

**United Technologies
Research Center**

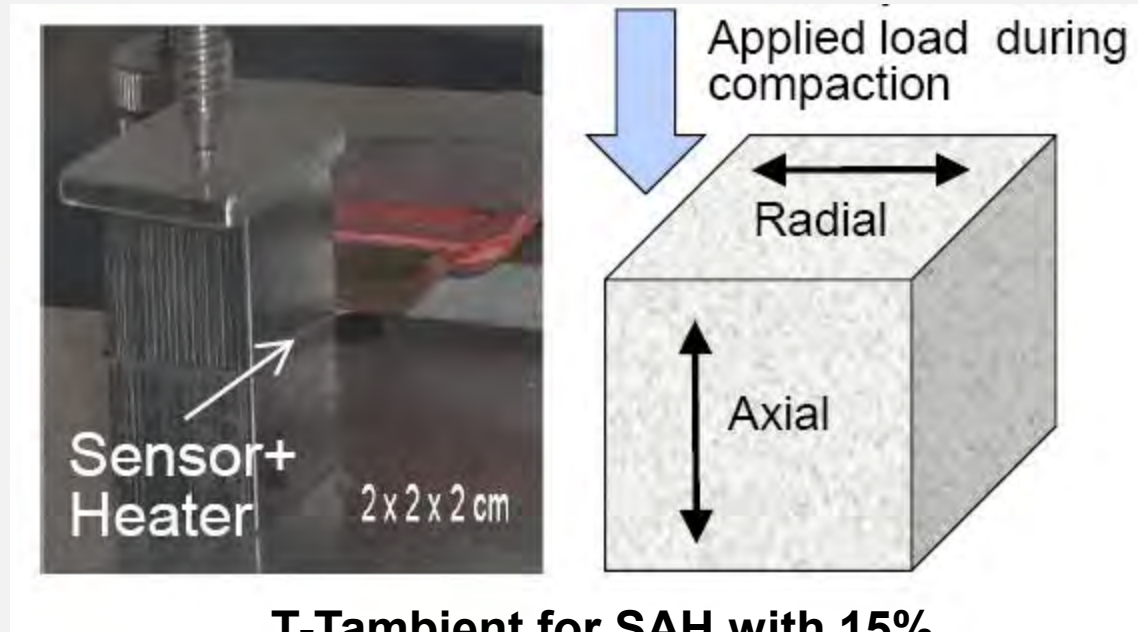
**Solution of Inverse Thermal Problem for
Assessment of Thermal Parameters of
Engineered H₂ Storage Materials**

Igor I Fedchenia and Bart A van Hassel

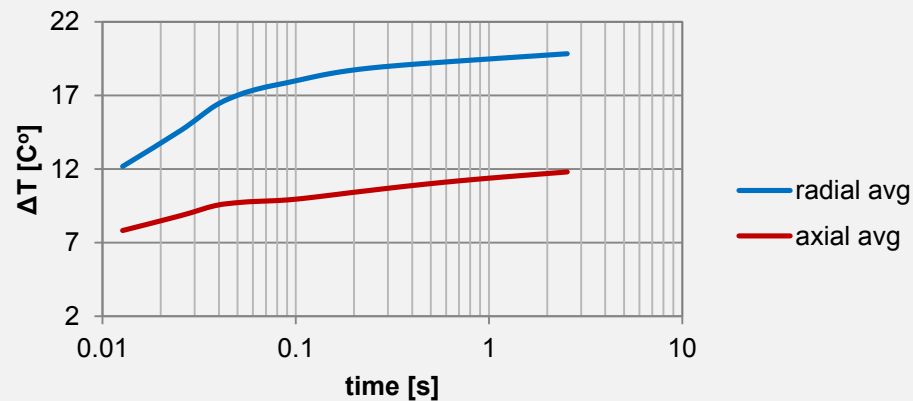
Presented at the COMSOL Conference, Boston October 14th, 2011

