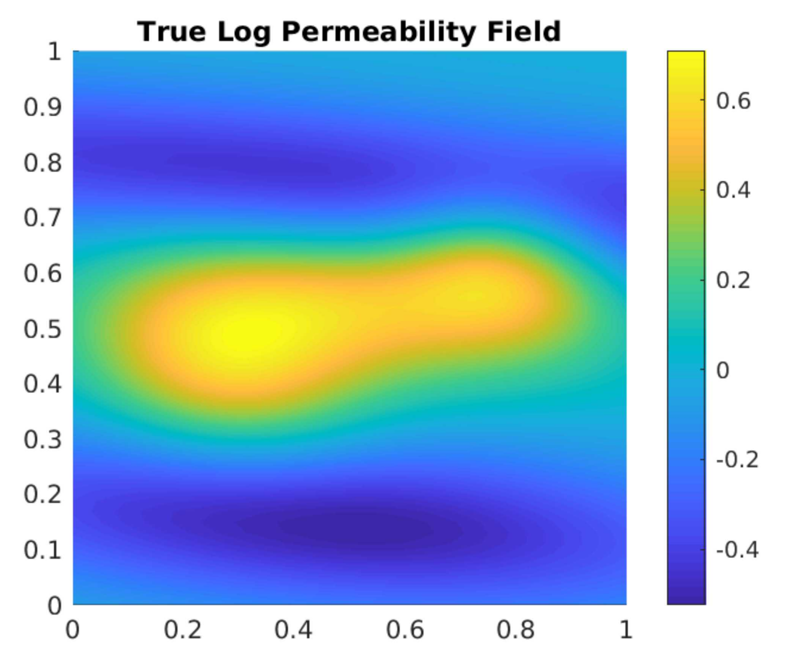
- e_i^k - basis element of parameter space $\Theta = \Theta_1\times\Theta_2\times\ldots\times\Theta_K$

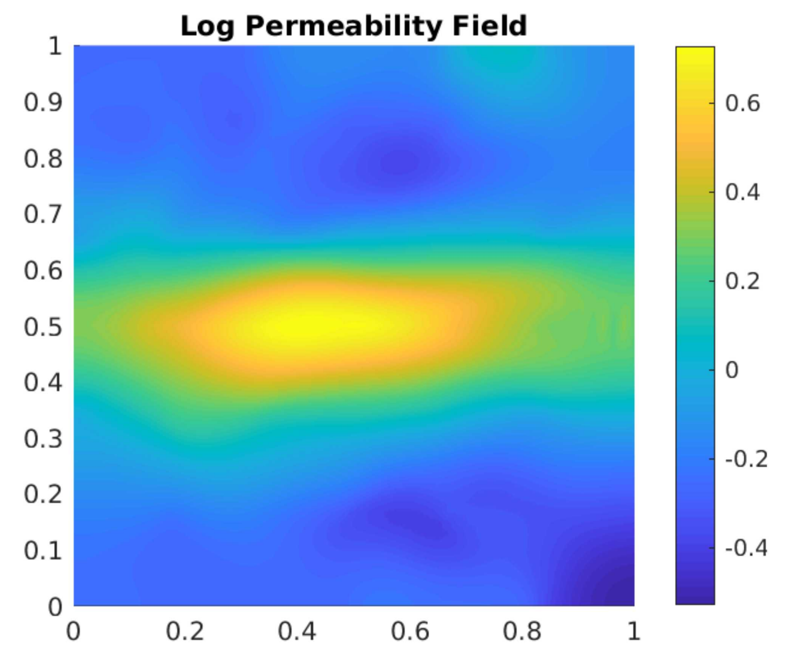
Generalized sensitivity indicies measure the maximum change in the solution w.r.t a norm-1 perturbation of the k^{th} parameter.

