ITEA Office
High Tech Campus 69 - 3
5656 AG Eindhoven
The Netherlands
T + 31 88 003 6136
E info@itea3.org
W www.itea3.org

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Deliverable 6.3: Best practice guidelines

COMPAS

Compact modelling of high-tech systems for health management and optimization **a**long the **s**upply chain

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Leading Authors		
Name	*Beneficiary name*	*Contact email*
Ghanshyam Gadhiya	Fraunhofer ENAS	ghanshyam.gadhiya@enas.fraunhofer.de
Reviewers		
Name	*Beneficiary Name*	*Contact email*
Martin Niessner	Infineon Technologies AG	martin.niessner@infineon.com
Michiel van Soestbergen	NXP Semiconductors	michiel.van.soestbergen@nxp.com

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List of abbreviations and acronyms

Abbreviations	
CTE	Coefficient of Thermal Expansion
CSED	Creep Strain Energy Density
Dx.y	Deliverable x.y of the COMPAS project
FC	Flip Chip
FE	Finite Element
FEA	Finite Element Analysis
FEM	Finite Element Model / Method
FMEA	Failure Mode and Effect Analysis
FMI	Functional Mock-up Interface
FOM	Full Order Model
IC	Integrated Circuit
PCB	Printed Circuit Board
PSED	Plastic Strain Energy Density
RDL	ReDistribution Layer
ROM	Reduced Order Model
Tg	Glass transition Temperature
Tx.y	Task x.y of the COMPAS project
UBM	Under Bump Metallization
WLCSP	Wafer Level Chip Scale Package
WPx	Work package x of the COMPAS project

Partner acronyms			
FhG-ENAS	Fraunhofer ENAS	MSC	MSC Software
Eesy	Eesy-Innovation	NXP	NXP Semiconductors NL B.V.
IFAG	Infineon	Reden	Reden B.V.
JADE	JADE Hochschule	SIEM	Siemens Munich
KU Leuven	Katholieke Universiteit Leuven	SISW	Siemens Industry Software
MCE	MicroConsult Engineering	TUD	Delft University of Technology
		Tue	Eindhoven University of Technology

Executive Summary

Thermomechanical Finite Element Analysis (FEA) is a crucial tool for understanding how microelectronic components behave under thermal and mechanical stress. The analysis focuses on three levels of reliability: 1st level (inside the package), 2nd level (board-level reliability on an unconstrained PCB), and 3rd level (board-level reliability on a PCB constrained inside a housing). The workflow of thermomechanical FEA involves three main stages: preprocessing, processing, and post-processing. In preprocessing, various steps such as defining material properties, geometry, meshing, loading, and boundary conditions are undertaken. The processing or solution stage solves the analysis based on the prepared model, and post-processing is utilized for analysing, plotting, evaluating, verifying, and reporting results.

The first step in preprocessing is defining the geometry and mesh. Different model types (2D, 3D) and boundary conditions can be chosen based on structure geometry. The focus of this deliverable is on full 3D FE models because the final aim is generating compact models that can be reintegrate into a larger 3rd level 3D FE model. The next step consists of defining material properties. Material modelling is crucial and involves material properties for different materials using appropriate constitutive models. The material orientation, time, temperature, and rate dependency need to be considered as the material responses can be anisotropic, viscoelastic, or hyperelastic. The final step is to apply boundary conditions. Here, mechanical constraints need to prevent rigid body motion. Recommendations include considering clamping during high-temperature steps and accounting for residual stresses. Finally, an appropriate temperature profile is applied to the model.

After preprocessing, the solution stage can be started. Solution settings depend on the chosen FEA software and involve selecting solver algorithms and settings. Automatic time-stepping controls are recommended for accurate rate-dependent responses, and considerations for viscoelastic material models and large deflection effects are discussed.

When results are available, the post-processing starts. Assessing results and model verification involve techniques such as contour plots and graphs. Recommendations include checking simulation convergence, comparing results with existing data, and assessing time steps. Clear result reporting includes comprehensive details about the FE model, material properties, boundary conditions, loading, results, and simulation time. This deliverable focusses on solder joint fatigue as an example. Factors influencing solder joint fatigue, damage parameters, and empirical models for predicting lifetime are discussed. Validation of simulation results through comparison with experiments is highlighted, showcasing an example of simulation verification against observed failure locations in experiments.

When extracting a reduced order model (ROM) from a 3D full order models (FOM), it is recommended to use for the ROM a vendor-independent exchange format and to validate the quality of the stand-alone ROM using displacement information. An extended validation can be done by comparing results from hybrid ROM-FOM against those from FOM simulations.

In conclusion, the meticulous application of thermomechanical FEA is crucial for ensuring the reliability and performance of microelectronic components, with a specific focus on solder joint fatigue as a key area of study. This deliverable provides detailed guidelines and recommendations for each step of the analysis process, emphasizing the importance of accurate modelling and verification.

1. Focus of the model

Thermomechanical finite element analysis (FEA) serves as a vital tool for exploring the thermal and mechanical characteristics of microelectronic components. The choice of model focus and simulation type depends on the specific level under investigation, as illustrated in Figure 1. The first level is focused on the characteristic inside the package; for example, analyzing the stress that is exerted by the mold compound onto the package. The second level entails assessing the board-level reliability. An example is investigating the reliability of solder joints on an unconstrained printed circuit board (PCB). The third level focuses on the board-level reliability of an PCB constrained inside a housing. These distinct levels provide a framework for tailoring the analysis to the specific challenges and conditions encountered at different stages of microelectronic device integration.

