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COMPUTATIONAL SYSTEM FOR PHYSICALLY NON-LINEAR THERMAL ANALYSIS

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Abstract. *The present work concerns the inclusion of functionalities into the free software INSANE - INteractive Structural ANalysis Environment for the physically non-linear thermal analysis in solid bodies by the Finite Element Method when the physical properties of the material are temperature dependent. INSANE is a multi-platform object-oriented computational system being developed at the Federal University of Minas Gerais - UFMG. Once the physical properties are temperature dependent, Newton's iterative method is used to calculate the desired solution. The implementation was tested comparing the numerical results to analytical solutions available in the literature. The segmentation and generalization of the INSANE's numerical core allowed the reuse of the existing classes to support the software expansion.*

Keywords: *Non-linear Thermal Analysis, Finite Element Method, INSANE System*

1. INTRODUCTION

In many practical applications industrial machinery is subjected to temperature variations during its operational cycle. In general, the temperature variation is inherent to the process purposes and has strong influence on the equipment's structure behavior, as in the case of molten metal handling equipment into the steel industry, for example.

For common engineering materials, their physical properties express significant changes on wide temperature ranges. The material's thermal properties dependence upon the temperature introduces a physical non-linearity into the thermal analysis (Reddy, 2004). To obtain the temperature field in a situation where the material physical properties depend upon the temperature itself, a numerical iterative method is usually applied, and Newton's iterative method is one possible solution algorithm.

According to Bergman *et al.* (2011), the knowledge of the temperature field and of the thermomechanical response of a solid body is of great importance for safe and efficient machinery design, since it allows, for instance, the optimization of refractory linings and the prediction of the equipment's behavior under conditions closer to reality.

However, the temperature field calculation is not a trivial task to accomplish, especially when the body geometry is complex and the medium presents a non-linear behavior. In some situations, this calculation may be even impossible using analytical methods, being necessary to resort numerical methods (Bergman *et al.*, 2011).

As better described by Zienkiewicz and Taylor (2000), the Finite Element Method (FEM) is a numerical technique based on the subdivision of the domain into individual components, or 'elements', whose behavior is readily understood. These components are then assembled in a proper way to rebuild the original system in order to determine the approximate behavior of the body.

This subdivision of the domain, called discretization, simplifies the solution by transforming the continuous problem, governed by partial differential equations, into a discrete problem, governed by a set of algebraic equations. Since the quality of this approximation improves as the number of individual components increase, it is necessary to solve large systems of equations in situations of practical application, justifying the computational implementation of the method.

The present work concerns the implementation of functionalities into INSANE's numerical core to solve non-linear heat transfer problems. The computational system INSANE (INteractive Structural ANalysis Environment) is a multi-platform free software, written in Java following the Object-Oriented Programming (OOP) paradigm, intended to be used as a didactic and researching tool, among other purposes. This software is being developed by the Structural Engineering Department of the Federal University of Minas Gerais (UFMG) and is available at http://www.insane.dees.ufmg.br. It has a segmented and generic numerical core independent from the graphical interfaces for pre and post-processing allowing reuse of the existing source code to support the software expansion.

Problems of different fields of engineering can be solved by INSANE since the software conception is abstract. The particularities related to each physics can be gradually included into the numerical core by the introduction of new entities following an OOP inheritance mechanism.

INSANE's development initially focused on solid mechanics. The first resources for solving heat transfer problems by the Finite Element Method were included into the software by Botelho *et al.* (2015) and the analysis was limited to the linear case. The work described in this paper is an extension of the referred work by allowing the analysis of physically non-linear heat transfer problems.

2. THEORETICAL BACKGROUND

2.1 FEM Formulation of the Heat Transfer Problem

As better described by Logan (2007), the Finite Element Method approach for heat transfer problems starts by approximating the temperature field within a finite element by the interpolation of the temperature values at nodes of this element. This approximation can be expressed mathematically as shown in Eq. 1.

$$\mathbf{u} = \mathbf{N}\hat{\mathbf{u}} \ , \tag{1}$$

where $\mathbf{u}$ is the temperature field within the finite element domain, $\hat{\mathbf{u}}$ is a vector containing the temperature values at the finite element's nodes and $\mathbf{N}$ is a matrix containing pre-determined interpolating functions. The matrix $\mathbf{N}$ has different forms depending upon the number of nodes, the spatial domain of the element and the interpolation scheme chosen. The appropriate matrix $\mathbf{N}$ for each type of element can be easily found in the literature (e.g. Zienkiewicz and Taylor, 2000; Reddy, 2004; Logan, 2007; Weaver and Johnston, 1984).

