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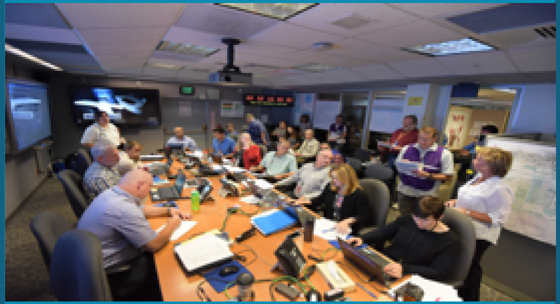
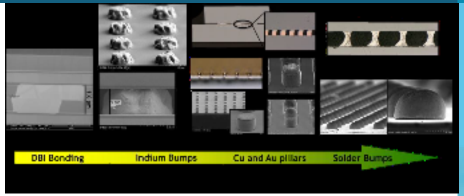
SAND2021-5689C

Assessment of Material Bond Integrity via Inversion for Thermophysical Properties



RAPID OPTIMIZATION LIBRARY



Summer Heat Transfer Conference

June 16-18, 2021

Presented by

Benjamin C. Treweek, Wyatt Hodges,
Elbara Ziade, and Timothy F. Walsh

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Outline

Heterogeneously Integrated (HI) Electronics Systems

Sierra Mechanics, Rapid Optimization Library (ROL), and Inverse Methods

Verification and Example Inversion for Thermophysical Properties

Conclusions and Future Work

Heterogeneously Integrated (HI) Electronics Systems

Heterogeneously Integrated (HI) Electronics Systems

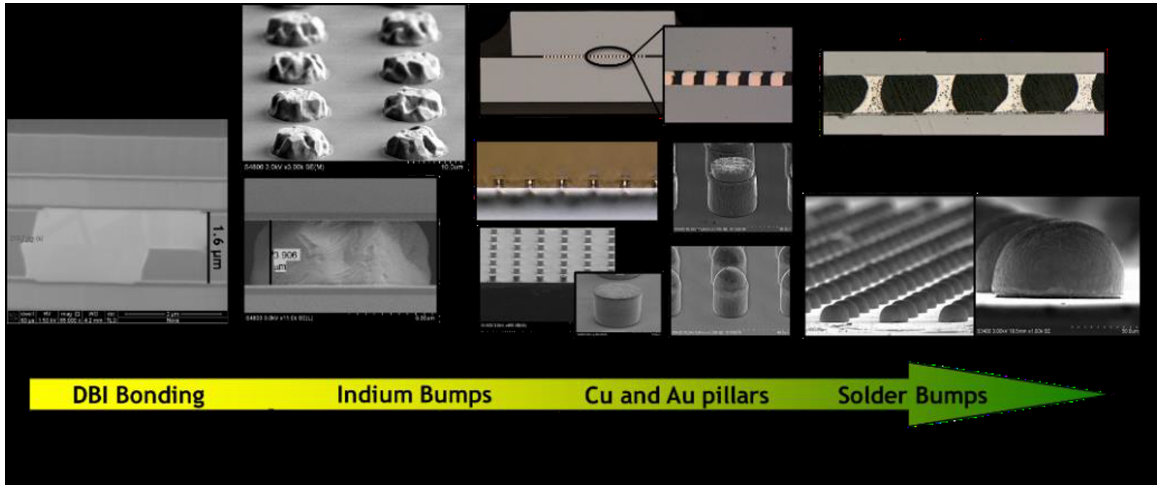
Connecting multiple chiplets from different manufacturing processes key to improving microsystem functionality