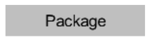
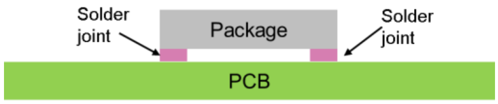
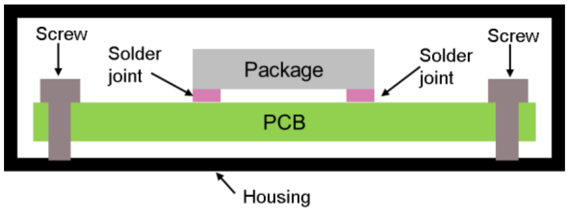
Reliability level	Schematic visualization of test setup
1^{st} level	
2^{nd} level	
3^{rd} level	

Figure 1: Visualization of the nomenclature used for the different reliability levels. The 1^{st} level considers only the package carrying the chip with its internal interconnects, the 2^{nd} level considers an assembly of package and PCB, the 3^{rd} level adds the housing.

The workflow of the thermo-mechanical finite element analysis (FEA) is outlined in Figure 2. The workflow may differ slightly depending on the FEA software used. In general, it can be divided into preprocessing, processing and post-processing. For preparing the FEA, preprocessing involves different steps like defining material properties, geometry, meshing, loading and boundary conditions. Based on the prepared model, the processing or solution section solves the analysis depending on the analysis type and solution settings. Finally, the post processing is used for analyzing, plotting, evaluating, verifying and reporting of the results of interest. Results can be validated or calibrated using experimental data. Iterations improving the FE model may be necessary during the pre- and processing steps if the solution is not converging or results are not satisfactory or explainable by engineering judgement. These different steps are explained in following sections of this document using examples.

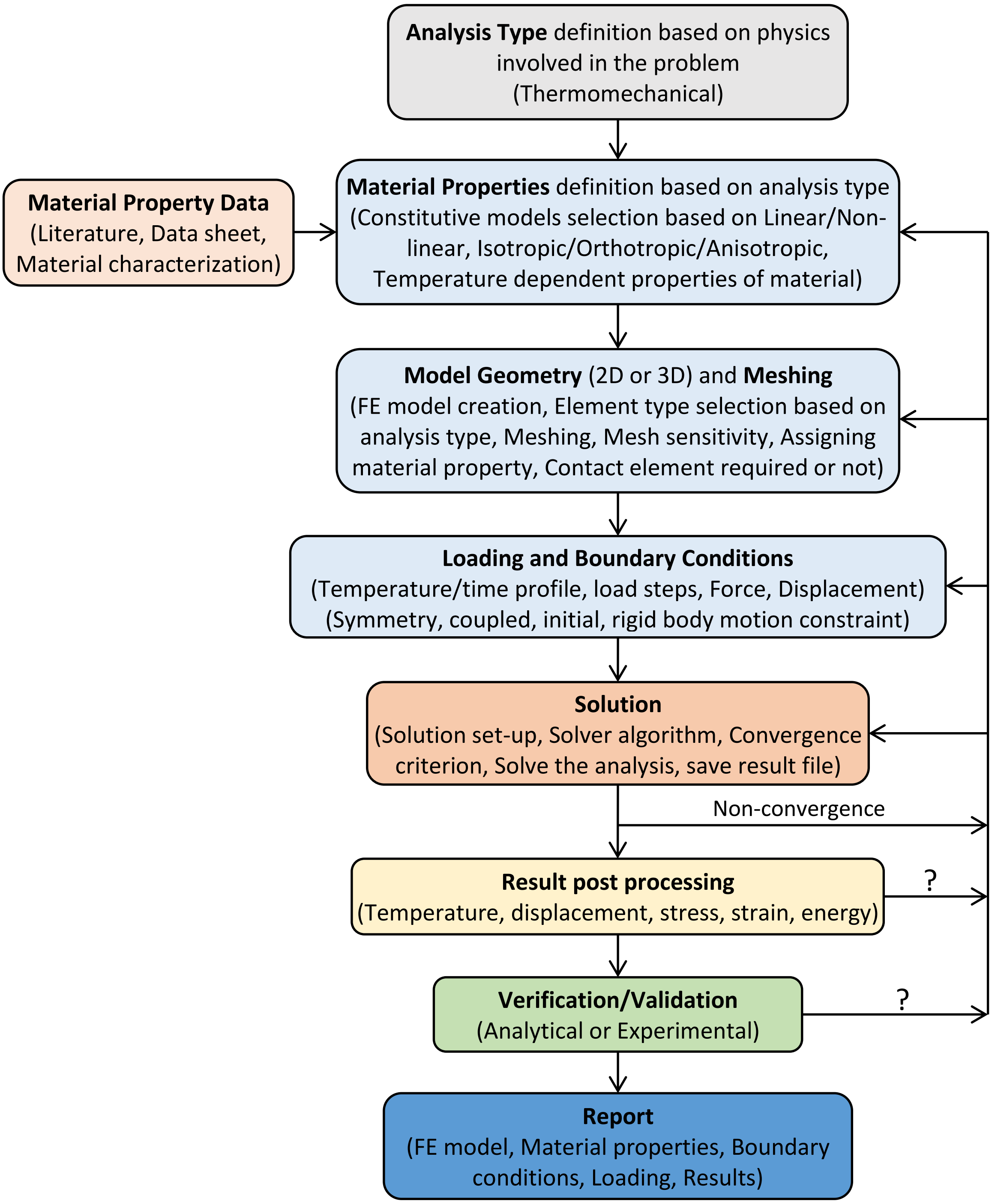


Figure 2: Typical Thermomechanical Finite Element Analysis Set-up

2. Geometry and meshing

For finite element (FE) analysis, a user has to create a virtual solid model of the package or the assembly considering the actual dimensions. For complex geometries, it might be necessary to simplify the geometry keeping in mind its effect on the accuracy of the result. The input for this step can be a CAD model which is then subdivided into many finite elements by discretization, creating a mesh of the model. Depending on the structure geometry, different types of FE model could be generated as shown in the Figure 3 for a PBGA component. For example, a 2D model, full 3D model, half, quarter, octant, strip or slice model. Different boundary conditions are necessary for different model types. There are pros and cons of using different model types in terms of simulation time, accuracy and scalability which is discussed in the IPC/JEDEC-9301 [1]. Our focus will be on full 3D FE model because we aim at generating a reduced-order models (ROMs) from 3D full order models (FOMs) of high quality and to reintegrate this model in a larger 3rd level 3D FE model.