In the case of isotropic materials, the heat flux per unit area in each direction of the global coordinate system is determined by the Fourier law and can be expressed by Eq. 2.

$$\mathbf{q}'' = -\mathbf{D}\mathbf{g} \ , \tag{2}$$

where $\mathbf{q}''$ is the heat flux per unit area in each direction of the global coordinate system, $\mathbf{D}$ is the constitutive matrix, shown illustratively in Eq. 3 for an isotropic material, and $\mathbf{g}$ is a vector containing the temperature gradient in each direction of the global coordinate system.

$$\mathbf{D} = \begin{bmatrix} k & 0 & 0 \\ 0 & k & 0 \\ 0 & 0 & k \end{bmatrix} \ , \tag{3}$$

where k is the thermal conductivity. It should be pointed out that the conductivity varies with the temperature in non-linear heat transfer problems. In the present work this relationship between the thermal conductivity and the temperature is expressed by a polynomial as:

$$k(x, y, z) = a_0 + a_1\mathbf{u}(x, y, z) + a_2\mathbf{u}^2(x, y, z) + \ldots + a_n\mathbf{u}^n(x, y, z) \ , \tag{4}$$

being a_0 , a_1 , ... , a_n polynomial coefficients.

The temperature gradient vector mentioned in Eq. 2 can be expressed, for a cartesian system, by the matrix equation:

$$\mathbf{g} = \left\{ \frac{\partial \mathbf{u}}{\partial x} \, , \, \frac{\partial \mathbf{u}}{\partial y} \, , \, \frac{\partial \mathbf{u}}{\partial z} \right\}^T \ . \tag{5}$$

Writing the derivative operator, $\mathbf{L}$, in matrix form,

$$\mathbf{L} = \left[\frac{\partial}{\partial x} \, , \, \frac{\partial}{\partial y} \, , \, \frac{\partial}{\partial z} \right]^T \tag{6}$$

and substituting Eq. 1 into Eq. 5 we get:

$$\mathbf{g} = \mathbf{L}\mathbf{N}\hat{\mathbf{u}} = \mathbf{B}\hat{\mathbf{u}} \ , \tag{7}$$

where $\mathbf{B}$ is the internal variables operator calculated as the matrix product between $\mathbf{L}$ and $\mathbf{N}$.

The relationship between the actions on a finite element and the nodal temperatures is given by Eq. 8:

$$\mathbf{c}\hat{\mathbf{u}} = \mathbf{f} \ , \tag{8}$$

where $\mathbf{c}$ is the element's conductivity matrix and $\mathbf{f}$ is a vector arising from the potentials for heat transfer acting in the finite element volume and on its surfaces. The vector $\mathbf{f}$ is called an equivalent nodal flux vector and has the three following components:

$$\mathbf{f} = \mathbf{f_Q} + \mathbf{f_q} + \mathbf{f_h} \tag{9}$$

where $\mathbf{f_Q}$ is the potential for heat transfer due to heat sources or heat sinks in the finite element's volume, $\mathbf{f_q}$ is the potential for heat transfer due to flux per unit area prescribed on any surface of the finite element, and $\mathbf{f_h}$ is the potential due to the heat transfer by convection prescribed on any surface of the finite element.

The element's conductivity matrix can be calculated as described in Eq. 10.

$$\mathbf{c} = \int_V \mathbf{B}^T \mathbf{D} \mathbf{B} dV + \int_{S_h} h \mathbf{N}^T \mathbf{N} dS \tag{10}$$

where h is the convective heat transfer coefficient.

The equivalent nodal flux vectors are calculated by Eq. 11, Eq. 12 and Eq. 13 :

$$\mathbf{f_Q} = \int_V \mathbf{N}^T Q dV \tag{11}$$

where Q is the heat sink or heat source per unit volume;

$$\mathbf{f_q} = \int_S \mathbf{N}^T q^* dS \tag{12}$$

where q^* is the heat flux per unit area prescribed on a surface of the element;

$$\mathbf{f_h} = \int_{S_h} \mathbf{N}^T h U_{\inf} dS \tag{13}$$

where $U_{\inf}$ is the fluid temperature.