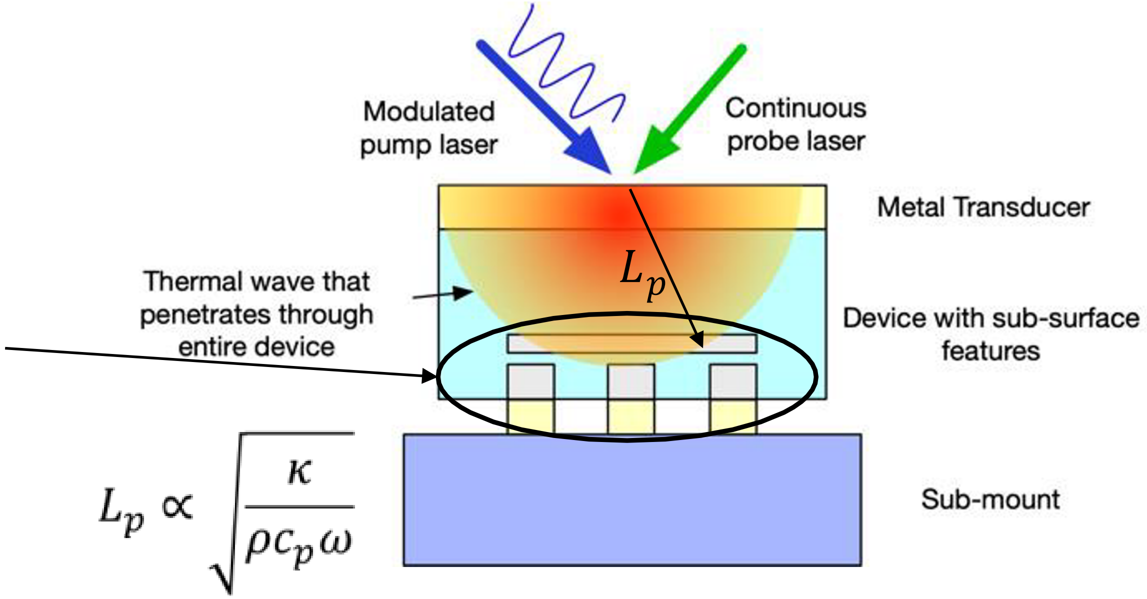
High-density interconnects needed for performance with variety of chips, components, and operating conditions

Need methods to test interconnect viability both after manufacturing and after use

Frequency-domain thermoreflectance (FDTR)

Given **complex microelectronic structure**, use **inverse methods** to assess **integrity of microbumps**

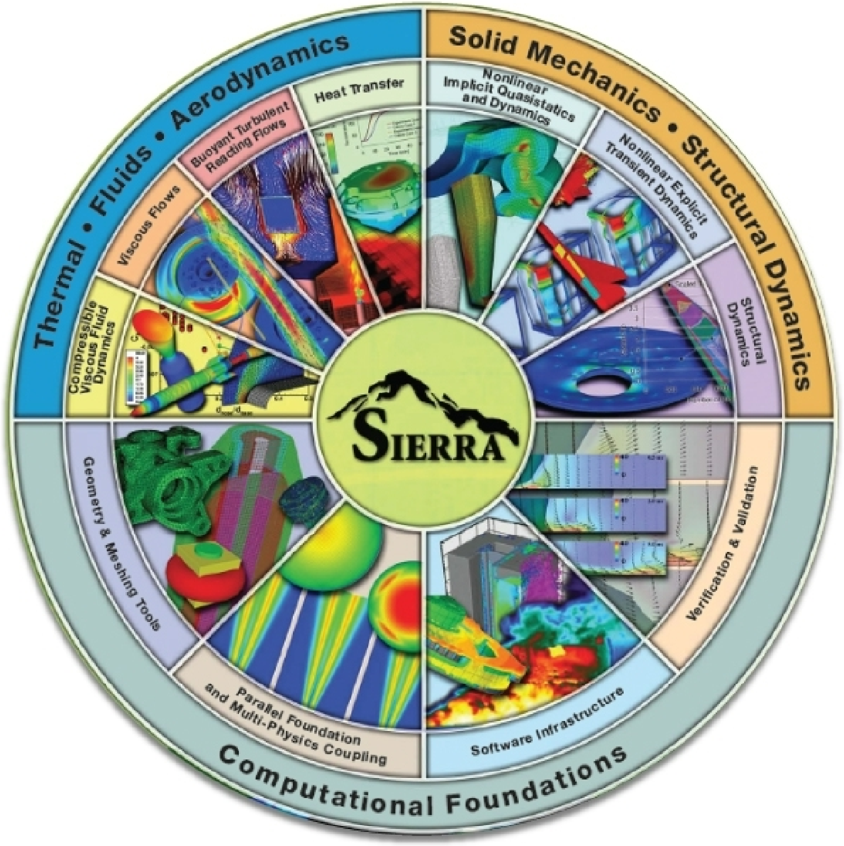




Sierra/SD, Rapid Optimization Library (ROL), and Inverse Methods

Inverse Methods in Sierra Mechanics

Inverse solution types via Sierra/SD linked to Rapid Optimization Library (ROL)