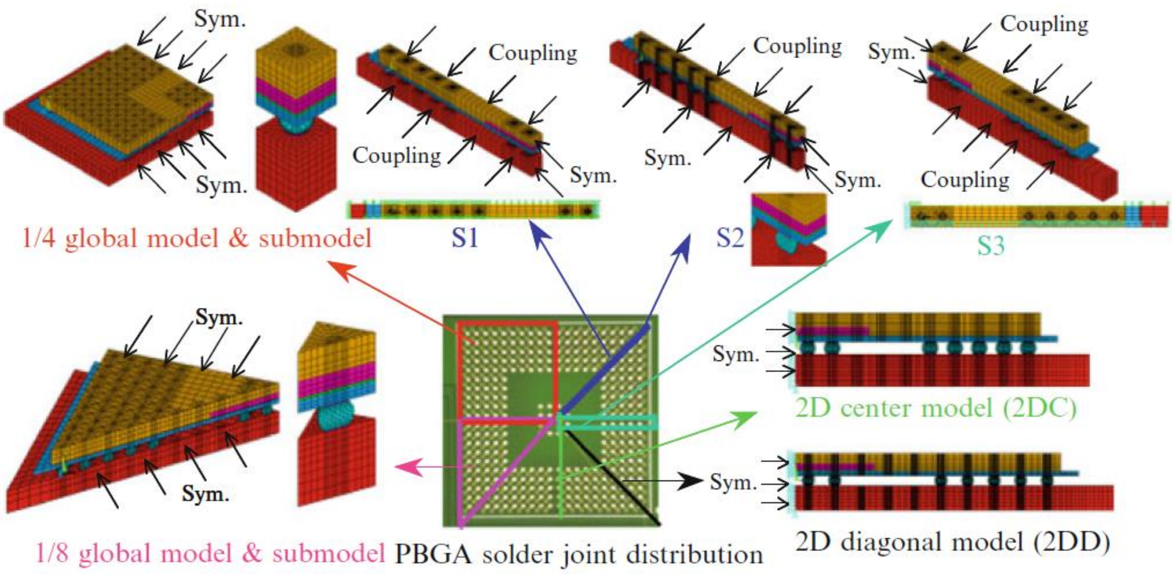


Figure 3: Typical FE model types with different boundary conditions [2]

The element types should be defined depending on the geometry and physical phenomena involved in the problem which is thermomechanical in this case. Different element formulations are available for thermal, mechanical or coupled analysis. Also, element types could be classified as 1D (Beam), 2D (triangular, quadrilateral) and 3D (tetrahedron, triangular prism, pyramid, hexahedron) with linear or quadratic ansatz functions.

Recommendations for FE modelling:

- Leadframe designs have to be used including the correct half etches and downsets.
- Substrate designs may be homogenized if the modeled question is not concerning the substrate design details.
- For solder joint analysis of wafer-level type packages, the RDL design must be included when available as it is determining the stiffness near the solder joint.
- Homogenization techniques can be applied with the restriction that stress relief slots, hinges and other mechanically important features are not homogenized away (e.g. they should still be visible after homogenization).
- Try to avoid using contact if possible. Keep contacts away from locations of interest

Recommendations for meshing:

- When creating a mesh, the mesh density should be sufficient to accurately capture the stress gradients in the areas of interest. Mesh sensitivity study is certainly recommended; especially in the case of limited experience with the type of simulation at hand.
- When using extrusion or volume meshing with linear elements, there need to be at least 3 elements in the thickness direction.
- Linear tetrahedral elements (w/ 4 nodes) should be avoided (or the volume occupied by such elements should be minimized) because of shear locking/poor bending behavior [3]. Converting to quadratic elements is needed when using tetrahedral elements. Linear

tetrahedrals cannot be used for parts that exhibit significant shear deformation (e.g. solder bumps, gels), and cannot be used for parts that warp/bend under loading (e.g. molded packages). For these cases quadratic elements are required, or a mesh dominated by hexahedral elements are required (volume of bricks should be >80%).

3. Material modeling

For different types of materials, the material properties are defined using the constitutive models available in the FE software. Required material properties depend on the type of analysis that needs to be carried out. For quasi-static thermomechanical analysis, Young's modulus, CTE and Poisson's ratio are required. Due to the internal structure of materials (e.g. crystal orientations or fibers) materials can have different properties in different directions. It is important to confirm the material orientation in the FE model and the assigned material properties. Also, these properties could be time, temperature and rate dependent for many materials. Different material characterization methods are used to measure these material properties. Also, various material properties are available in the literature.
In general, the aim is to accurately capture the time, temperature and deformation behaviour of each material. Therefore, material models used should be kept in line with the matrix given below as much as possible. A basic summary for common materials used in the microelectronics components is provided in Table 1.

Table 1 - Material classes and material models

Material group	Preferred material model	Backup material model
Silicon	Anisotropic elasticity (elastic constants)	Isotropic elastic
Ceramics	Linear elastic	-
Solders	Viscoplastic / creep / elastic plastic	*Linear elastic is not allowed*
Other metals	Elastic-plastic (with hardening where applicable)	
Adhesives	Viscoelastic	Linear elastic temperature dependent with at least two Young's moduli, two CTE's and Tg
Moulding compounds	Viscoelastic	
Gels	Hyperelastic	Linear elastic
Substrates / PCB's	Linear elastic orthotropic temperature dependent	Linear elastic isotropic

Figure 4 shows typical stress-strain response for linear elastic and different elastic-plastic material models. An elastic material shows a linear relationship between stress and strain. But, this material could be orthotropic (e.g. PCBs) or anisotropic (e.g. silicon) and also temperature dependent. For metals such as copper, different elastic-plastic constitutive models are available with isotropic or kinematic hardening. In elastic-perfect plastic model, stress does not change as strain increases after yield point. For models with the bilinear hardening option, a second (lower stiffness) relationship between stress and strain beyond yield can be defined. Complex hardening relationships could also be used with the multilinear approach. Selection of the material model should be based on the actual material response.

