Some Researches of Thermal Problem in 3D ICs

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Outline

1. Thermal analysis problems in 3D ICs
2. Deterministic analysis of the thermal problems
3. Uncertainty analysis of the thermal problems
4. Interval inversion analysis of the thermal problems
5. Summary
3D ICs

Die stacked by TSV

TSV

TSV photo

F2B TSV process
1. Thermal problem in 3D ICs

• Heat dissipation is obstructive due to multi-die structure of 3D ICs. Accumulated hot point within 3D IC can worsen the performance or even destroy the ICs.

• It is difficult or even impossible to measure temperature or thermal stress in the interior of 3D ICs. Therefore, numerical simulation is a popular way to analyze the thermal problems of 3D ICs.

• A lots of literatures about numerical analysis of thermal problems in 3D ICs have been published in recent years. But there also exists quite big difference among them. So, the analysis methodology still needs to be studied.
Outline

1. Thermal analysis problems in 3D ICs
2. Deterministic analysis of the thermal problems
3. Uncertainty analysis of the thermal problems
4. Interval inversion analysis of the thermal problems
5. Summary
2. Deterministic analysis of thermal problem

- Firstly, deterministic numerical simulation with Finite Element Analysis (FEA) is studied to be a bases for uncertainty analysis.
- A model with certainty parameters, as an example, is shown as following:

- Heat sink is on die 1 and the ambient temperature is 25°C.
- Die 4 is the heating source with heating power of 1mW.
- The diameter of TSV is 5 µm and the pitch between two TSV is 70 µm.
How to make a compatible mash between TSV and dies

Diagram showing two squares with dots and arrows pointing downwards to shaded areas.
Temperature and Thermal stresses around TSV

model

temperature

thermal stress
Affection of TSV parameters

Temp. vs different diameters and pitches of TSVs

Stress. vs different diameters and pitches of TSVs
Deficiency of the deterministic FEA

- In general, there are some bigger errors between FEA and experimental measurement results.
- That is mainly because that, in practice engineering problems, material properties, geometry and boundary conditions of a structure may experience fluctuations, due to measurement and manufacturing errors, model inaccuracies and/or physical imperfections, which may significantly affect the response.
- Even though uncertainty factor of single parameter may be in a smaller range, the total uncertainties of all parameters may induce a bigger errors to the analysis, especial to analyze a composited structure like 3D ICs.
3. Uncertainty analysis of the thermal problems

- It has been recognized that there are three main approaches to describe uncertainties:
  - The first one and possibly the most widely used method is the probabilistic approach. But it gives reliable results only when sufficient experimental data are available.
  - The other more recent uncertainty analysis is based on concept of fuzzy sets which introduces the notation of a membership function which characterizes the degree of belonging to a set.
  - The third methodology is known as set-theoretic approach including in it convex modeling, ellipsoidal modeling, and interval analysis.
- Specifically, interval analysis may be considered as the most widely adopted analytic tool among non-probabilistic analysis.
The mathematical definitions and notations of IAs are extended from set theory and order numerical sets called intervals.

IA represents the uncertainty by replacing single values (fixed-point) with intervals to deal with presence of approximate numbers, fluctuating parameters, error bounds, uncertain experimental data and so on.

IA provides both upper and lower bounds on the effects all uncertainties have on a computed quantity.

IA is extremely attractive due to its philosophy of simplicity providing analytically rigorous enclosures of the solution.
Principle of interval analysis

- Contrary to the field of real numbers which is denoted by $R$, the field of all closed real interval numbers is denoted by a subset of $R$ of the form:

$$x \equiv [x] = [\underline{x}, \overline{x}] = \{x | \underline{x} \leq x \leq \overline{x}, x \in R\}$$

is called an interval variable with upper and lower bounds $[\underline{x}, \overline{x}]$.

- The interval could be represented by its midpoint (or central value or mean) and by the deviation (or half-width) i.e.:

$$\text{mid}\{x\} \equiv x^C = \frac{\underline{x} + \overline{x}}{2}; \quad \text{dev}\{x\} \equiv \Delta x = \frac{\overline{x} - \underline{x}}{2}$$
Principle of interval analysis

Therefore, interval can be also represented as:

\[ x = \text{mid}\{x\} + \text{dev}\{x\} = x^C + \Delta x = \frac{-}{2} + \frac{-}{2} \]

• The major focus of IA is to develop practical interval algorithms that produce sharp (as narrow as possible) or nearly sharp bounds on the solution of numerical computing problems.
Based on the concept of interval analysis, original FEA equations should be firstly changed into a new one for interval analysis.