The contributions of each finite element can be properly assembled to obtain an algebraic system of equations representing the global behavior of the body. The assembling process is based on the principles of equilibrium and continuity and is described in details by Logan (2007). The resulting set of equations can be written as:

$$\mathbf{CU} = \mathbf{F} \tag{14}$$

where $\mathbf{C}$ is the global conductivity matrix of the body, $\mathbf{U}$ is a vector containing the temperatures at each node of the finite element mesh and $\mathbf{F}$ is the vector containing the flux prescribed on the nodes of the finite element mesh. This later vector ($\mathbf{F}$) contains heat flux from the element's equivalent nodal flux vectors and from concentrated heat flux prescribed directly onto the nodes of the finite element mesh.

2.2 FEM Formulation of the Non-linear Heat Transfer Problem

In a physically non-linear analysis the global conductivity matrix C given by Eq. 14 depends upon the temperature, thus:

$$[C(\mathbf{U})]\mathbf{U} = \mathbf{F} \tag{15}$$

Since the temperatures vector $\mathbf{U}$ is not readily known, the matrix $\mathbf{C}$ can only be an approximation based on a guessed temperature distribution. This approximation causes the left side of Eq. 15 to differ from the right side. This inequality is called residue, $\mathbf{R}$, and can be calculated as the difference between the left and right sides (Reddy, 2004):

$$\mathbf{R} = \mathbf{CU} - \mathbf{F} \tag{16}$$

As described in detail by Reddy (2004), Newton's iteration procedure consists of a technique for minimizing the residue along the iterations. Since the residue vector is a function of the temperature vector, it can be expanded in a Taylor series close to the solution U_s as:

$$\mathbf{R}(\mathbf{U_s}) = \mathbf{R}(\mathbf{U}_{(p-1)}) + \left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)_{(p-1)} \cdot \delta \mathbf{U} + \ldots \tag{17}$$

The subscript $(p-1)$ refers to the previous iteration. In the imminence of the solution the residue is null, thus:

$$\mathbf{R}(\mathbf{U_s}) \equiv [C(\mathbf{U_s})]\mathbf{U_s} - \mathbf{F} = \mathbf{0} \ . \tag{18}$$

Substituting Eq. 18 into Eq. 17 and omitting the terms of order 2 and higher we obtain:

$$\left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)_{(p-1)} \cdot \delta \mathbf{U} = -\{\mathbf{R}(\mathbf{U}_{(p-1)})\} \tag{19}$$

The first term in the Eq. 19 is called tangent matrix, named $\mathbf{\Lambda}$:

$$\mathbf{\Lambda}(\mathbf{U}_{(p-1)}) \equiv \left(\frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right)_{(p-1)} \tag{20}$$

The terms of the tangent matrix of a finite element can be calculated by Eq. 21, where lowercase symbols $\hat{\mathbf{u}}$ and $\mathbf{c}$ accompanied by indices were employed to indicate terms of the corresponding matrices and vectors.

$$\mathbf{\Lambda}_{ij} = \sum_{m=1}^{n} \frac{\partial \mathbf{c}_{im}}{\partial \hat{\mathbf{u}}_j} \hat{\mathbf{u}}_m + \mathbf{c}_{ij} \tag{21}$$

The negative of the residue after the $(p-1)$st iteration, present in Eq. 19, can be calculated as:

$$-\{\mathbf{R}(\mathbf{U}_{(p-1)})\} \equiv \mathbf{F} - [C(\mathbf{U}_{(p-1)})]\mathbf{U}_{(p-1)} \tag{22}$$

The approximation for the temperature field at the pth iteration is then given by:

$$\mathbf{U}_p = \mathbf{U}_{(p-1)} + \delta \mathbf{U} \tag{23}$$

This iterative process continues until a convergence criterion is reached.

3. IMPLEMENTATION REMARKS

3.1 Analysis of INSANE's Object-Oriented Design

The analysis of INSANE's object-oriented design focused on identifying:

- The necessary modifications into the classes for data input and output;
- The execution flow and the entities involved during the solution of physically non-linear problems by the software;
- Available classes for the management of the solution of physically non-linear problems by iterative methods;
- The classes to be extended and the methods to be overloaded to represent the particularities associated to the physically non-linear problem.

3.2 Expansion of the computational system

To allow the analysis of non-linear heat transfer problems by INSANE it was necessary to implement three new classes into the numerical core as briefly described below. Besides, modifications were made in the methods responsible for data input and output from the class PersistenceAsXml.