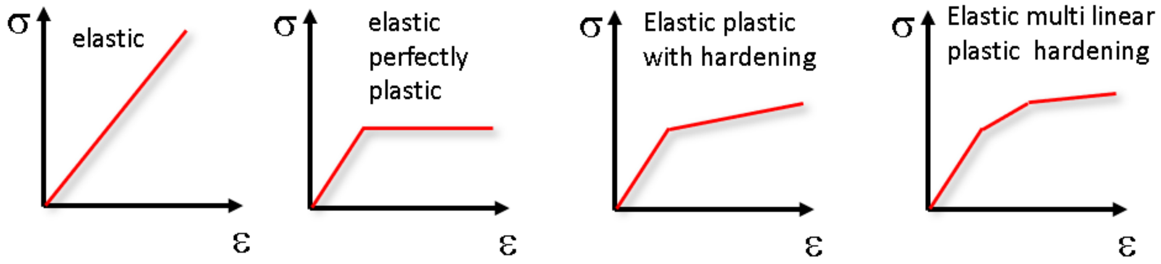


Figure 4: Different material response types. Source [1]

For molding compounds, it is highly recommended to use viscoelastic material models were available because viscoelastic material models are able to account for the relaxation effects in the glass transition region of a moulding compound. Figure 5 compares the displacement result of a bi-material beam consisting of moulding compound and silicon, once computed with a linear-elastic material model and a viscoelastic one to experimental data. The linear-elastic material model shows high deviation to the experimental data when cooling down from high temperature through the glass transition (Tg) region whereas the viscoelastic material model does not.

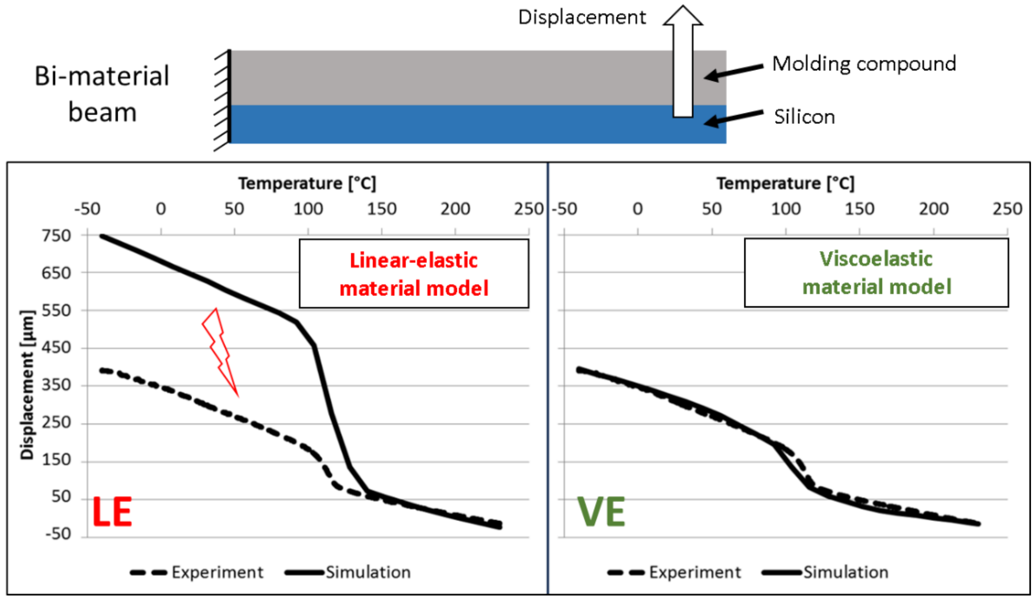


Figure 5: Simulation of a bi-material beam consisting of moulding compound and silicon. Left: A linear-elastic material model is used for the moulding compound. Right: A viscoelastic material model is used for the moulding compound which shows significantly better agreement with the measured data.

For viscoplastic material such as solder, the material exhibits creep behavior which is stress, strain, time and temperature dependent. Different material models are available in the FE software to account for viscoplastic behavior. For example, the Anand model, the Garofalo hyperbolic sine law and the power law. An example of a simple tensile test simulation is shown in Figure 6. The stress-strain response for SAC305 solder using Anand model parameters [4] is illustrated for different temperatures and one strain rate. As this model is strain rate dependent, Anand model parameters are usually calculated using measurements at different strain rates. Also, the response of a widely used Garofalo model of SAC387 is plotted which clearly demonstrates the effect of temperature on the stress level. For different solder alloys, various such parameters are available as Anand and Garofalo models in the literature [5-8]. It is recommended to perform such a simulation with simple stripe model to check material response at different strain rates and temperatures, to confirm its convergence stability and usability for the FE analysis. It is important to pay attention to the unit system a material model is reported in the publication of interest and the unit system which is used for defining the parameters of the respective material model in the FE simulation software: Mixing up different unit system is known to be a common source of error.

