Recent developments in MADS algorithms: ABAGUS and *Squads*

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Model analysis and decision support (MADS) for complex problems

Complex problems:

- Large number of model parameters
- Nonlinear and hysteretic parameter correlations
- Multiple maxima/minima
- Flat response surface regions (portions of parameter space with low parameter sensitivity)
- Long execution times
- Require efficient and robust model analyses strategies

Model analysis and decision support (MADS) for complex models

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- Model analysis
  - Calibration/parameter estimation
  - Uncertainty quantification
  - Parameter sensitivities and correlations
  - Predictive analysis
  - Model selection
  - Model averaging

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  - Predictive analysis
  - Model selection
  - Model averaging
- Decision support
  - Robust and/or optimal decisions

Agent-Based Analysis of Global Uncertainty and Sensitivity

ABAGUS features:

- "Agent-based" model analysis
- Extends Particle Swarm Optimization (PSO) to uncertainty and sensitivity analysis
- Collects all model evaluation results in KD-Tree for efficient restart and hierarchical analysis
- Response surface sculpting discourages reinvestigation of "collected" regions of the parameter
- Discretized parameter space
- Automated discretization refinement

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- Identify acceptable parameter ranges
- Sensitivity analysis

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ABAGUS uses:

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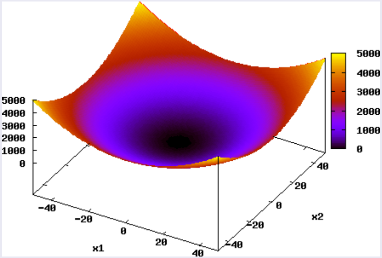
- Sensitivity analysis
- Identify parameter correlations
- Parameter uncertainty analysis
- Predictive analysis
- Decision support
- Information for these are contained in the results from a single ABAGUS run

Harp, D.R. and V.V. Vesselinov (2011), An agent-based approach to global uncertainty and sensitivity analysis, *Computers & Geosciences*, doi:10.1016/j.cageo.2011.06.025.

Monte Carlo vs ABAGUS: Estimation of probability of success/failure based

Example: parabola function



$$f(x_1, x_2) = x_1^2 + x_2^2$$

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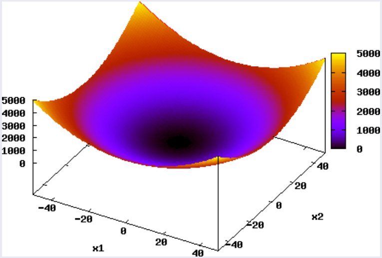
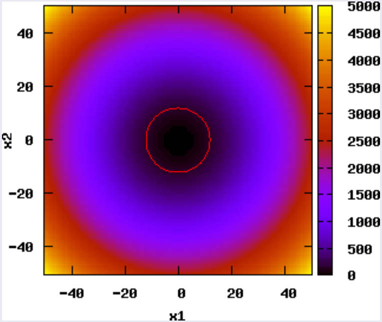


$$f(x_1, x_2) = x_1^2 + x_2^2$$

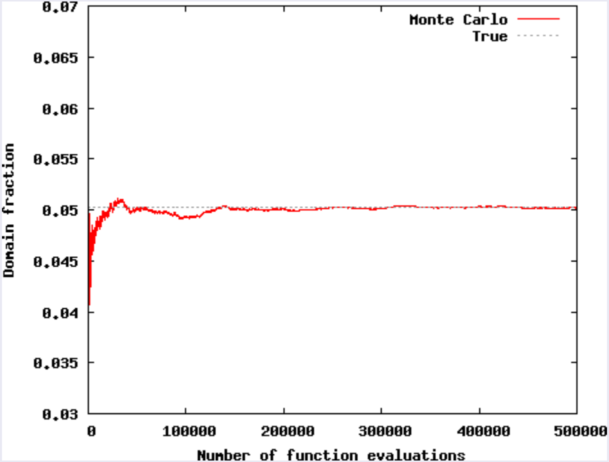
Goal: estimate area where $f(x_1, x_2) \leq 160$, (red circle)



- $f(x_1, x_2) \leq 160$ is approximately 5% of domain
- **x** uniformly distributed
- Domain: $\mathbf{x} = [-50 : 50]$