Fabrication and measurement

New materials for H₂ storage requires accurate estimation of thermal parameters



T-Tambient for SAH with 15% worms



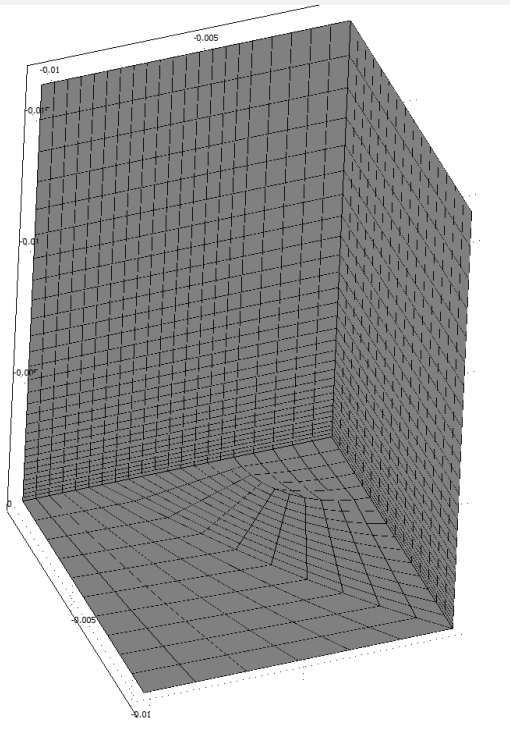
Inverse problem

Find PDE parameters that match solution of forward problem

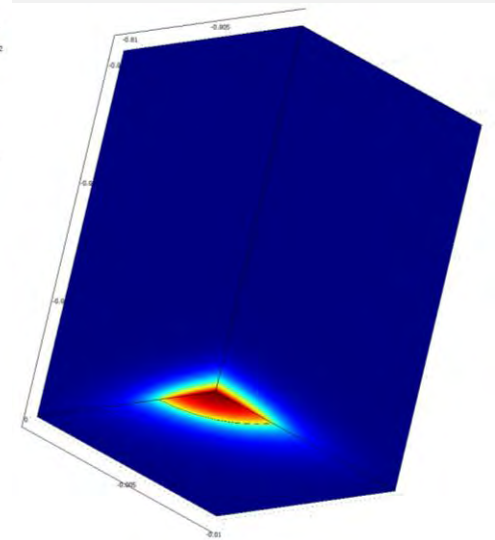
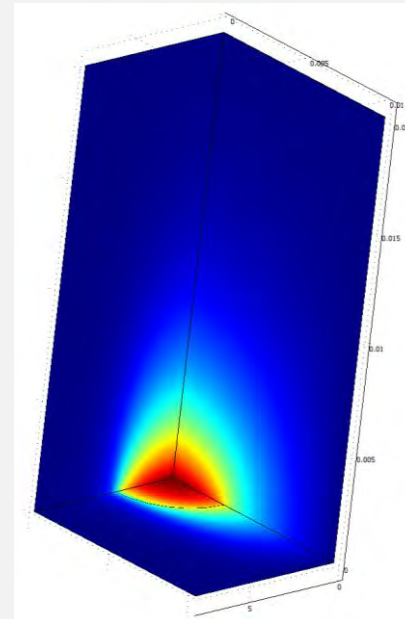
$$\rho_{sensor} \cdot C_{sensor} \cdot d_{sensor} \cdot \frac{\partial T_{sensor}}{\partial t} + \nabla(-d_{sensor} \cdot k_{sensor} \cdot \nabla T_{sensor}) = d_{sensor} \cdot q + h \cdot (T_{sample} - T_{sensor})$$

$$\rho_{sample} \cdot C_{sample} \cdot \frac{\partial T_{sample}}{\partial t} + \nabla(-k_{sample} \cdot \nabla T_{sample}) = 0$$

$$-\mathbf{n} \cdot (-k_{sample} \cdot \nabla T_{sample}) = h \cdot (-T_{sample} + T_{sensor})$$