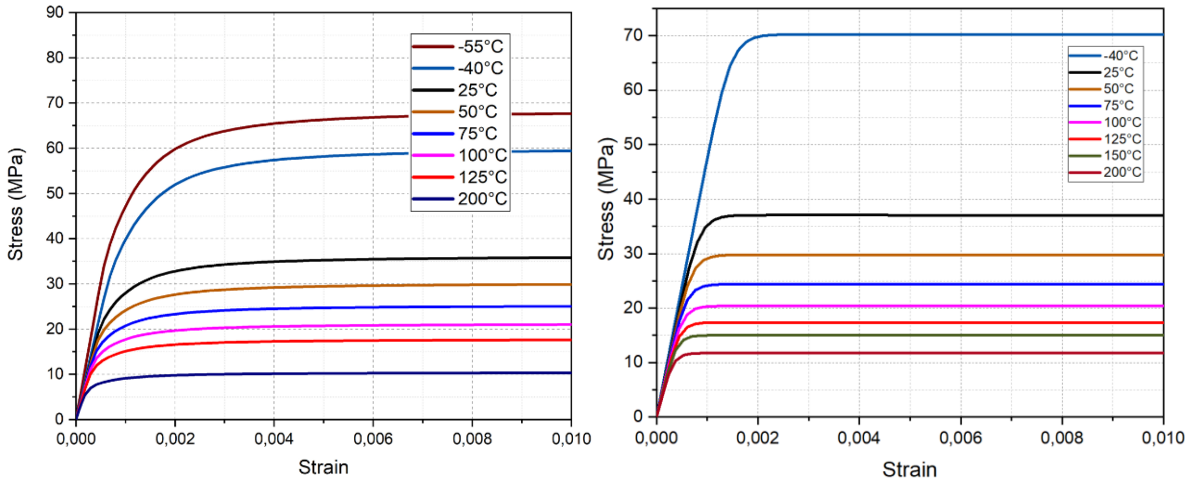


Figure 6: Stress-strain response of solder under tensile simulation at different temperatures (strain rate of 10^{-4}/s), Left: Anand model parameters used for SAC305 [4], Right: Garofalo model parameters used for SAC387 [5].

4. Boundary conditions

Mechanical boundary conditions are necessary to prevent rigid body motion or rotation. Insufficient mechanical constraints may allow parts to 'float off' and to cause convergence issues in the simulation. Basic mechanical constraints for full, half and quarter models are given in Figure 7.

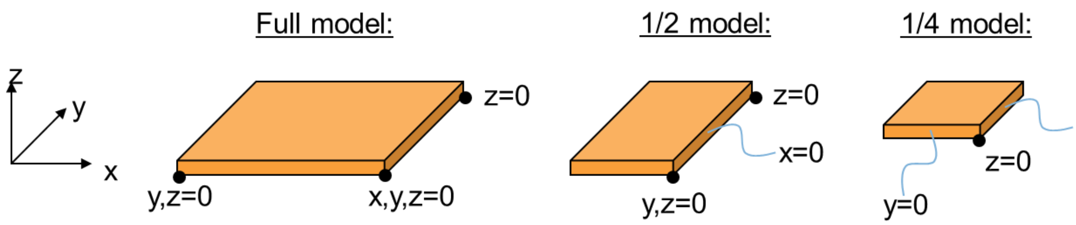


Figure 7: Constraints and symmetry conditions on different types of FE model

- A full model is normally constrained using the "1,2,3" rule. Constrain one node in all 3 directions, another in 2 directions, and the third in 1 direction. The model can now freely expand and warp but does not suffer from rigid body motion or rotation.
- Half symmetry is obtained using the rules for a simply supported beam. Constrain one node in 2 directions, the opposite corner in 1 direction, and finally the cross-sectional area fully in the remaining direction.
- Quarter symmetry models are constraint in one point in 1 direction and the 2 cross-sectional areas in the other 2 directions.

Mechanical loading conditions such as force or displacements are used to apply tension, compression, bending or shear loads. However, for thermomechanical simulations of microelectronics components, temperature needs to be applied as load depending on the temperature profile the component has gone through or will be tested for. Figure 8 shows an example of a characteristically used profile with temperatures from -40°C to 125°C.

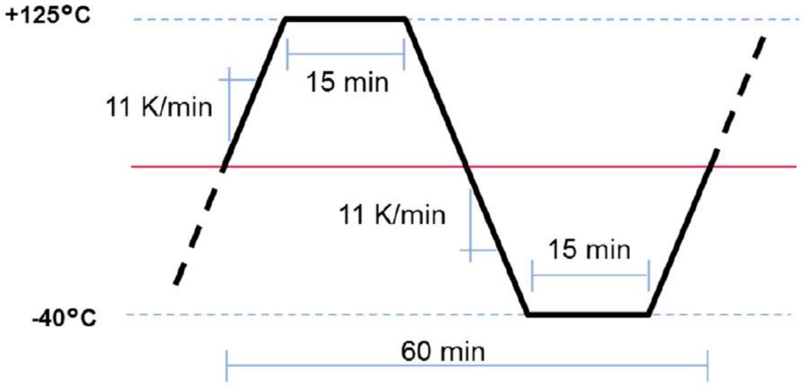


Figure 8: Typical temperature profile example for 2nd level (board-level reliability) [8-11]

Recommendations for boundary conditions:

- The initial conditions shall reflect the manufacturing process stress free temperatures for all backend parts. This means gels are set to the cure temperature, solders are set stress free to the solidification temperature and mold compounds to their mold temperatures. Cure/chemical shrinkage may be included where applicable.
- Room temperature is only an acceptable assumption for the stress-free temperature in very few cases. Residual stresses may sequentially build up during manufacturing process history and may have to be considered using element birth and death options. In Ansys this is for example done using 'EKILL/EALIVE,' in Marc Mentat this is done using '(de)activation.'
- Boundary conditions should be chosen such that they represent reality as much as possible. For most thermomechanical models of individual microelectronics packages this means an isothermal assumption is valid.
- Clamping during high temperature steps of maps or products has a significant impact on the warpage and stress state and must be included.
- For thermal cycling, multiple cycles need to be computed to prove that the increase in energy or inelastic strain is settling to a reproducible number per cycle.