Monte Carlo estimation of probability of success/failure

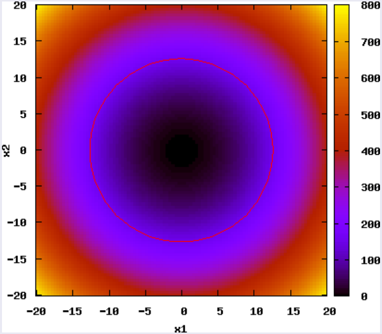
Estimation of parameter space with $f(x_1, x_2) \leq 160$



- Probability of success/failure (i.e. domain fraction) estimated by fraction of random samples in "red circle"
- Monte Carlo uses an Improved Distance Latin Hypercube Sampling

ABAGUS estimation of probability of success/failure

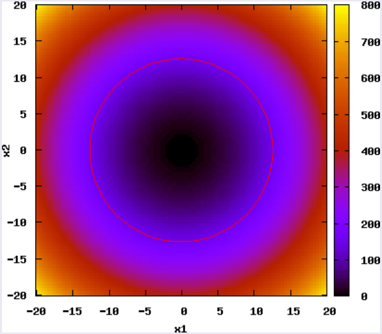
Before exploration



- $f(x_1, x_2) = 160$ indicated by red circle
- Zoomed into $x_1, x_2 = [-20 : 20]$

ABAGUS estimation of probability of success/failure

Before exploration



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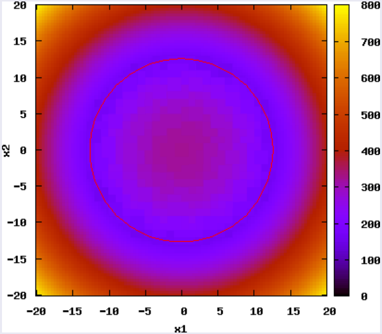
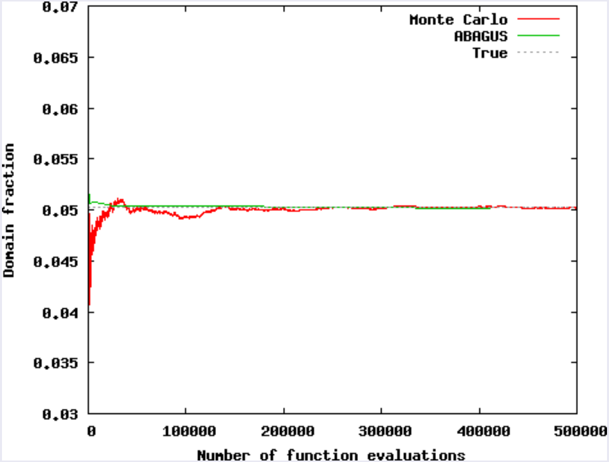
After exploration



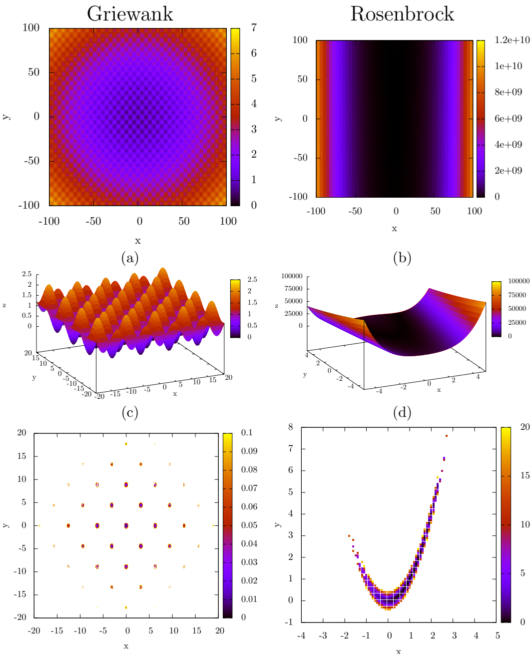
- Response surface sculpted
- "Acceptable" parameter sets collected

ABAGUS estimation of probability of success/failure

Estimation of parameter space with $f(x_1, x_2) \leq 160$

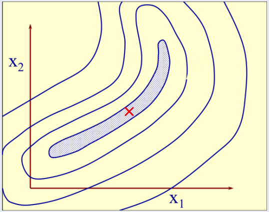


ABAGUS results on more complicated response surfaces...