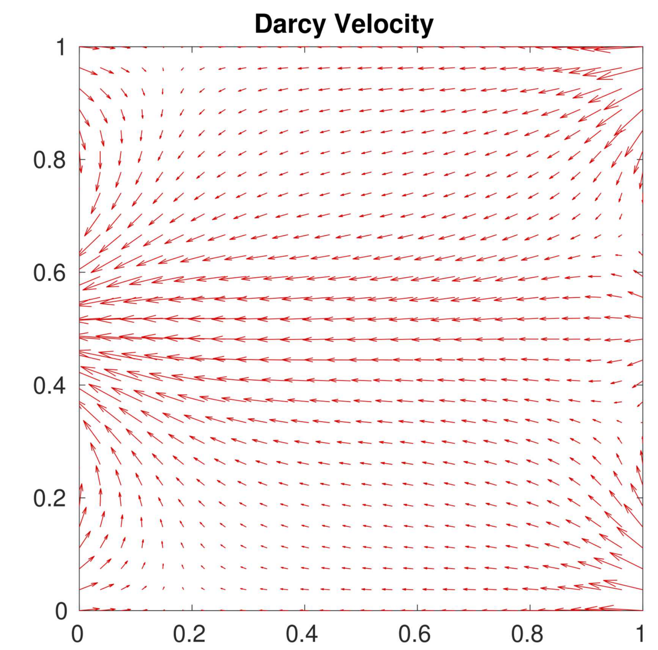
$$S^k = \max_{\theta\in\Theta}\frac{\|\mathcal{D}\mathcal{T}_k\theta\|_{\mathcal{M}}}{\|\theta\|_{\Theta}}$$