5. Solution settings

The solver algorithms and settings may differ depending on the FE software used. The simulation engineer must identify recommended practices for the respective software used. Recommendations for the solver settings:

- Automatic time-stepping controls is recommended. It should be ensured that the time step size is small enough to capture rate-dependent responses adequately with minimum bisections of the load step. Therefore, it is still better to divide cooling or heating step in sufficiently small steps. Also, optimum substeps should be allowed in each steps to avoid time step bisection leading to more iterations and more simulation time.
- When using visco-elastic material models, e.g. for taking into account the relaxation effects within the glass transition (Tg) region of molding compound, a time-stepping control or a respective time-stepping should be used which ensures sufficient time steps inside the glass transition region. Otherwise, in case of very large time steps, the solver might miss the glass transition region and, hence, not account for the relaxation effects.
- FE solver usually generates a solver output log file. The solver log file can provide many useful information about the solution. For example, summary of applied solver settings,

convergence behavior, warnings and errors. It is recommended to get familiar with the content of this file for FE software.

6. Assessing results and model verification

Post-processing brings the results from simulation into an understandable format. Software packages offer various output methods. Examples are contour plots onto the geometry, graphs or text files with values. Recommendations for assessing the results:

- Check the solver output log to see if any errors during the run were reported by the software, e.g. whether the simulation run started at the intended initial conditions and converged.
- Use for viewing the data in SI-units or derivatives thereof (such as MPa).
- Compare the results with existing simulation data on similar model and check for deviations that cannot be explained by engineering judgement: Are the overall values for the results of the same order of magnitude as intuitively to be expected?
- Are there regions of interest with very high gradients in the results but a (very) coarse mesh (singularities)? Material edges and corners cause mathematical singularities in mechanical models. Stress values must not be evaluated in the vicinity of singularities.
- Plot the results as a function of time (if applicable) and assess if the time steps were not too large.
- To evaluate stresses near/on the interface of a material, isolation techniques might be necessary to prevent errors by nodal averaging.

7. Solder fatigue simulations

The envisioned thermo-mechanical compact models are anticipated to find significant application in the study of solder joint fatigue. A discussion on the simulation of solder joint fatigue is presented in this section.

In scenarios involving cyclic temperature variations, the discrepancy in coefficients of thermal expansion (CTEs) between materials in the microelectronics package and the PCB leads to a mismatch in thermal expansion. Consequently, mechanical stress is imposed on the solder joints, resulting in fatigue, thus limiting the assembly's lifetime.

To quantify cyclic damage in finite element (FE) analysis, the change in creep strain or creep strain energy density per cycle serves as a damage parameter. Nodal values of this parameter depend on the mesh (number of elements) near the region of interest. Therefore, volume averaging techniques are recommended to average results over multiple elements, mitigating dependence on element size and singularities.

The mean number of cycles to failure of a solder joint is commonly determined using various empirical models. Coffin-Mason-type and Morrow-type models are widely employed, utilizing volume-averaged creep strain or energy, respectively [5]. There are no universally applicable pass or fail thresholds. For solder joints, the allowable damage parameter depends on factors such as the solder material type and the soldering process profile used in the assembly. Nonetheless, analyzing trends within a consistent solder setup reveals a clear correlation: a higher damage parameter corresponds to a shorter solder joint lifetime. Translation of the damage parameter into a lifetime requires careful consideration, as empirical models often rely on constants derived from references that may not align with the specific situation.

Validation of simulation results through comparison with experiments, including failure analysis, deformation or strain measurements, and characteristic lifetime data, is crucial to ensure the accuracy of the underlying model physics. Figure 9 illustrates an example of simulation verification against experimental observations. The simulation accurately depicts the bending of a copper pad, mirroring experimentally observed pad deformation. Additionally, it predicts plastic strain maxima at the same location where pad failure is observed. Similarly, the simulation indicates the highest accumulation of creep strain in the solder near under bump metallization, aligning with the crack location observed in testing.

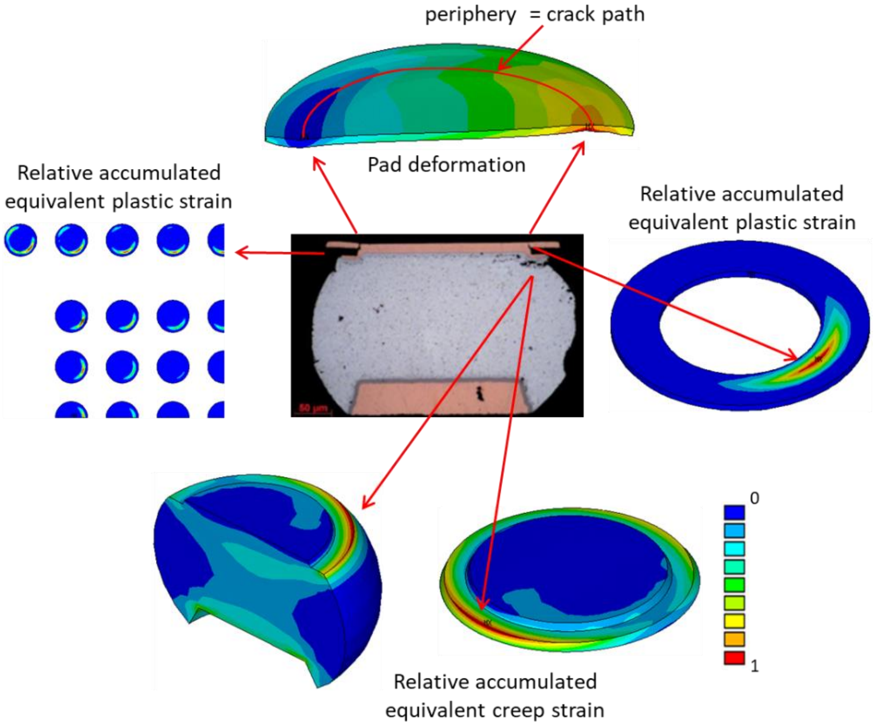


Figure 9: Simulation result validation using experimental observation [9]

8. Extraction and validation of reduced-order models

Once a validated full order model (FOM) is established, it can be reduced using different techniques, such as component mode synthesis or the Kylov subspace method, to a reduced order model (ROM). A discussion of methods for thermo-mechanical compact models is available in [12][13][14] and the public deliverable D2.6 of the COMPAS project.
In order to enable the use of the resulting ROM across different FEM simulation tools from different vendors, it is recommended to use for ROM the FMI 3.0 based exchange format, which is presented in the public COMPAS deliverable D6.2. Figure 10 shows the overall workflow for using the exchange format developed in the COMPAS project.

