Recent developments in MADS algorithms: ABAGUS and Squads

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Model analysis and decision support (MADS) for complex problems

<table>
<thead>
<tr>
<th>Complex problems:</th>
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<tbody>
<tr>
<td>Large number of model parameters</td>
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<tr>
<td>Nonlinear and hysteretic parameter correlations</td>
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<tr>
<td>Multiple maxima/minima</td>
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<tr>
<td>Flat response surface regions (portions of parameter space with low parameter sensitivity)</td>
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<tr>
<td>Long execution times</td>
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<td>Require efficient and robust model analyses strategies</td>
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Model analysis and decision support (MADS) for complex models

Why do we care?

- Model analysis
- Calibration/parameter estimation
- Uncertainty quantification
- Parameter sensitivities and correlations
- Predictive analysis
- Model selection
- Model averaging
- Decision support
  - Robust and/or optimal decisions
Model analysis and decision support (MADS) for complex models

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**Robust and/or optimal decisions**
Model analysis and decision support (MADS) for complex models

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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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### ABAGUS uses:
- Identify acceptable parameter ranges
- 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

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

Example: parabola function

\[ f(x_1, x_2) = x_1^2 + x_2^2 \]
Monte Carlo vs ABAGUS: Estimation of probability of success/failure based

Example: parabola function

\[ f(x_1, x_2) = x_1^2 + x_2^2 \]

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: \( x = [-50 : 50] \)
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 method (encoded in MADS as well)
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

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

After exploration

- Response surface sculpted
- “Acceptable” parameter sets collected
Estimation of parameter space with $f(x_1, x_2) \leq 160$
ABAGUS results on more complicated response surfaces...

Griewank

Rosenbrock

(a) (b)

(c) (d)
Identify “plausible” region based on 1st criterion
ABAGUS as predictive analyzer

Identify “plausible” region based on 1st criterion

Gradient contours of 2nd criterion
ABAGUS as predictive analyzer

Identify “plausible” region based on 1st criterion

Gradient contours of 2nd criterion

Max/min values of 2nd criterion within 1st criterion
w wells (circles) - existing wells

d wells (stars) - proposal wells

Uncertain parameters: source location \((x_s, y_s)\) dispersions \((a_x, a_y, a_z)\)
Parameter histograms produced from ABAGUS:
Plausible source locations collected by ABAGUS:

- Min OF at each source location plotted
Predictive analysis of concentrations at proposal wells:

(a) d01  (b) d02  
(c) d03  (d) d04
Adaptive Optimization: *Squads*

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

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

Comparison details:
- 2D, 5D, and 10D Rosenbrock and Griewank test functions
- Domain: $x = [-100: 100]$ for each optimization run
- 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
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Squads: Rosenbrock comparisons

2D Rosenbrock

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<tr>
<th>Method</th>
<th>Function evaluations</th>
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<tbody>
<tr>
<td>LM</td>
<td>360 runs</td>
</tr>
<tr>
<td>PSO</td>
<td>992 runs</td>
</tr>
<tr>
<td>TRIBES</td>
<td>982 runs</td>
</tr>
<tr>
<td>hPSO</td>
<td>1000 runs</td>
</tr>
<tr>
<td>SQUADS</td>
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- 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

Global minimum: $x = 1$
**Squads: Rosenbrock comparisons**

### Function evaluation boxplots

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<th>10,000 runs</th>
<th>20,000 runs</th>
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<td>360</td>
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<tr>
<td>LM</td>
<td>44</td>
<td>5D</td>
<td></td>
</tr>
<tr>
<td>PSO</td>
<td>139</td>
<td></td>
<td></td>
</tr>
<tr>
<td>TRIBES</td>
<td>18</td>
<td></td>
<td></td>
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<tr>
<td>LM</td>
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<td>10D</td>
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<tr>
<td>PSO</td>
<td>6</td>
<td></td>
<td></td>
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**2D Rosenbrock function**

- Global minimum: \( x = 1 \)
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

Global minimum: $x = 0$
Squads: Griewank comparisons

Function evaluation boxplots

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<tr>
<td>3D</td>
<td>27 runs</td>
<td>824 runs</td>
<td>835 runs</td>
<td>1000 runs</td>
<td>1000 runs</td>
</tr>
<tr>
<td>5D</td>
<td>106 runs</td>
<td>11 runs</td>
<td>38 runs</td>
<td>0 runs</td>
<td>805 runs</td>
</tr>
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2D Griewank function

Global minimum: $x = 0$
Conclusions

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