Objective function,
Derivative operators

→

←

Next iteration
of design variables

RAPID OPTIMIZATION LIBRARY

PDE-Constrained Optimization

Abstract optimization formulation

$$\underset{\boldsymbol{u},\boldsymbol{p}}{\text{minimize}} \quad J(\boldsymbol{u},\boldsymbol{p})$$

$$\text{subject to} \quad \boldsymbol{g}(\boldsymbol{u},\boldsymbol{p}) = 0$$

Objective function

PDE constraint

$$\mathcal{L}(\boldsymbol{u},\boldsymbol{p},\boldsymbol{w}) := J + \boldsymbol{w}^T\boldsymbol{g}$$

Lagrangian

$$\begin{Bmatrix} \mathcal{L}_u \\ \mathcal{L}_p \\ \mathcal{L}_w \end{Bmatrix} = \begin{Bmatrix} J_u + g_u^T w \\ J_p + g_p^T w \\ g \end{Bmatrix} = \{0\}$$

First order optimality conditions

$$\begin{bmatrix} \mathcal{L}_{uu} & \mathcal{L}_{up} & g_u^T \\ \mathcal{L}_{pu} & \mathcal{L}_{pp} & g_p^T \\ g_u & g_p & 0 \end{bmatrix} \begin{Bmatrix} \delta u \\ \delta p \\ w^\star \end{Bmatrix} = - \begin{Bmatrix} J_u \\ J_p \\ g \end{Bmatrix}$$

Newton iteration

$$W\Delta p = -\hat{J}',$$

$$W = g_p^T g_u^{-T}(\mathcal{L}_{uu}g_u^{-1}g_p - \mathcal{L}_{up}) - \mathcal{L}_{pu}g_u^{-1}g_p + \mathcal{L}_{pp}$$

Hessian calculation

$\boldsymbol{u}$ ~ response
$\boldsymbol{p}$ ~ design parameters
$\boldsymbol{w}$ ~ Lagrange multipliers

Discrete Equations for Inverse Problem

	Objective Functions	Governing Equations
Time	$J(\{\boldsymbol{u}\},\{\boldsymbol{p}\}) = \frac{\kappa}{2}\left(\{\boldsymbol{u}\} - \{\boldsymbol{u}_m\}\right)^{\mathrm{T}}[Q]\left(\{\boldsymbol{u}\} - \{\boldsymbol{u}_m\}\right) + \mathscr{R}(\{\boldsymbol{p}\})$	$\boldsymbol{g}(\boldsymbol{u},\boldsymbol{p}) = \boldsymbol{C}(\boldsymbol{p})\dot{\boldsymbol{u}} + \boldsymbol{K}(\boldsymbol{p})\boldsymbol{u} - \boldsymbol{f}(\boldsymbol{p})$
Frequency	$J(\{\tilde{\boldsymbol{u}}\},\{\boldsymbol{p}\}) = \frac{\kappa}{2}\sum_{k=1}^{N}\left(\tilde{\boldsymbol{u}}_k - \tilde{\boldsymbol{u}}_{mk}\right)^{\mathrm{H}}[Q]\left(\tilde{\boldsymbol{u}}_k - \tilde{\boldsymbol{u}}_{mk}\right) + \mathscr{R}(\{\boldsymbol{p}\})$	$\boldsymbol{g}(\boldsymbol{u},\boldsymbol{p}) = \left[\boldsymbol{K}(\boldsymbol{p}) + i\omega\boldsymbol{C}(\boldsymbol{p})\right]\boldsymbol{u} - \boldsymbol{f}(\boldsymbol{p})$

Choose frequency domain to attempt inversion with FDTR data

Optimization Procedure

PDE and Objective

$$\boldsymbol{g}(\boldsymbol{u},\boldsymbol{p}) = \left[\boldsymbol{K}(\boldsymbol{p}) + i\omega \boldsymbol{C}(\boldsymbol{p})\right]\boldsymbol{u} - \boldsymbol{f}(\boldsymbol{p})$$

$$J(\boldsymbol{u}) = \frac{1}{2}\left|\boldsymbol{u} - \boldsymbol{u}_m\right|^2$$