In general, three types of governing equations of heat transfer for interval analysis should be took out:

- **Steady** state heat transfer equation of interval analysis
- **Transient** state heat transfer equation of interval analysis
- **Hyperbolic** state (heat wave) heat transfer equation of interval analysis
Governing equation of interval analysis - Steady state

\[ K(\varphi)T = F(\varphi) \]

where:

\[
\begin{aligned}
K(\varphi) &= K(\varphi^c) + \Delta K \\
F(\varphi) &= F(\varphi^c) + \Delta F
\end{aligned}
\]

Decompose formula:

\[ K(\varphi^c)T = F(\varphi^c) \]
\[ K(\varphi^c)\Delta T = \Delta F - \Delta K \cdot T \]

where:

\[
\begin{aligned}
K(\varphi^c) &= \sum_{j=1}^{N} K_j(\varphi^c) \\
\Delta K &= \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\partial K_j}{\partial \varphi_i} \Delta \varphi_i e_{ji} \\
F(\varphi^c) &= F_T + F_q + F_h + F_Q \\
\Delta F &= \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\partial F_j}{\partial \varphi_i} \Delta \varphi_i e_{ji}
\end{aligned}
\]

Upper and lower bounds of temperatures:

\[ \overline{T} = T^c + \Delta T \quad T = T^c - \Delta T \]
Governing equation of interval analysis - Transient state

\[ C(\varphi) \dot{T} + K(\varphi)T = F(\varphi) \]

Where:

\[ C(\varphi) = C(\varphi^c) + \Delta C \]
\[ K(\varphi) = K(\varphi^c) + \Delta K \]
\[ F(\varphi) = F(\varphi^c) + \Delta F \]

Decompose formula:

\[ C(\varphi^c) \dot{T} + K(\varphi^c)T = F(\varphi^c) \]
\[ C(\varphi^c) \Delta \dot{T} + K(\varphi^c)\Delta T = \Delta F_t \]

Where:

\[ \Delta F_t = \Delta F - (\Delta C \cdot \dot{T} + \Delta K \cdot T) \]
\[ C(\varphi^c) = \sum_{j=1}^{N} C_j(\varphi^c) \]
\[ \Delta C = \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\partial C_j}{\partial \varphi_i} \Delta \varphi_i e_{ji} \]
\[ K(\varphi^c) = \sum_{j=1}^{N} K_j(\varphi^c) \]
\[ \Delta K = \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\partial K_j}{\partial \varphi_i} \Delta \varphi_i e_{ji} \]
\[ F(\varphi^c) = F_T + F_q + F_h + F_Q \]
\[ \Delta F = \sum_{j=1}^{N} \sum_{i=1}^{n} \frac{\partial F_j}{\partial \varphi_i} \Delta \varphi_i e_{ji} \]

Upper and lower bounds of temperatures:

\[ \overline{T}_t = T_t^c + \Delta T_t \quad \underline{T}_t = T_t^c - \Delta T_t \]
Governing equation of interval analysis - Hyperbolic state

\[ \tau C(\varphi) \ddot{T} + C(\varphi) \dot{T} + K(\varphi) T = F(\varphi) \]

Where:
\[
\begin{align*}
C(\varphi) &= C(\varphi^c) + \Delta C \\
K(\varphi) &= K(\varphi^c) + \Delta K \\
F(\varphi) &= F(\varphi^c) + \Delta F
\end{align*}
\]

Decompose formula:

\[ \tau C(\varphi^c) \ddot{T} + C(\varphi^c) \dot{T} + K(\varphi^c) T = F(\varphi^c) \]
\[ \tau C(\varphi^c) \Delta \ddot{T} + C(\varphi^c) \Delta \dot{T} + K(\varphi^c) \Delta T = \Delta F_1 \]

Upper and lower bounds of temperatures:

\[ \overline{T}_t = T_t^c + \Delta T_t \]
\[ \underline{T}_t = T_t^c - \Delta T_t \]
Model of interval analysis for TSV temperature field

- The thickness of TSV, SiO2, and Silicon is 2.5µm, 0.7µm and 25µm, respectively. The height of TSV is 50µm.
- Assuming the up die is equivalent heat source and bottom die is in the consistent temperature of 40°C.
- Try to obtain the temperature distribution of TSV in steady, transient, and hyperbolic states.
Interval parameters for the calculation