3.2.1 Expansion in the Problem Driver package

The Problem Driver package groups the classes responsible for calculating, at element level, the matrices and vectors related to the mathematical problem being solved (Fonseca, 2008). In the field of heat transfer, these matrices are the element's conductivity and capacitive matrices and the vectors are the ones arising from the loadings applied into the element's volume and over its surfaces (Botelho *et al.*, 2015).

Once in non-linear problems it is necessary to mount a tangent matrix for the iterative solution process, as shown in Eq. 20, a new class descending from HeatTransferPd, called NonLinearHeatTransfer, which can be seen in Fig. 1, overloaded two methods: *getIncrementalC()* and *getC()*. Both classes descend from the Parametric class because the present work focuses on the parametric formulation of the Finite Element Method. A complete description of the parametric formulation can be found in Weaver and Johnston (1984) and in Navarra (1995).

The method *getC()* mounts the element's conductivity matrix, matrix $\mathbf{c}$ in Eq. 8. This method had to be overloaded because in non-linear problems the thermal conductivity is temperature dependent, and in the general case the temperature field along the element's geometrical space is not constant. This implies a different constitutive matrix at each element's integration point, what requires the evaluation of the temperature at the integration point before requesting the Constitutive Model to mount the constitutive matrix. This later process of mounting the constitutive matrix by the Constitutive Model will be further explained in this paper.

The method *getIncrementalC()* mounts the tangent matrix as described in Eq. 21.

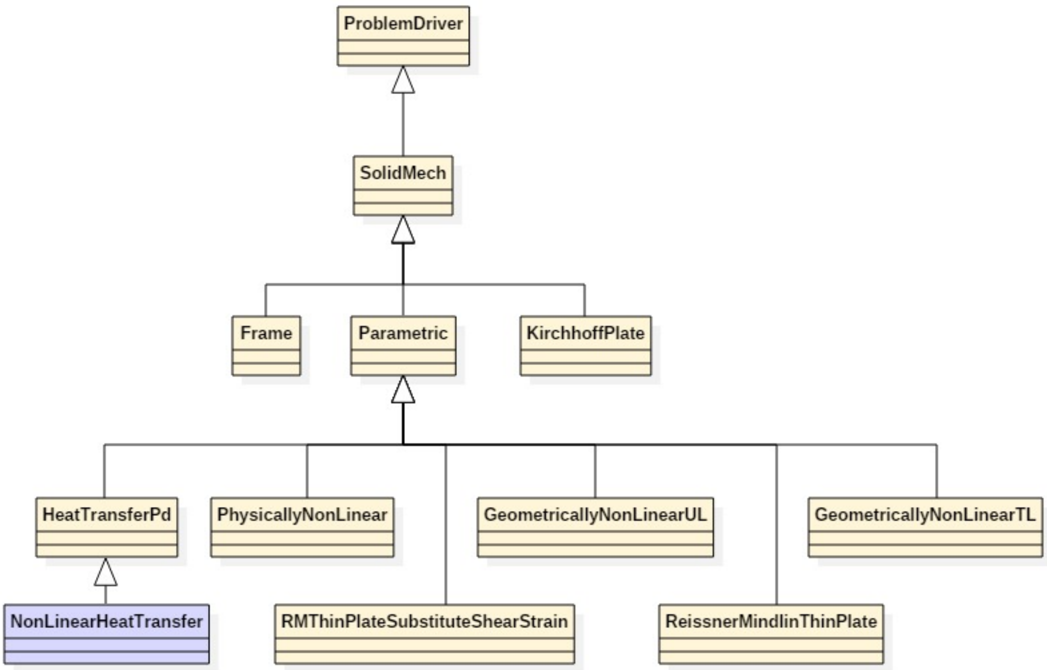


Figure 1. Problem Driver package expansion.

3.2.2 Expansion in the Material package

The Material package contains classes to represent the physical properties of the material that constitutes the medium. The new class NonLinearThermalIsotropicMaterial, shown in Fig. 2 extended the class ThermalIsotropicMaterial. Heir classes of the existing classes weren't shown in Fig. 2. In the new class the material's physical properties temperature dependence is described by polynomials. The new class also contains two new methods for obtaining the secant and the tangent physical properties at a given temperature.