1. Solve PDE for $\boldsymbol{u}$ (forward solution)

2. Use forward solution with J and $J_{\boldsymbol{u}}$ (known) to find $\boldsymbol{w}$ (adjoint solution)

3. Use adjoint solution along with $J_{\boldsymbol{p}}$ and $\boldsymbol{g}_{\boldsymbol{p}}$ (both known) to find current gradient

4. Pass current objective, gradient to ROL

Optimality conditions

$$\mathcal{L}_{\boldsymbol{u}} = J_{\boldsymbol{u}} + \boldsymbol{g}_{\boldsymbol{u}}^T \boldsymbol{w} = 0$$

$$\mathcal{L}_{\boldsymbol{p}} = J_{\boldsymbol{p}} + \boldsymbol{g}_{\boldsymbol{p}}^T \boldsymbol{w} = 0$$

$$\mathcal{L}_{\boldsymbol{w}} = \boldsymbol{g} = 0$$

ROL

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Frequency-Domain Material and Force Optimization

Governing equation for time-harmonic temperature oscillations:

$$i\omega\rho c_p T - \kappa\nabla^2 T = 0$$

Discretized heat equation:

$$\mathbf{g}(\mathbf{u},\mathbf{p}) = [\mathbf{K}(\mathbf{p}) + i\omega\mathbf{C}(\mathbf{p})]\,\hat{T} - \mathbf{f} = \mathbf{0}$$

Thermal conductivity, heat capacity, heat flux:

$$\mathbf{K}(\mathbf{p}) = \int_\Omega \kappa \boldsymbol{\nabla}\mathbf{N} \cdot \boldsymbol{\nabla}\mathbf{N}^T\, dV$$

$$\mathbf{C}(\mathbf{p}) = \int_\Omega \rho c_p \mathbf{N}\mathbf{N}^T\, dV$$

$$\mathbf{f} = -\int_{\partial\Omega} \mathbf{q}\cdot\mathbf{n}\mathbf{N}^T\, dS$$

Discretized temperature field:

$$\hat{T}(\mathbf{x}) = \sum_{k=1}^{n} \hat{T}_i N_i(\mathbf{x})$$

Derivatives with respect to κ, c_p:

$$\mathbf{K}_\kappa = \frac{1}{\kappa}\mathbf{K}$$

$$\mathbf{C}_{\rho c_p} = \frac{1}{\rho c_p}\mathbf{C}$$

Verification and Inversion for Thermophysical Properties

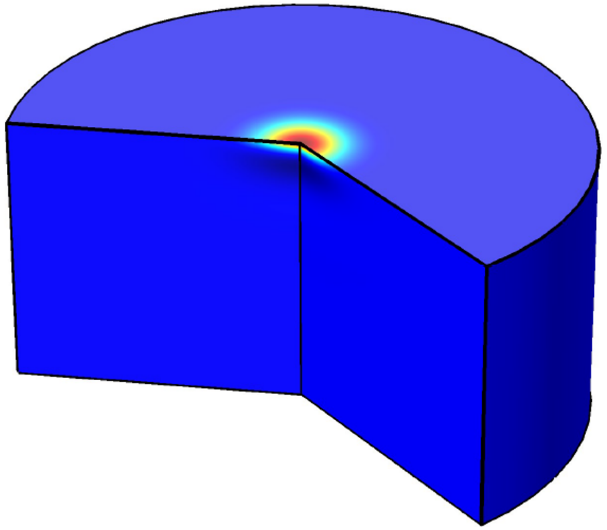
Verification: Sierra/SD vs COMSOL

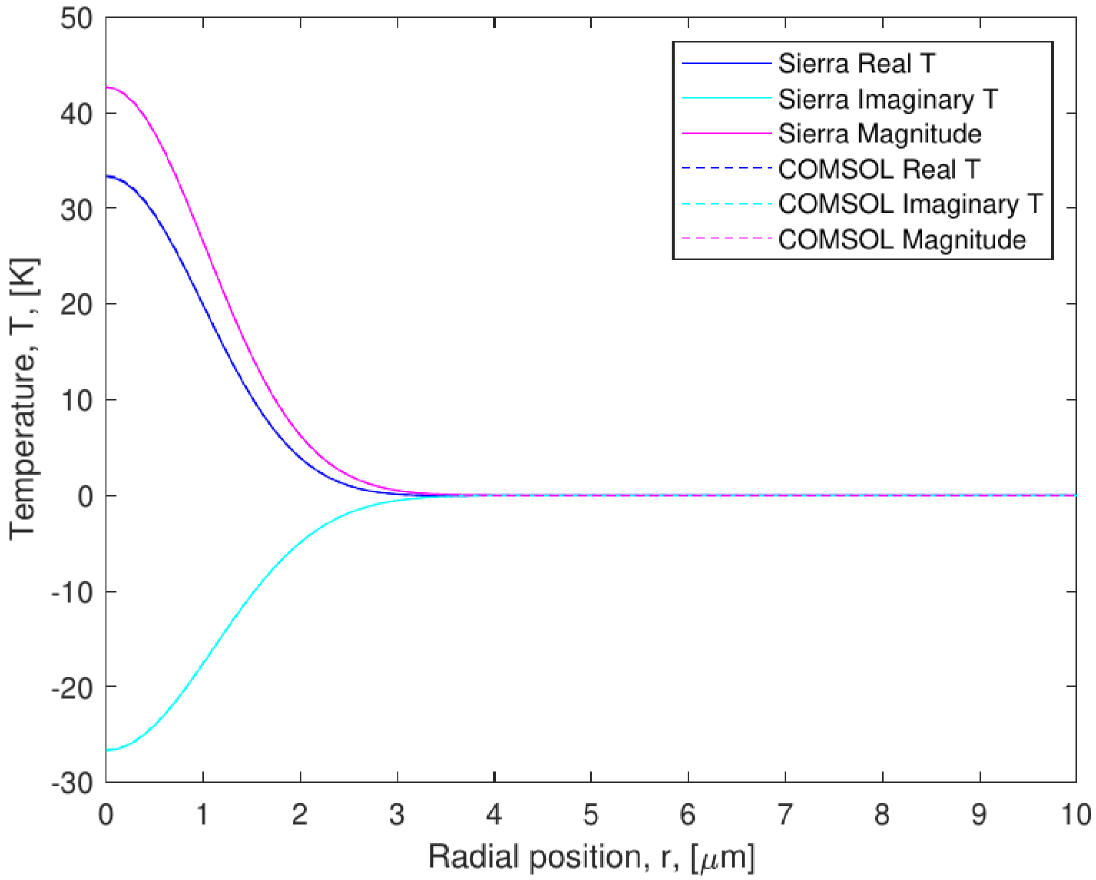
Cylinder with uniform material properties