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Interval values (Cu   SiO2  Si polymer)</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>[8843.67,9022.33;2178.99,2223.01;2306.7,2252.3;1132.6,1155.4]</td>
<td>Kg/m²</td>
</tr>
<tr>
<td>Sp. heat</td>
<td>$c$</td>
<td>[382.14, 398.66; 702.9, 717.1; 695.97, 710.03; 1683.00, 1717.00]</td>
<td>J/(Kg · °C)</td>
</tr>
<tr>
<td>Heat</td>
<td>$q$</td>
<td>[7.992e7,8.008e7]</td>
<td>W/m²</td>
</tr>
<tr>
<td>Co. ht Cond.</td>
<td>$k$</td>
<td>[394.02,401.98; 1.386,1.414; 151.47,154.53; 24.75,25.25]</td>
<td>W/(m · °C)</td>
</tr>
<tr>
<td>Co. ht Conv.</td>
<td>$h$</td>
<td>[29.7, 30.3]</td>
<td>W/(m² · °C)</td>
</tr>
<tr>
<td>Initial temp.</td>
<td>$T_0$</td>
<td>[24.5, 25.5]</td>
<td>°C</td>
</tr>
<tr>
<td>Bound. temp.</td>
<td>$\bar{T}$</td>
<td>[36, 44]</td>
<td>°C</td>
</tr>
<tr>
<td>Ambient temp.</td>
<td>$T_a$</td>
<td>[24.5, 25.5]</td>
<td>°C</td>
</tr>
</tbody>
</table>
Results of interval analysis - Steady state

Temperature (°C)

Distance to the center of TSV (um)

Upper bound

Lower bound

ANSYS certainty Analysis

Path 2
Result of interval analysis - Transient state

Temperature °C vs Response time

- Cu 下限
- Cu 上限
- SiO2 下限
- SiO2 上限
- Si 下限
- Si 上限

×1.5E-6s
Result of interval analysis - Hyperbolic state
Different high aspect ratio vs. temperature distribution of TSV array
Different TSV pitches vs. temperature distribution of TSV array
4. Interval inversion analysis

• In some cases, inversed analysis is particularly needed for tackling the problems where the inhomogeneities of the sample are insufficiently well understood.

• Because inversed analysis typically involves the estimation of certainty quantities based on indirect measurements, in order to avoid the estimation process ill-posed, inversed analysis should be combined with interval analysis to ensure efficiency and correctness.
Procedures of interval inversion analysis

• Any unknown reversal parameter can be written as a vector (object function):

\[
\{\varphi\}^T = \left\{\{k\}^T, \{\bar{k}\}^T, \{q\}^T, \{\bar{q}\}^T, \{T\}^T, \{\bar{T}\}^T\right\}
\]

• Then Gaussian-Newton iteration method can be used to solve the inversed problem

• The concept of Gaussian-Newton iteration method is to use series expansion to replace the mathematic model and to minimize the sum of squared residuals during many times of iteration
Flow chart for computation of interval inversion analysis

start

Input interval variables, n=0

Interval FEA equations

Building object function

Gaussian-Newton reversal

Convergence test

n=n+1

end

N

Y
How to balance the calculation time and accuracy

- Temperature is a bridge parameter to connect the other thermal parameters during the analysis.

- The temperature during the calculation can be written as:

\[ T_p = (1 + \sigma) \cdot T_e \]

Where \( T_p \) is temperature with error, \( T_e \) is the true temperature, and the \( \sigma \) is so called information error that determines the calculation time and accuracy.

- Therefore, the analysis results is dependent on the input value of information error.
The thickness of TSV, SiO2, and Silicon is 2.5µm, 0.7µm and 25µm, respectively. The height of TSV is 50µm. Assuming the up die is equivalent heat source and bottom die is in the consistent temperature of 40°C.

Reversal start values are $k = 35 \text{ W/(m} \cdot \text{oC)}$, $q = 500 \text{ W/m}^2$, $\bar{T} = 5.0\text{oC}$