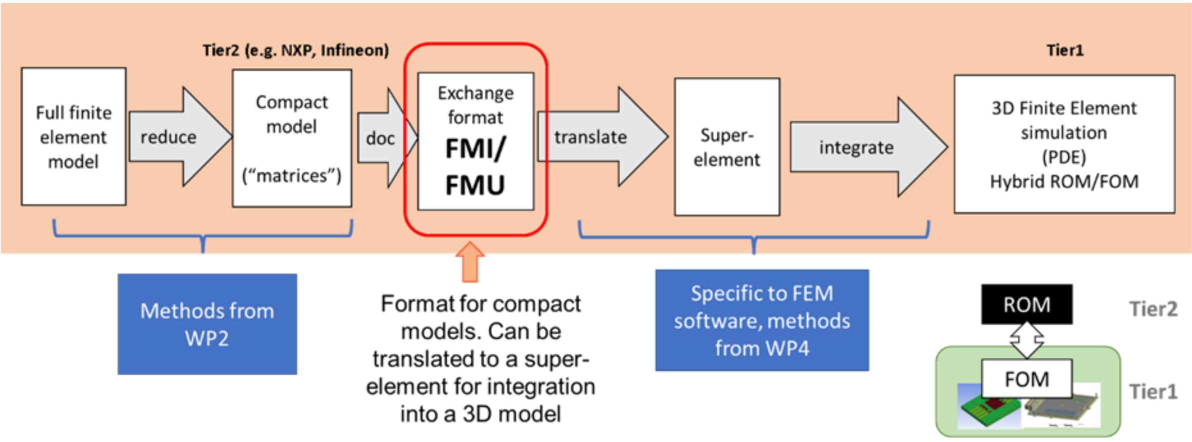


Figure 10: Overall workflow for the generation, exchange, and re-integration of thermo-mechanical compact models according to deliverable D6.2 of the COMPAS project

In order to validate the quality of the extracted ROM vs. the reference FOM, it is recommended to perform verification simulations, which compare the displacement at a monitoring node, as shown in [12][13][14]. For illustration, Figure 11 depicts a 3D FOM and a ROM re-integrated in a 3D simulation environment as a superelement and Figure 12 the boundary conditions and the total displacement magnitude values extracted at a monitoring node.

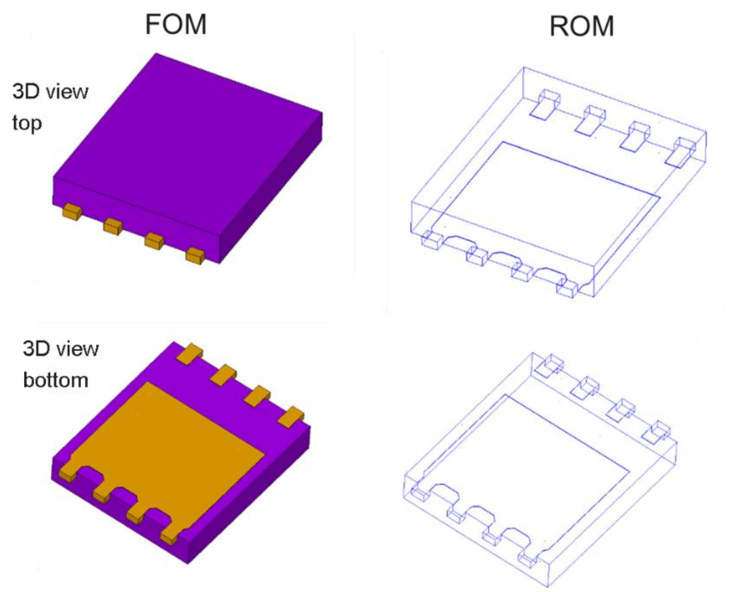


Figure 11: Views of the full order model (FOM) and the reduced order model (ROM) of a electronics component investigated in the COMPAS project