Gaussian heat flux applied to top surface

Insulating condition applied to bottom and outer surfaces

Agreem
precisio





Inverse Problem: Geometry

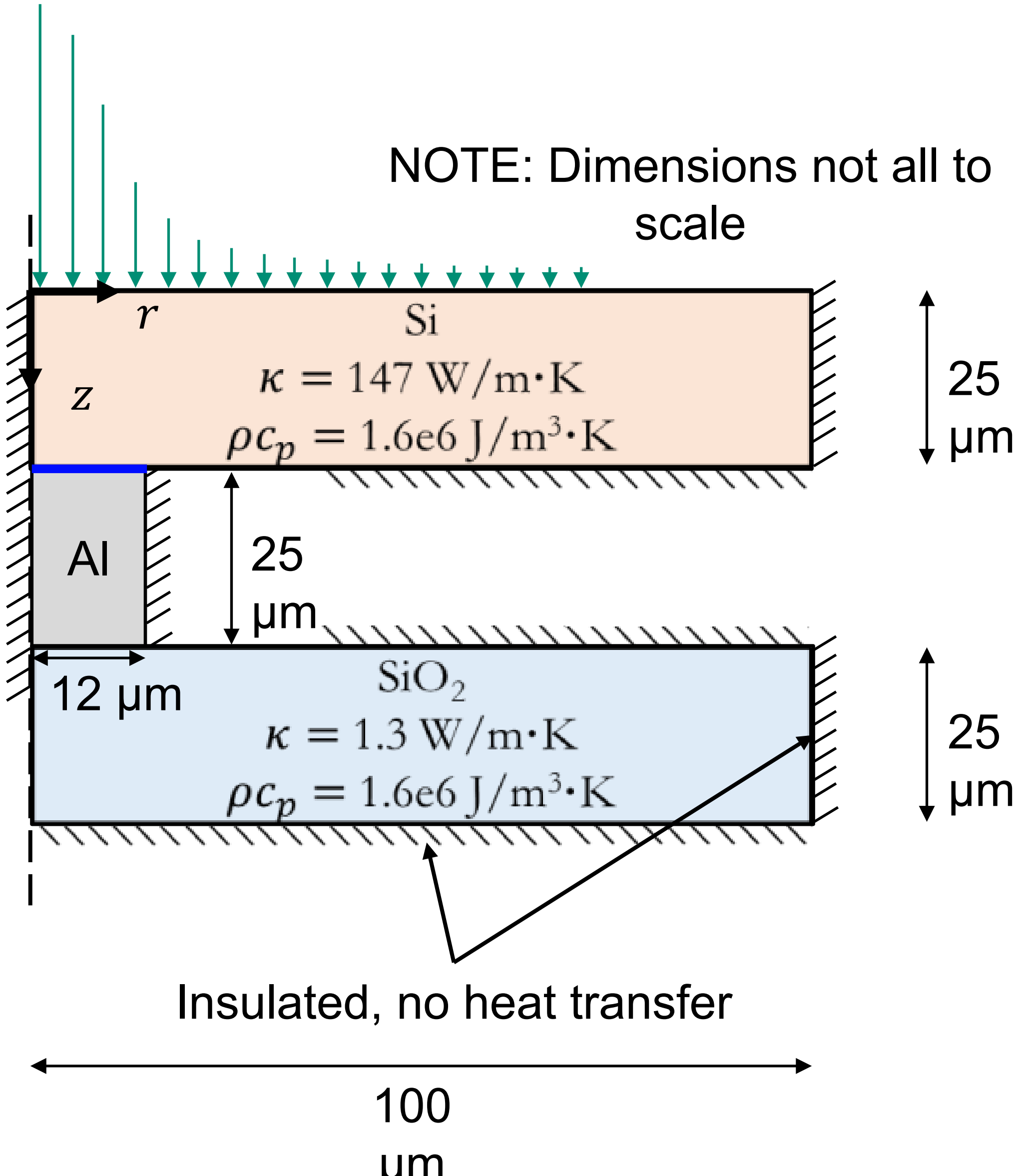
Cylindrical geometry separated into three layers:
- Top: silicon
- Middle: aluminum
- Bottom: silicon dioxide

Thin layer (100 nm) representing possible de-bond
- Bonded: aluminum
- De-bonded: air

Gaussian heat source applied to small region on top surface (2 μm beam radius, $1/e^2$)