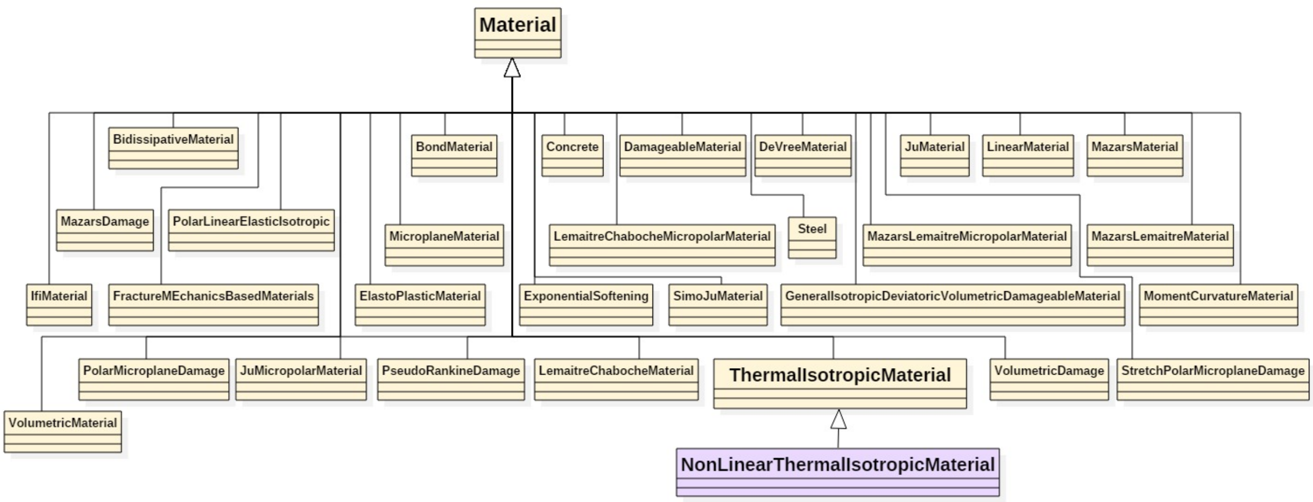


Figure 2. Material package expansion.

3.2.3 Expansion in the Constitutive Model package

The Constitutive Model package arranges the classes engaged in describing the relationship between the inner variables. In heat transfer problems this law is the relationship between the heat flux per unit area and the temperature gradient. Since in non-linear heat transfer the constitutive law has a dependence upon the temperature, a new class named *NonLinearHeatTransferCm* was implemented extending the class *LinearHeatTransferConstitutiveModel*.