ABAGUS as predictive analyzer

Identify "plausible" region based on 1^{st} criterion



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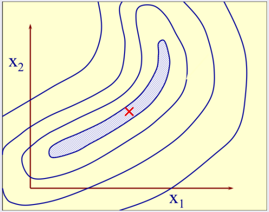
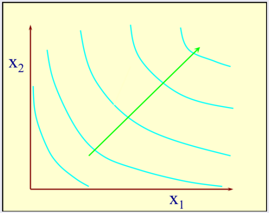


Gradient contours of 2^{nd} criterion



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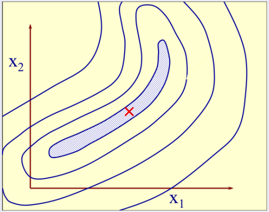

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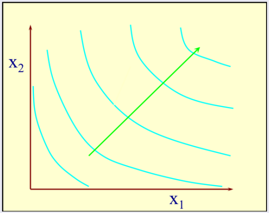
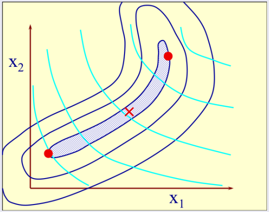
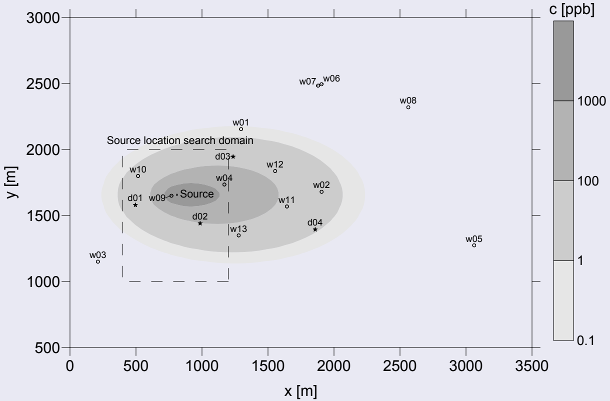


Max/min values of 2^{nd} criterion within 1^{st} criterion



ABAGUS application

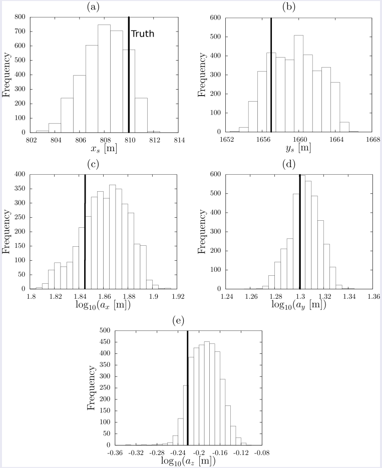
Contaminant plume in aquifer...



- w wells (circles) - existing wells
- d wells (stars) - proposal wells
- Uncertain parameters: source location (x_s, y_s) dispervities (a_x, a_y, a_z)

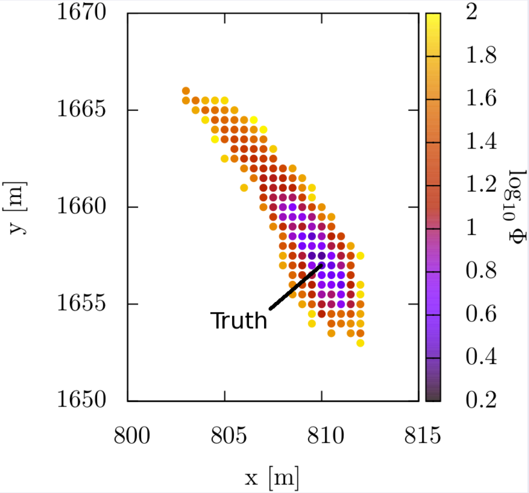
ABAGUS application

Parameter histograms produced from ABAGUS:



ABAGUS application

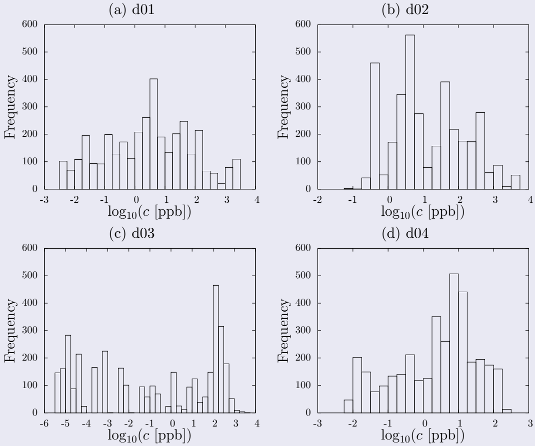
Plausible source locations collected by ABAGUS:



- Min OF at each source location plotted

ABAGUS application

Predictive analysis of concentrations at proposal wells:



Adaptive Optimization: *Squads*

Squads

- Global optimization with local optimization speedup
- Global strategy: Adaptive Particle Swarm Optimization (APSO)
- Local strategy: Levenberg-Marquardt (LM)
- Adaptive rules balance strategies

Vesselinov, V.V. and D.R. Harp, Adaptive hybrid optimization strategy for calibration and parameter estimation of physical model, *Computers & Geosciences*, In Review.

Squads comparisons

Squads is compared to:

- Levenberg-Marquardt (LM) - local strategy
- Particle Swarm Optimization (PSO) Standard 2006 - global strategy
- TRIBES Adaptive PSO - global strategy
- hPSO (PSO + simplex) - alternative hybrid strategy

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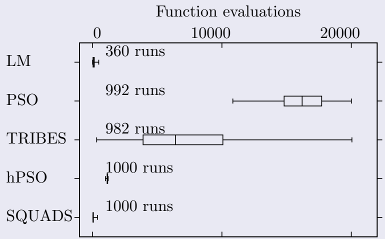
Comparison details:

- 2D, 5D, and 10D Rosenbrock and Griewank test functions
- Domain: $\mathbf{x} = [-100 : 100]$
- 20,000 allowable function evaluations for each optimization run
- 1000 runs per strategy for each test function
- Success: all parameters within 0.1 of optimal parameters

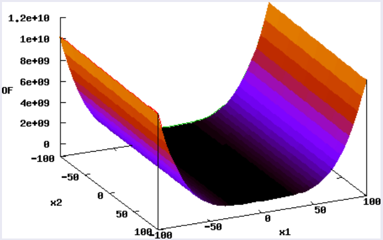
Squads: Rosenbrock comparisons

2D Rosenbrock

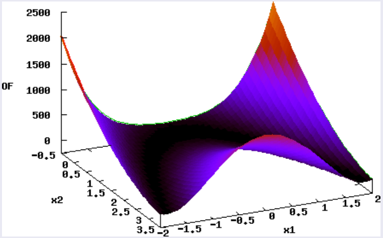


- Boxes indicate 25th to 75th percentile range for number of evaluations needed to achieve success
- Vertical lines in boxes indicate median value
- "Whiskers" indicate max and min values
- Number of successful runs out of 1000 are indicated above boxes