Simultaneous runs at 500 Hz and 1 kHz

Nodal temperature data considered in small region on top surface



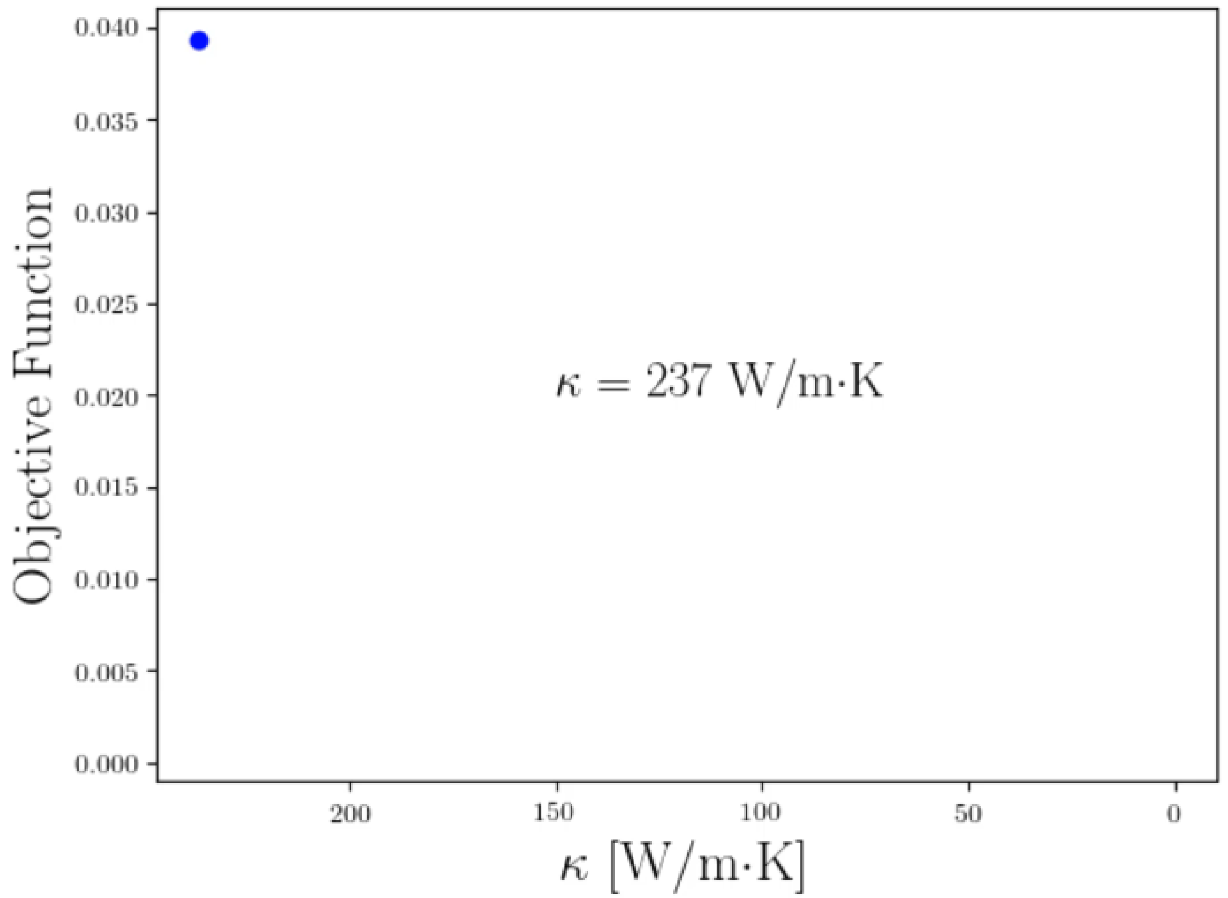
Inverse Problem: Results

Flat objective function for much of parameter space

Rapid convergence to objective as material properties in thin de-bond approach material properties of air

Simple material identification: **thousands of iterations** to converge

Damage identification: **only a couple of iterations** to converge



$$\kappa = \kappa^{\text{lo}} + (\kappa^{\text{hi}} - \kappa^{\text{lo}})\phi^{p_1}$$

$$\rho c_p = \rho c_p^{\text{lo}} + (\rho c_p^{\text{hi}} - \rho c_p^{\text{lo}})\phi^{p_2}$$

$$\phi \in [0, 1]$$

```
Quasi-Newton Method with Limited-Memory BFGS
Line Search: Cubic Interpolation satisfying Null Curvature Condition
  iter  value          gnorm          snorm          #fval     #grad     ls_#fval  ls_#grad
  0     1.239728e-04   1.957024e-06
  1     1.239728e-04   1.957021e-06   1.957024e-06   2         2         1         0
  2     1.812705e-24   0.000000e+00   9.915583e-01   3         3         1         0
Optimization Terminated with Status: Converged
```

Conclusions and Future Work

Conclusions and Future Work

Conclusions

- FDTR may be used to assess material bond integrity
- Sierra/SD can be used for massively parallel thermal simulations in frequency domain
- Inverse methods may be effective in determining unknown material properties in practical geometries

Future Work

- Investigate different frequencies for heat flux applied to top surface
- Examine different thicknesses for top layer
- Use temperature phase data (instead of more ideal nodal temperature data) from top surface
- Try more complicated geometries (e.g., less symmetry, an array of interconnects, etc.)
- Try to detect partial de-bonds (i.e., heterogeneous properties in thin layers)

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LDRD
LABORATORY DIRECTED
RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS

Coworkers at SNL

- Greg Pickrell (PI)

Questions?