- $\mathcal{T}_k$ - projection operator onto the k^{th} parameter space

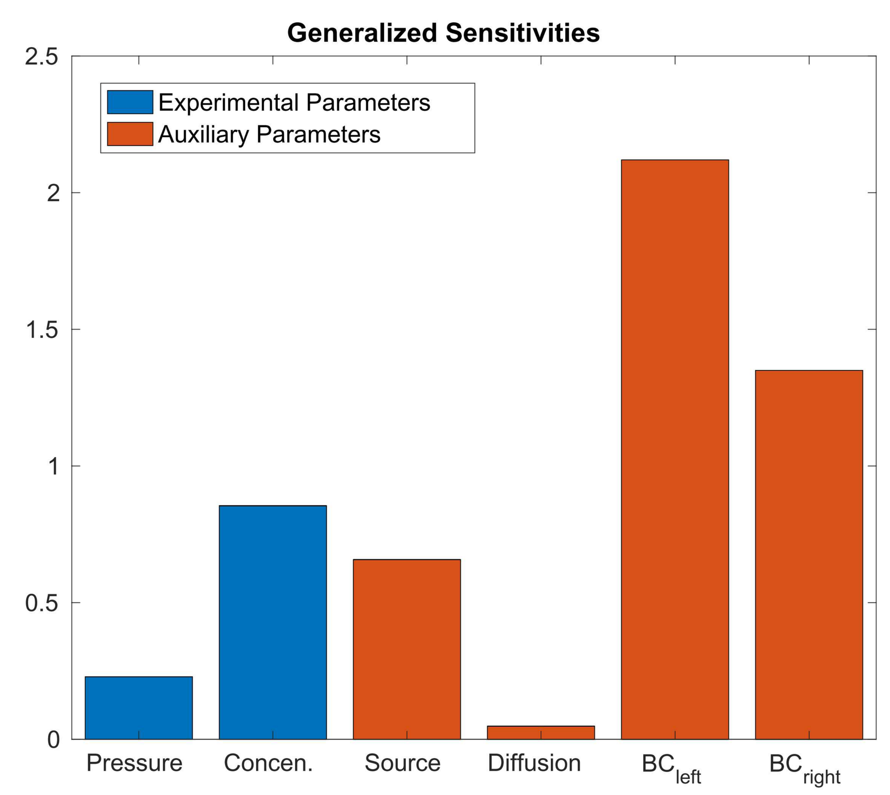
Inverse Problem

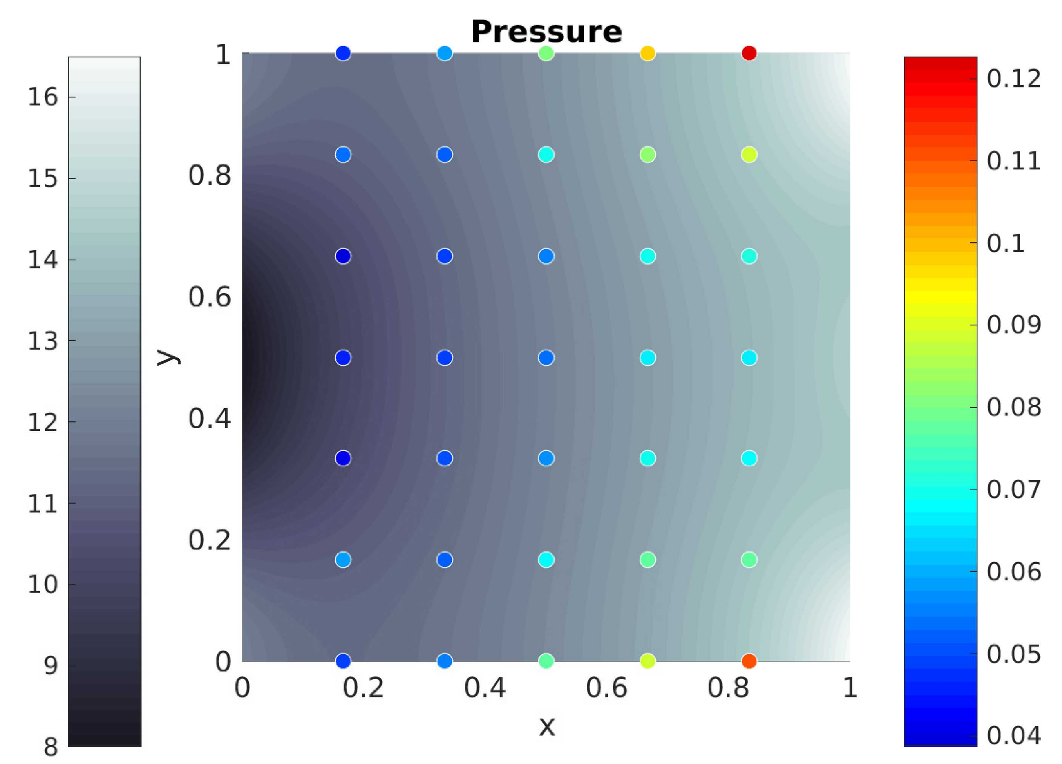


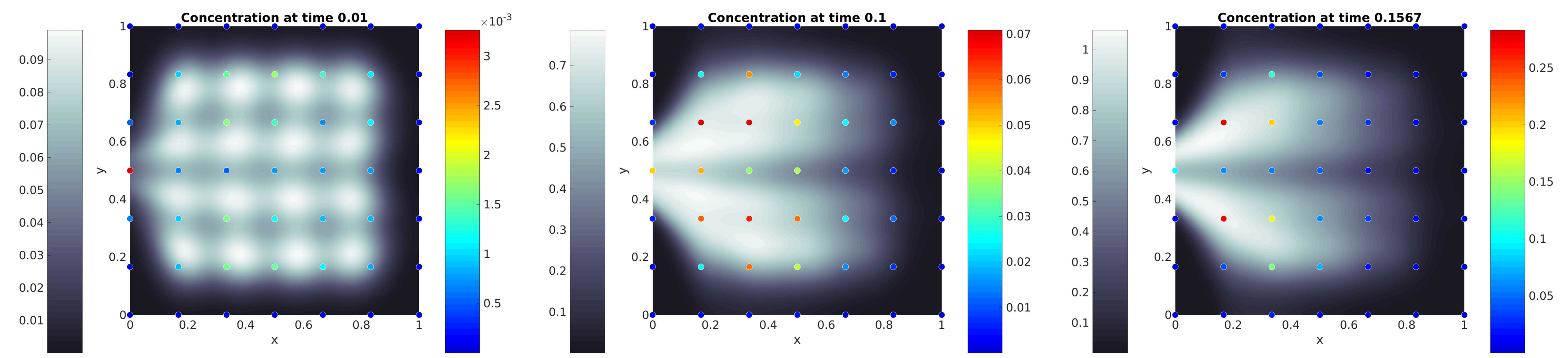


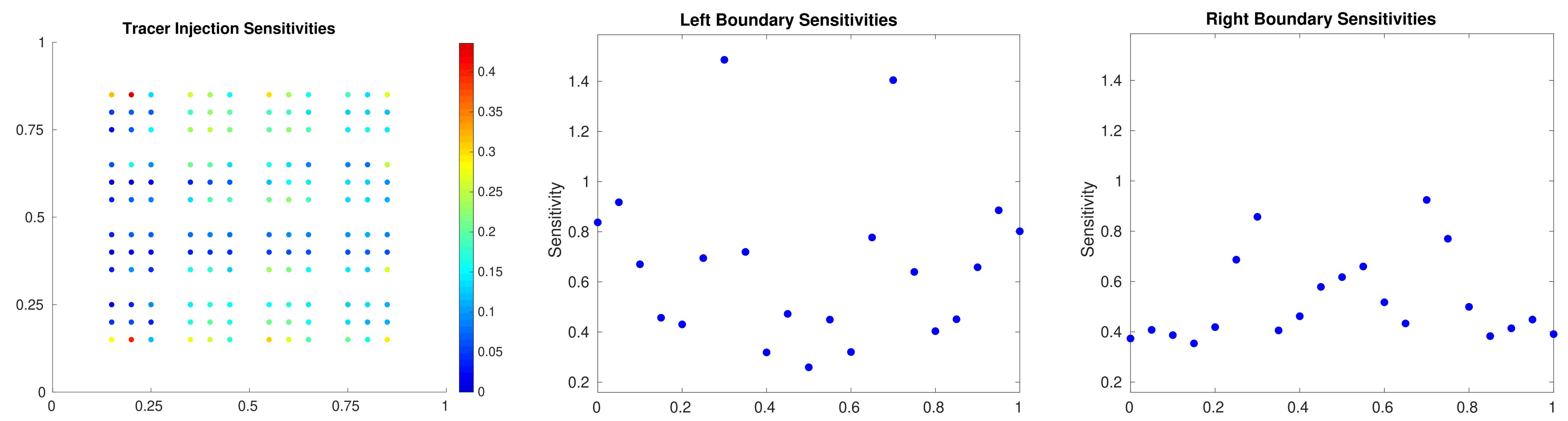


Sensitivity Results









Discussion

Generalized Sensitivities

- Boundary conditions are most important and drive flow through the domain
- Diffusivity coefficient is relatively unimportant
- Concentration measurements are more important than pressure measurements
- Used for parameter reduction and model specification
- Compares the relative importance of different parameters

Experimental Sensitivities

- Continuously injected tracer moves from right to left, splitting at y=0.5 into two concentration masses
- Both tracer concentration and sensitivities to consentration increase with time
- Pressure has higher sensitivity than concentration early in time, but is surpassed as concentration becomes increasingly important later in time
- High concentration sensitivity on the left side of the domain and low sensitivity on the right side
- High concentration sensitivity at sensors observing large amounts of tracer flow or a change in the contaminant mass
- Inverse problem relies on pressure data to reconstruct the solution on the right side of the domain where there is little concentration data
- Informs experimental design and sensor specification

Auxiliary Sensitivities

- Source injection sensitivities are generally higher in regions with low darcy velocity
- Boundary condition sensitivities are highest around y=0.3 and y=0.7, which cooresponds to the region of transition between the high and low permeability and darcy velocity regions
- Informs model specification and increases understanding of the relationship between complicated multi-physics systems and the inverse problem

Future Work

- How robust are the sensitivities to perturbations in the experimental design?
- Global HDSA
- HDSA for Bayesian inverse problems

References/Acknowledgments

[1] Joseph Hart, Bart van Bloemen Waanders, and Roland Herzog. Hyper-differential sensitivity analysis of uncertain parameters in PDE-constrained optimization. International Journal of Uncertainty Quantification, 2020.

[2] Kerstin Brandes and Roland Griesse. Quantitative stability analysis of optimal solutions in PDE-constrained optimization. Journal of Computational and Applied Mathematics, 2007.

[3] Ambrosetti A and Prodi G. 1995 *A Primer of Nonlinear Analysis* (Cambridge University Press).

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND No: SANDXXXX

This work was supported by the National Science Foundation under grant DMS-1745654

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.