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**Title:** W14\_CONTAMINANTREMEDIATION: High Performance Computing (HPC) for Multi-scale Decision Analyses: From Pore-scale Processes to Field-scale Contaminant Remediation

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## W14\_CONTAMINANTREMEDIATION: High Performance Computing (HPC) for Multi-scale Decision Analyses: From Pore-scale Processes to Field-scale Contaminant Remediation

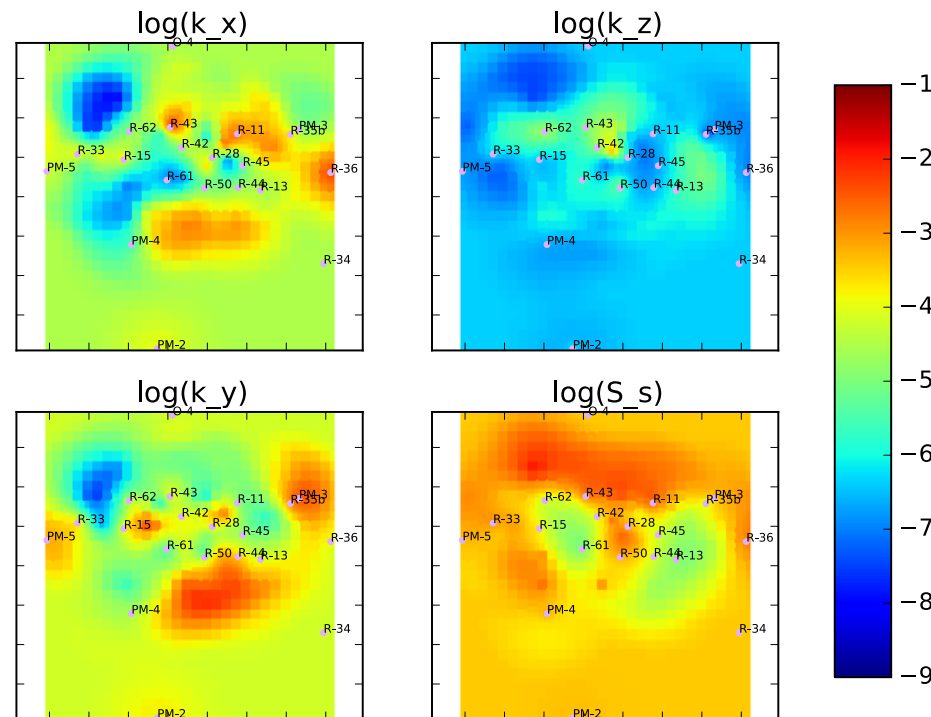
- LANL chromium site is one of the most complex, data-rich, highly visible sites within the Department of Energy (DOE) complex.
- The modeling work for the site requires high-performance computational (HPC) dealing with large data sets ( $>10^7$  datum), complex models ( $>10^6$  computational grid points), ambiguous uncertainties and challenging decisions.
- **ZEM** is designed to provide on-the-fly analysis, assimilation and integration of the site data into a series of tools and models to perform various types of data- and model-based analyses
- **ZEM** data streams include (1) hydraulic and barometric pressure data streamed in real-time to web servers, (2) pumping rate records (updated monthly), and (3) geochemical concentration data from groundwater (updated weekly to quarterly)
- **ZEM** incorporates (1) data assimilation, model simulation (FEHM/PFLOTRAN) and model analysis tools including decision support techniques incorporated in **MADS**
- **MADS** (Model Analysis and Decision Support; <http://mads.lanl.gov>) is LANL-developed, high-performance, open-source framework
- **MADS** is coded in Julia, a novel, high-level, high-performance, dynamic, programming language for technical computing (<http://github.com/madsjulia>). Julia provides substantial benefits over the other programming languages and allows for relatively easy development of high-performance computational codes
- **MADS** is applied in several HPC projects at LANL
- **MADS** has been tested on jobs using up to 20,000 processors.

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**ZEM/MADS** have been applied to perform numerous tasks (accumulating more than 1,000 CPU-years of computational time) including:

- Tomography of aquifer heterogeneity
- Decision analysis related to contaminant source termination

Example tomographic (log-scale) images of key model parameters associated with aquifer heterogeneity related to anisotropy of hydraulic permeability ( $k_x$ ,  $k_y$ ,  $k_z$ ) and specific storage ( $S_s$ )



Robustness of alternative decision “choices” (operational scenarios where the contaminant source is terminated at different times) based on Bayesian Information Gap Decision Theory (BIGDT)