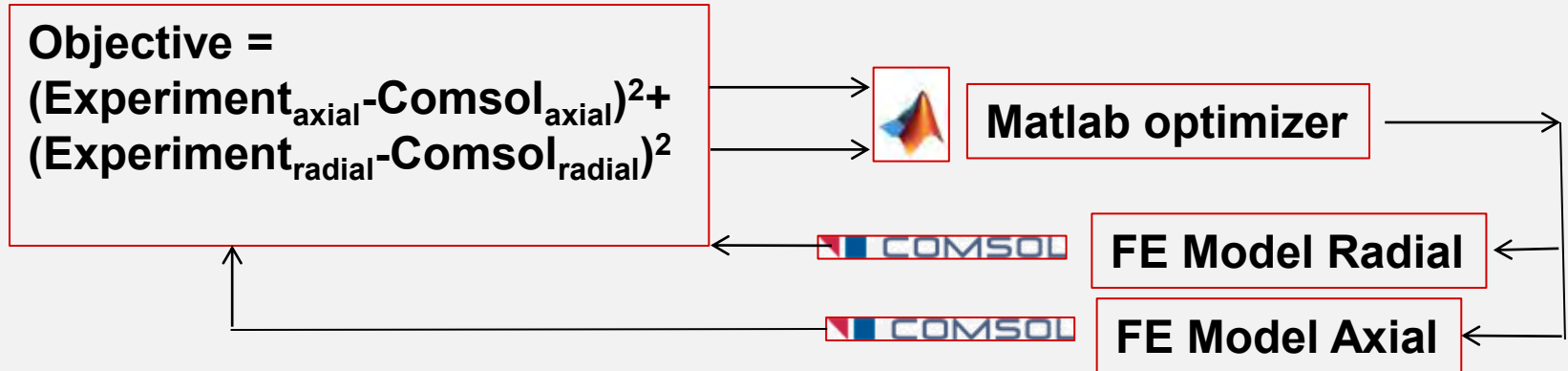
**2560
hexahedral
elements with
exponentially
changing
density**



**7 seconds to
solve on 4
processor
computer**

Inverse problem as optimization task

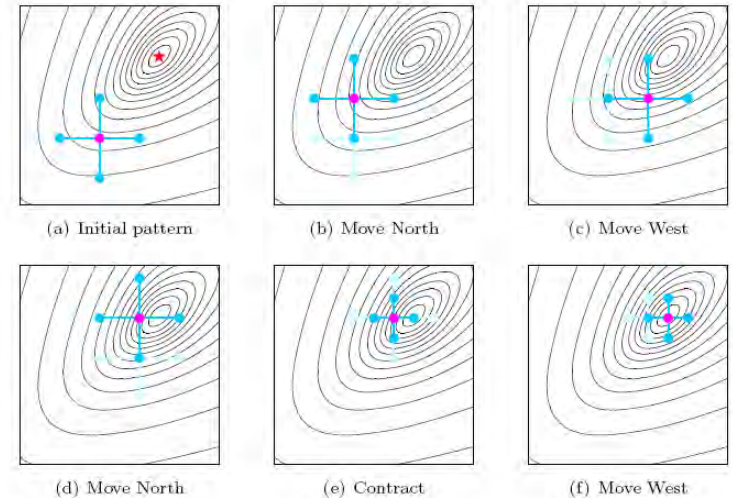
Forward problem: Comsol; Backward problem: Matlab Global Optimization Toolbox



Matlab optimization routine **patternsearch** implements derivative free direct search algorithm

- Fast to converge to vicinity of minimum
- Does not require derivatives
- Very robust
- Allows for work with different norms