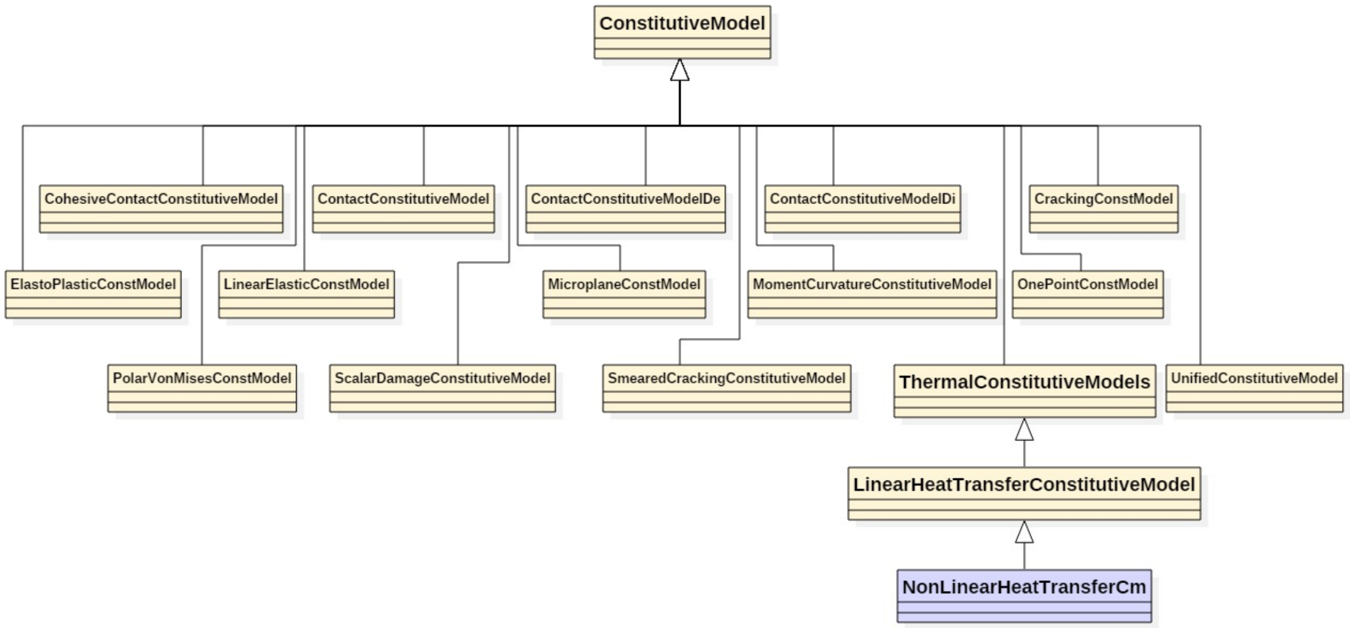


Figure 3. Constitutive Model package expansion.

This new class overloaded the methods responsible in charge of mounting the tangent and the secant constitutive matrices. The overloaded methods receive the temperature at the integration point and then request the Material entity to calculate the physical properties at the given temperature. Having the physical properties, the constitutive model requests an entity called Analysis Model to mount the constitutive matrix based on the problem's spatial dimension. A description of the entity Analysis Model for heat transfer problems can be found in Botelho *et al.* (2015).

4. NUMERICAL EXAMPLES

4.1 Reference problems for validation

To validate the software expansion, three different physically non-linear heat transfer problems whose analytical solutions are readily known were solved by INSANE. These problems, presented in the following subsections, consist on calculating the temperature field in situations where the temperatures are prescribed at the boundaries and the thermal conductivity has a linear dependence on the temperature.

4.1.1 Reference problem 1: Heat conduction in a rod

The rod shown in Fig. 4 has length L and cross section area A_c. The temperatures at the ending A, where $x = 0$ and at the ending B, where $x = L$, are T_a and T_b. The thermal conductivity is k_a and k_b for temperatures T_a and T_b, respectively. The analytical solution of this problem is explained in detail by Danish *et al.* (2011) and consists of solving eq. 24:

$$\frac{d}{dx}\left(A_c k(T)\frac{dT}{dx}\right) = 0 \ . \tag{24}$$

In eq. 24, $k(T)$ is the temperature-dependent thermal conductivity. For a linear interpolation between the values of k_a and k_b, $k(T)$ can be written as:

$$k(T) = k_a\left(1 + \beta\frac{T - T_a}{T_b - T_a}\right) \tag{25}$$

where β is calculated by:

$$\beta = \frac{k_b}{k_a} - 1 \ , \tag{26}$$

To allow the solution, the problem is transformed to the dimensionless variables ξ and θ:

$$\xi = \frac{x}{L} \ , \tag{27}$$

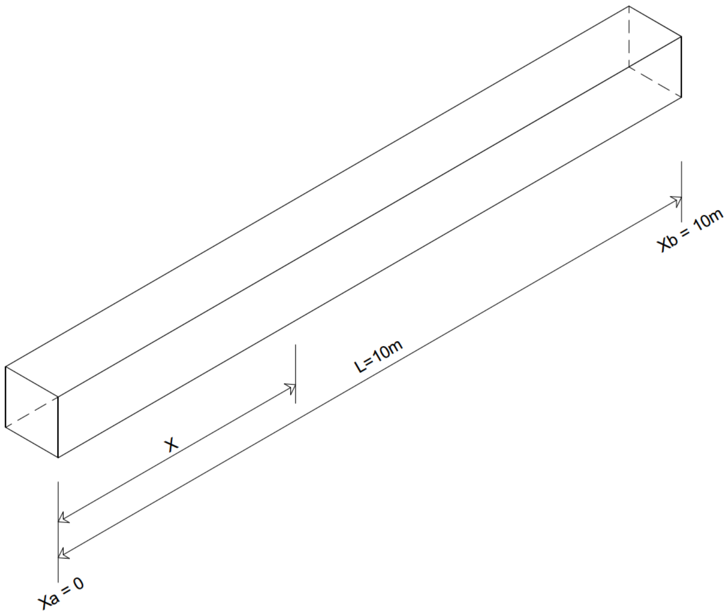


Figure 4. Rod with temperatures prescribed at the endings.