Try to find reversal interval
Interval parameters for TSV analysis

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Interval values (Cu SiO2 Si polymer)</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co. ht Condu.</td>
<td>$k$</td>
<td>[394.02,401.98; 1.386,1.414; 151.47,154.53; 24.75,25.25]</td>
<td>W/(m⋅°C)</td>
</tr>
<tr>
<td>Density</td>
<td>$\rho$</td>
<td>[8843.67,9022.33;2178.99,2223.01;2306.7,2252.3;1132.6,1155.4]</td>
<td>Kg/m²</td>
</tr>
<tr>
<td>Spec. heat</td>
<td>$c$</td>
<td>[382.14, 389.86; 702.9, 717.1; 695.97,710.03; 1683.00,1717.00]</td>
<td>J/(Kg⋅°C)</td>
</tr>
<tr>
<td>Heat</td>
<td>$q$</td>
<td>[7.992e7,8.008e7]</td>
<td>W/m²</td>
</tr>
<tr>
<td>Co. ht Condv.</td>
<td>$h$</td>
<td>[29.7, 30.3]</td>
<td>W/(m²⋅°C)</td>
</tr>
<tr>
<td>Initial temp.</td>
<td>$T_0$</td>
<td>[24.5, 25.5]</td>
<td>°C</td>
</tr>
<tr>
<td>Bound. temp.</td>
<td>$\bar{T}$</td>
<td>[36, 44]</td>
<td>°C</td>
</tr>
<tr>
<td>Ambient temp.</td>
<td>$T_a$</td>
<td>[24.5, 25.5]</td>
<td>°C</td>
</tr>
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</table>
# Results of interval inversion analysis—steady state

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>Reversed $k$</th>
<th></th>
<th></th>
</tr>
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<tbody>
<tr>
<td></td>
<td></td>
<td>$\sigma = 0.01$</td>
<td>$\sigma = 0.05$</td>
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</tr>
<tr>
<td></td>
<td>reversed value</td>
<td>relative error</td>
<td>reversed value</td>
<td>relative error</td>
</tr>
<tr>
<td>$k_1$</td>
<td>[394.02, 401.98]</td>
<td>381.14, 388.89</td>
<td>0.033</td>
<td>336.86, 343.91</td>
</tr>
<tr>
<td>$k_2$</td>
<td>[1.386, 1.414]</td>
<td>1.3724, 1.4001</td>
<td>0.010</td>
<td>1.3205, 1.3472</td>
</tr>
<tr>
<td>$k_3$</td>
<td>[151.47, 154.53]</td>
<td>147.65, 150.65</td>
<td>0.025</td>
<td>134.11, 136.90</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>Reversed $q$</th>
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<tbody>
<tr>
<td></td>
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<td>$\sigma = 0.01$</td>
<td>$\sigma = 0.05$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>reversed value</td>
<td>relative error</td>
<td>reversed value</td>
<td>relative error</td>
</tr>
<tr>
<td>$q$</td>
<td>[7.92e7, 8.08e7]</td>
<td>8.143e7, 8.305e7</td>
<td>0.028</td>
<td>9.033e7, 9.203e7</td>
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</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>Reversed $\tilde{T}$</th>
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<tbody>
<tr>
<td></td>
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<td>$\sigma = 0.01$</td>
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<td>relative error</td>
<td>reversed value</td>
<td>relative error</td>
</tr>
<tr>
<td>$\tilde{T}$</td>
<td>[36.00, 44.00]</td>
<td>36.380, 44.689</td>
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<td>37.804, 47.540</td>
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### Results of interval inversion analysis—steady state

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>Combined Reversed $K$ and $q$</th>
<th>$\sigma = 0.01$</th>
<th>$\sigma = 0.05$</th>
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<tbody>
<tr>
<td></td>
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<td></td>
<td>reversed value</td>
<td>reversed value</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>relative error</td>
<td>relative error</td>
</tr>
<tr>
<td>$k_1$</td>
<td>[394.02, 401.98]</td>
<td>[381.39, 389.14]</td>
<td>0.032</td>
<td>0.032</td>
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<tr>
<td>$k_2$</td>
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<td>[1.3729, 1.4010]</td>
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<td>0.009</td>
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<tr>
<td>$k_3$</td>
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<td>[147.74, 150.75]</td>
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<td>0.025</td>
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<tr>
<td>$q$</td>
<td>[7.92e7, 8.08e7]</td>
<td>[7.925e7, 8.085e7]</td>
<td>0.001</td>
<td>0.001</td>
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### Results of interval inversion analysis – transient state