- Very slow in vicinity of minimum
- Very slow in the long shallow valleys



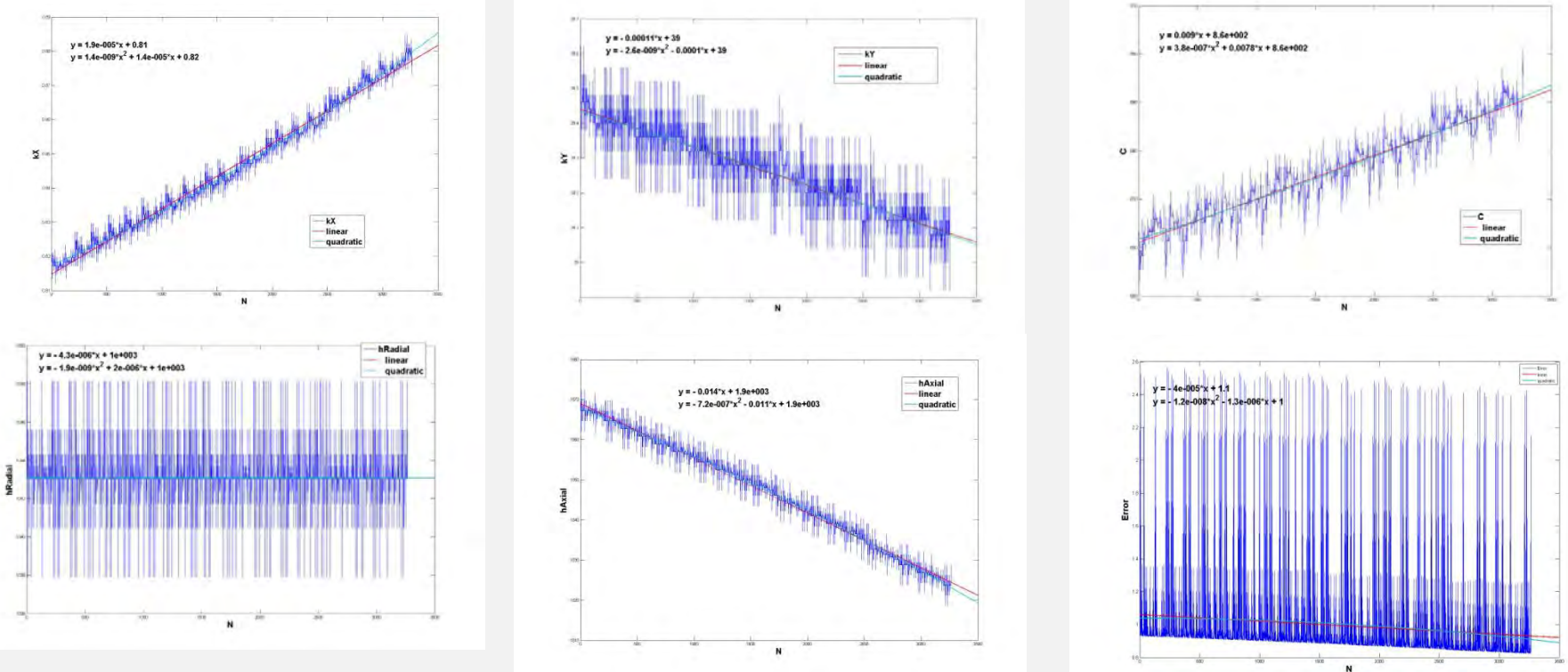
Kolda, Tamara G., Robert Michael Lewis, and Virginia Torczon.

Optimization by direct search: new perspectives on some classical and modern methods.

SIAM Review, Volume 45, Issue 3, 2003, pp. 385–482.

Acceleration strategies

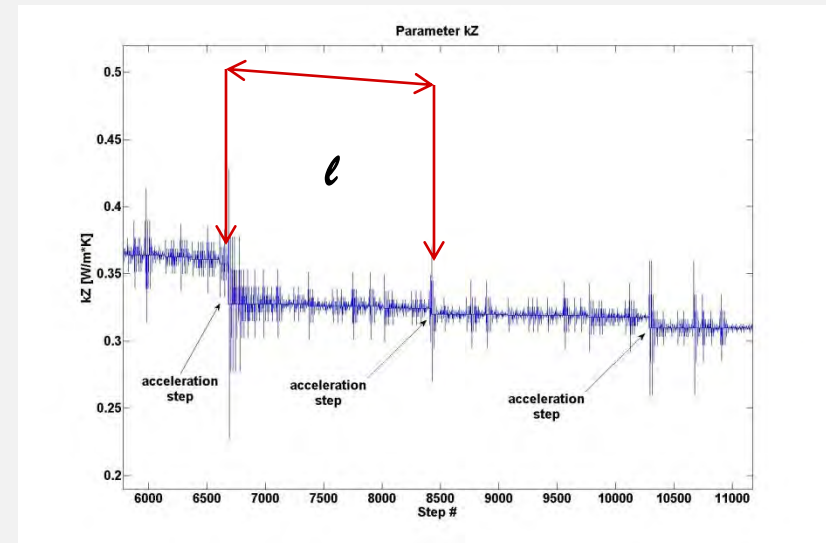
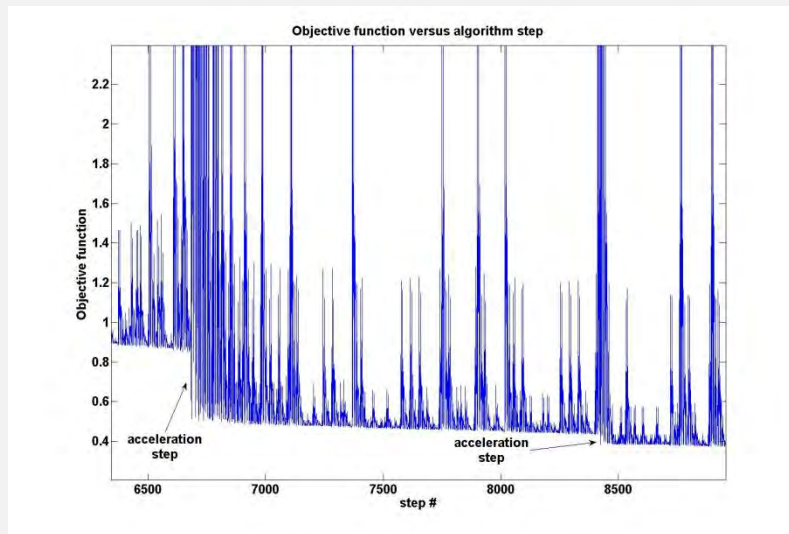
Reconstruct locally smoothed objective function manifold and move along