$$\theta = \frac{T - T_a}{T_b - T_a} \quad . \tag{28}$$

The solution obtained by direct integration after the coordinate transformation is given by eq. 29.

$$\theta = \frac{-1 + \sqrt{1 + 2\beta\xi + \beta^2\xi}}{\beta} \quad . \tag{29}$$

4.1.2 Reference problem 2: Heat conduction in a hollow disk

The hollow disk present in Fig. 5 has thickness t_d, inner raius R_a and outer radius R_b. The temperature at the inner radius is T_a, where the thermal conductivity is k_a, and T_b at the outer radius, where the conductivity is k_b. We can arrive at the analytical solution to this problem by solving eq. 30, following the technique presented by Danish *et al.* (2011):

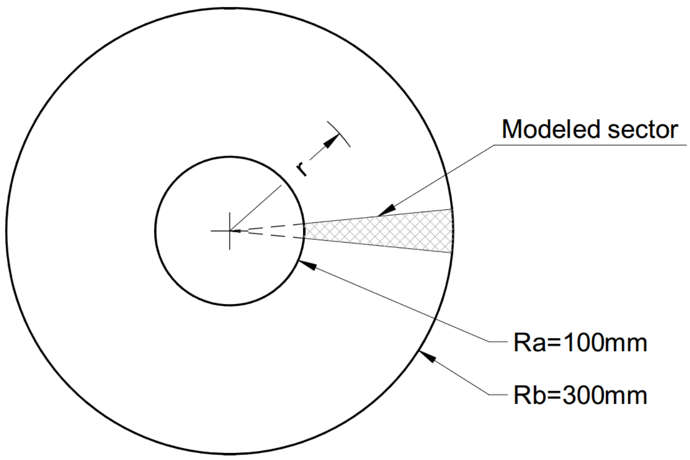


Figure 5. Disk with temperatures prescribed at the inner and outer radii.

$$\frac{1}{r}\frac{d}{dx}\left(rk(T)\frac{dT}{dr} \right) = 0 \quad . \tag{30}$$

The temperature-dependent thermal conductivity varies linearly in the same way described for the rod in equations 26 and 25.

In the case of the disk, a different coordinate transformation is employed. The dimensionless coordinate ξ_d for the disk can be written as:

$$\xi_d = \frac{r - R_a}{R_b - R_a} \quad . \tag{31}$$

The dimensionless temperature θ remains as described in eq. 28.

After the coordinate transformation and solution by direct integration the non-linear temperature distribution is:

$$\theta = \frac{-1 + \sqrt{1 + 2\beta\left(1 + \frac{\beta}{2}\right)\frac{ln\left(1 + \frac{R_b - R_a}{R_a}\xi_d\right)}{\ln\left(\frac{R_b}{R_a}\right)}}}{\beta} \quad . \tag{32}$$

4.1.3 Reference problem 3: Heat conduction in a hollow sphere

The hollow sphere seen in Fig. 6 has inner radius R_a and outer radius R_b. The temperature at the inner surface is T_a and at the outer surface is T_b. As in the cases of the rod and disk , the thermal conductivity at the temperature T_a is k_a and at the temperature T_b is k_b. Similarly to the solution of the problem of heat conduction in a disk, the analytical solution of this problem is obtained by the solution of the eq. 33 using the methodology described by Danish *et al.* (2011):

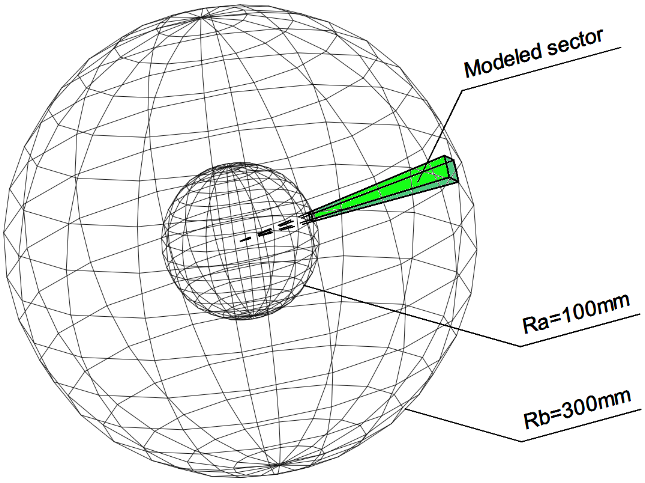


Figure 6. Sphere with temperatures prescribed on the inner and outer surfaces.