2D Rosenbrock function

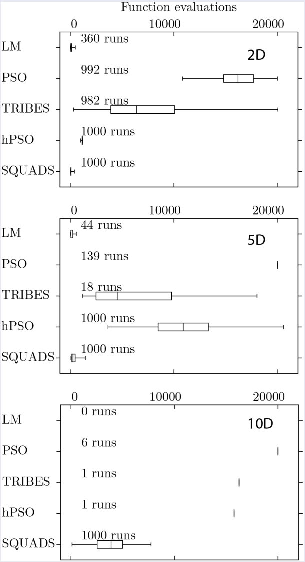


Global minimum: $\mathbf{x} = \mathbf{1}$

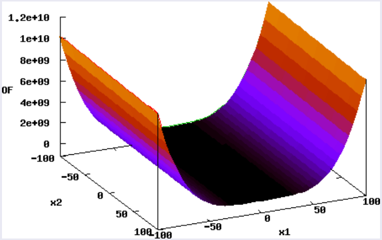


Squads: Rosenbrock comparisons

Function evaluation boxplots



2D Rosenbrock function



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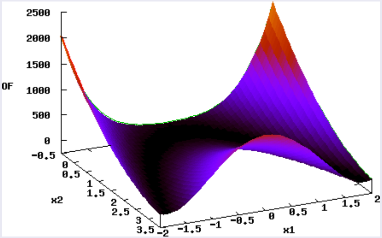
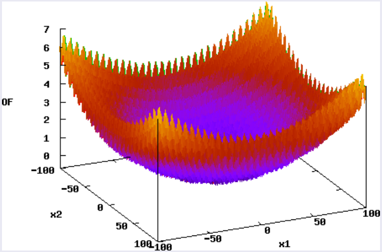


Squads: Griewank comparisons

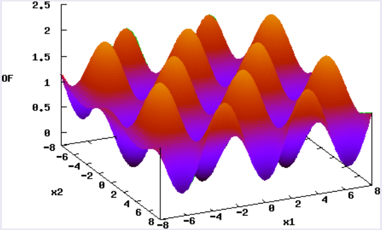
Griewank Function:

- Ideal for comparison of hybrid methods
- Becomes more difficult for global methods with increased dimensionality
- Becomes easier for local methods with increased dimensionality
- Hybrid methods should have a well balanced act

2D Griewank function



Global minimum: $\mathbf{x} = \mathbf{0}$



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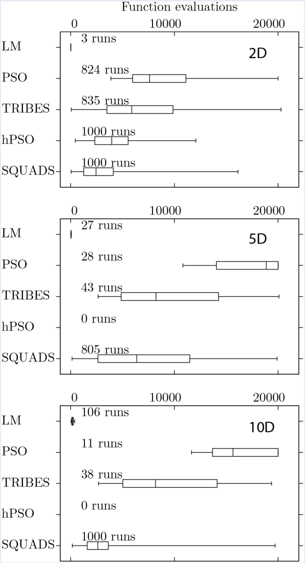

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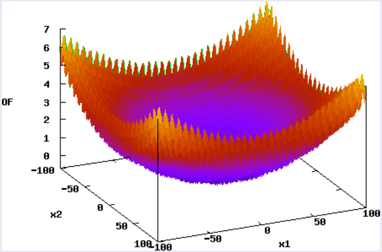

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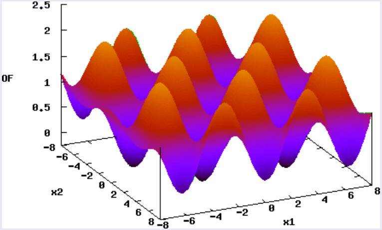
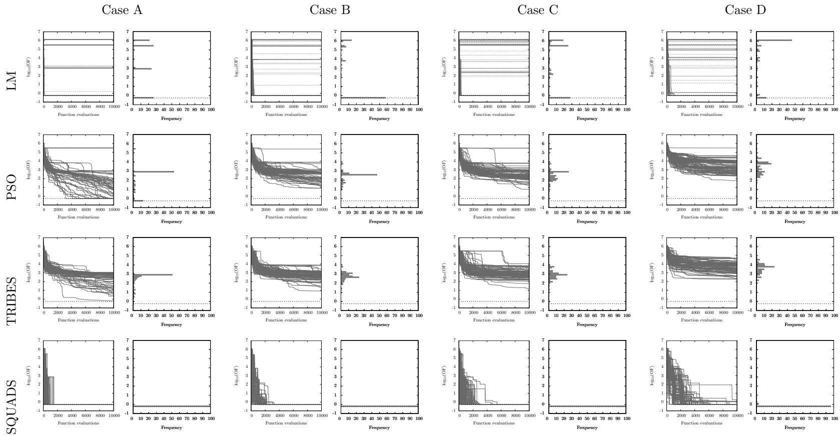


SQUADS application



Conclusions

- ABAGUS presents efficient approach for model-based uncertainty analyses
- *Squads* provides an efficient and robust optimization strategy