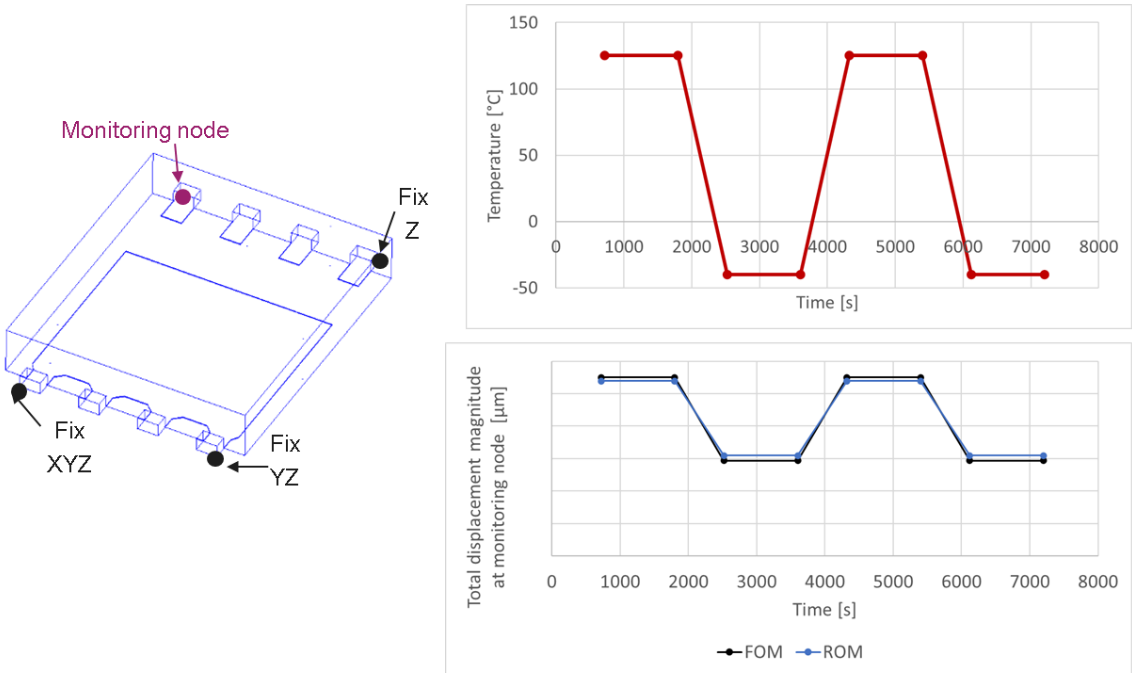


Figure 12: View of the displacement boundary conditions, and the monitoring point used for both the ROM and FOM (left) as well as the profile of the temperature loading (right, upper graph) and the total displacement magnitude at the monitoring node (right, lower graph)

For an extended validation of the ROMs quality, a hybrid ROM-FOM simulation can be performed which compares the in-elastic strain per temperature cycle described in the previous section for the FOM vs. the hybrid ROM-FOM simulation. Figure 13 illustrates an example for such a setup in the 3D FEM simulation environment ANSYS and Figure 14 and Table 2 show examples how the in-elastic strain results can be reported.

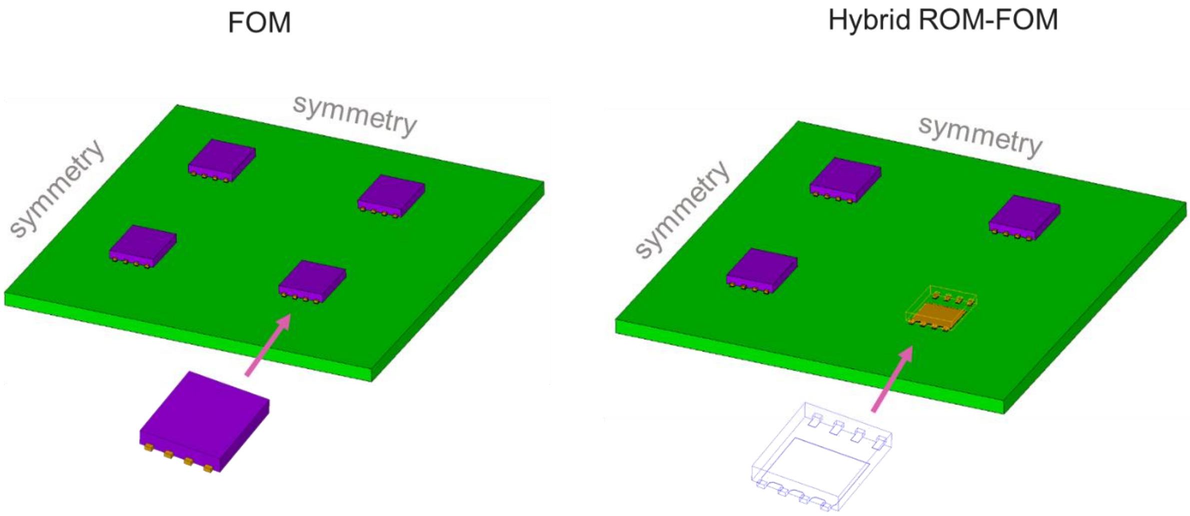


Figure 13: View of the FOM 3D simulation setup (left) and the hybrid ROM-FOM simulation setup (right) with one component modelled using a ROM

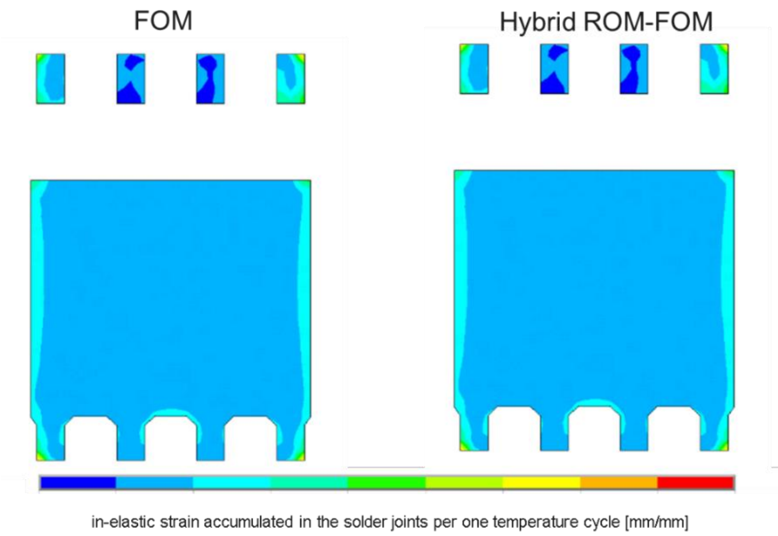


Figure 14: Distribution of in-elastic strain accumulated in the solder joints per one temperature cycle

	FOM	Hybrid ROM-FOM
Volume-weighted average of the accumulated creep strain at the critical gate solder joint	**100%**	**97%**

Table 2: Comparison of volume-weighted averaged in-elastic strain accumulated per temperature cycle for the FOM vs. hybrid ROM-FOM approach.

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