- Smoothed parameter dynamics allows for parametric reconstruction of objective function manifold for each parameter;
- The size of the leap step is computed from the smooth parametric reconstruction of error plot;
- The step is made for each parameter;
- The procedure is repeated until parameters stop changing.
- The length of direct search run is the algorithm adjustable parameter.

Optimization algorithm

Smooth local parametric representation of objective function manifold

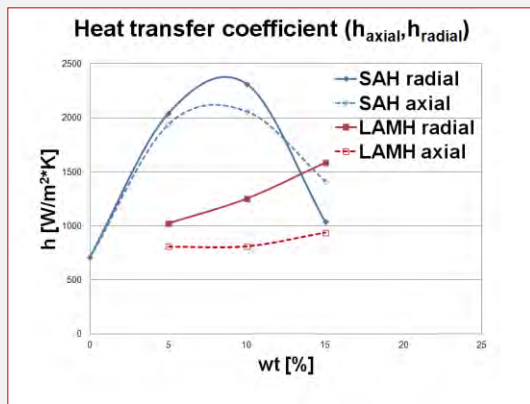
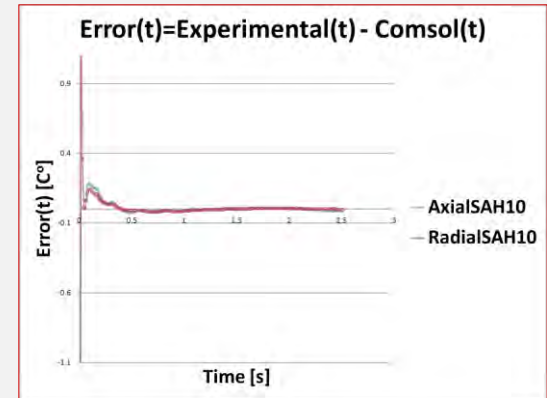
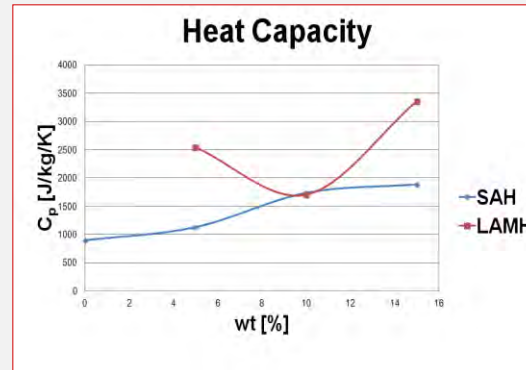
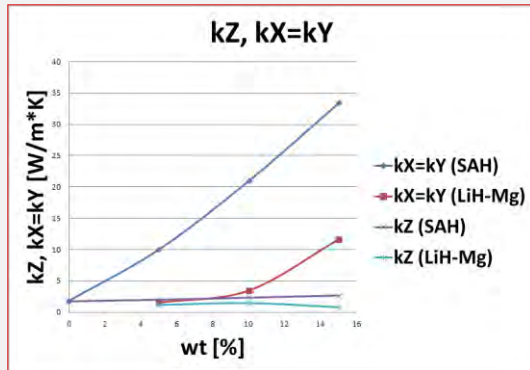


Step n :

- run direct search for ℓ steps; **slow**
- calculate smooth curve for each parameter as a function of step n ; **fast**
- run line search along the smooth parametrically represented line to find the minimum of objective function at the end of the line; **fast**
- Repeat at Step $n+1$

Results

Thermal parameters for 3 new materials have been reconstructed using Comsol Matlab combination



The first 0.2 [s] of experimental data have been discarded to keep complexity of the sensor model to minimum