<table>
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<tr>
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<th>Relative error ($\sigma = 0.01$)</th>
<th>Reversed value ($\sigma = 0.05$)</th>
<th>Relative error ($\sigma = 0.05$)</th>
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</thead>
<tbody>
<tr>
<td>$k_1$</td>
<td>[394.02, 401.98]</td>
<td>[398.48, 406.62]</td>
<td>0.011</td>
<td>[416.33, 425.18]</td>
<td>0.057</td>
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<tr>
<td>$k_2$</td>
<td>[1.386, 1.414]</td>
<td>[1.3713, 1.4034]</td>
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<td>[1.3155, 1.3629]</td>
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<td>[152.98, 156.16]</td>
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<td>[159.05, 162.70]</td>
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<table>
<thead>
<tr>
<th>Variable</th>
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<th>Relative error ($\sigma = 0.01$)</th>
<th>Reversed value ($\sigma = 0.05$)</th>
<th>Relative error ($\sigma = 0.05$)</th>
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</thead>
<tbody>
<tr>
<td>$q$</td>
<td>[7.92e7, 8.08e7]</td>
<td>[8.0799e7, 8.0801e7]</td>
<td>0.01</td>
<td>[8.3999e7, 8.4001e7]</td>
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<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>Reversed value ($\sigma = 0.01$)</th>
<th>Relative error ($\sigma = 0.01$)</th>
<th>Reversed value ($\sigma = 0.05$)</th>
<th>Relative error ($\sigma = 0.05$)</th>
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<tr>
<td>$k_1$</td>
<td>[394.02, 401.98]</td>
<td>[398.57, 406.67]</td>
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<td>[416.74, 425.43]</td>
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<td>[8.4840e7, 8.4853e7]</td>
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# Results of interval inversion analysis – hyperbolic state

<table>
<thead>
<tr>
<th>Variable</th>
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<th>$\sigma$</th>
<th>Reversed values</th>
<th>relative error</th>
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<tbody>
<tr>
<td>$k_1$</td>
<td>[394.02,401.98]</td>
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<td>[384.03,392.10]</td>
<td>[384.03,392.10]</td>
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<td>0.05</td>
<td>[346.65,352.41]</td>
<td>[346.65,352.41]</td>
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<td>$k_2$</td>
<td>[1.386,1.414]</td>
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<td>[1.3639,1.3925]</td>
<td>[1.3639,1.3925]</td>
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<td>[148.28,151.26]</td>
<td>[148.28,151.26]</td>
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<td>0.05</td>
<td>[136.57,139.38]</td>
<td>[136.57,139.38]</td>
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</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>$\sigma$</th>
<th>Reversed values</th>
<th>relative error</th>
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<tbody>
<tr>
<td>$\bar{T}$</td>
<td>[36.00, 44.00]</td>
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<td>[35.267, 43.408]</td>
<td>[35.267, 43.408]</td>
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<td>0.05</td>
<td>[32.336, 41.039]</td>
<td>[28.827, 31.060]</td>
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</table>
Results of interval inversion analysis – hyperbolic state

<table>
<thead>
<tr>
<th>Variable</th>
<th>True value</th>
<th>$\sigma$</th>
<th>$D_0$</th>
<th>$\overline{D}_0$</th>
<th>relative error</th>
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</thead>
<tbody>
<tr>
<td>$k_1$</td>
<td>[394.02,401.98]</td>
<td>0.01</td>
<td>[383.97,391.88]</td>
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<td>0.025</td>
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<tr>
<td></td>
<td></td>
<td>0.05</td>
<td>[346.51,351.35]</td>
<td>[346.51,351.35]</td>
<td>0.123</td>
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<td>$k_2$</td>
<td>[1.386,1.414]</td>
<td>0.01</td>
<td>[1.3813,1.4094]</td>
<td>[1.3813,1.4094]</td>
<td>0.003</td>
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<tr>
<td></td>
<td></td>
<td>0.05</td>
<td>[1.3639,1.3926]</td>
<td>[1.3639,1.3926]</td>
<td>0.016</td>
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<td>$k_3$</td>
<td>[151.47,154.53]</td>
<td>0.01</td>
<td>[148.29,151.28]</td>
<td>[148.29,151.28]</td>
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<td>[136.60,139.47]</td>
<td>[136.60,139.47]</td>
<td>0.098</td>
</tr>
<tr>
<td>$\overline{T}$</td>
<td>[36.00,44.00]</td>
<td>0.01</td>
<td>[35.533,43.137]</td>
<td>[35.533,43.137]</td>
<td>0.017</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.05</td>
<td>[28.827,31.060]</td>
<td>[28.827,31.060]</td>
<td>0.251</td>
</tr>
</tbody>
</table>
Summary

- Considering the uncertainties of thermal parameters in practice thermal problems of 3D ICs, interval and interval inversion analysis algorithms were given for studying heat conduction problems in steady, transient, and hyperbolic states.

- Even though the results of interval analysis may not be the exact values, they belong to the interval indeed. This is very important to design the operation limitation of 3D ICs.

- Interval inversion analysis can solve the problem that some material properties are unknown or can not be determined previously. That is very useful to thermal problems in 3D ICs.
Thank you very much for your attention!