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 k(T)\frac{dT}{dr}\right) = 0 \quad . \tag{33}$$

The same coordinate transformation as the employed for the disk, eq. 31, was performed for the sphere, as described by equation 34:

$$\xi_s = \frac{r - R_a}{R_b - R_a} \quad . \tag{34}$$

The dimensionless temperature θ remains as described in eq. 28.

The non-linear temperature distribution obtained by direct integration of eq. 33 after transformation to dimensionless variables is:

$$\theta = \frac{-1 + \sqrt{1 + 2\beta\left(1 + \frac{\beta}{2}\right)\frac{R_b}{R_b - R_a}\left[1 - \frac{1}{\left(\frac{R_b - R_a}{R_a}\right)\xi_s + 1}\right]}}{\beta} \quad . \tag{35}$$

4.2 Validation of the implementation

The reference problems described in the subsections 4.1.1 , 4.1.2 and 4.1.3 were modeled according to the Finite Element Method using INSANE. The new classes were then employed to solve these problems.

4.2.1 Solution using one dimension elements - Heat transfer in a rod

Figure 4 shows a rod modeled using 100 one dimensional straight elements of two nodes as depicted in Fig. 7. The temperature prescribed at the left ending was 0°C and at the right ending, 1000°C. The thermal conductivity at 0°C was considered 20 $W/(m \cdot K)$ and at 1000°C, 1020 $W/(m \cdot K)$. These values lead to the polynomial $k(T) = 20 + T$. The bar length is 10m.

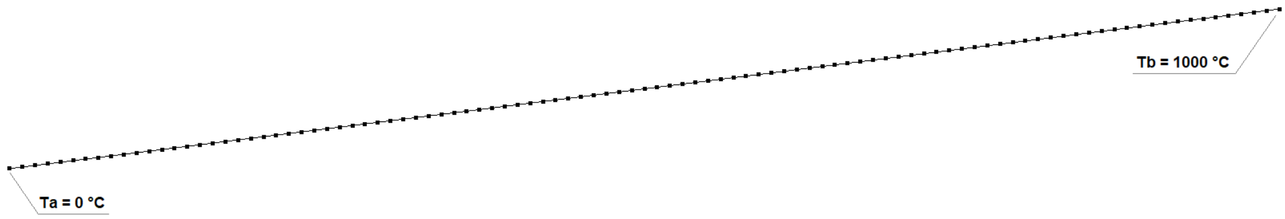


Figure 7. Finite Element Model for the rod.

The comparison between the analytical and the numerical results is shown in Fig. 8. As it can be seen, a good agreement between the solutions was obtained.

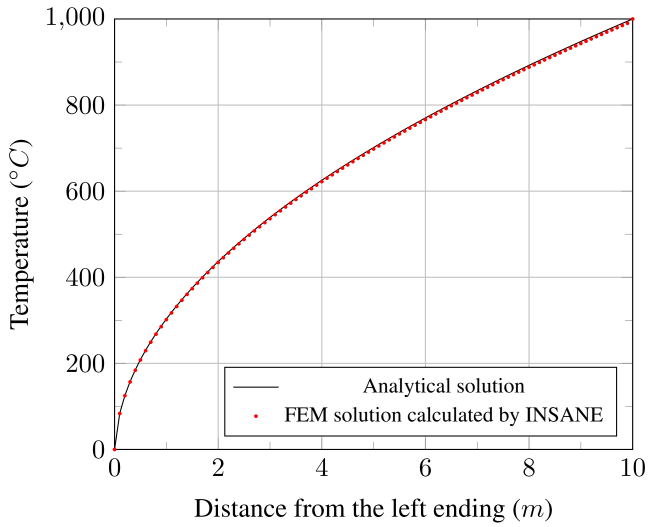


Figure 8. Results comparison between analytical and numerical solutions

4.2.2 Solution using two dimension elements - Heat transfer in a hollow disk

Figure 5 depicts a hollow disk modeled using 500 two dimensional quadrilateral elements of four nodes as depicted in Fig. 9 - (a). The boundary conditions, prescribed at the inner and at the outer radii, were the temperatures 0°C and 1000°C, respectively. The temperature-dependent thermal conductivity was described by the same polynomial that was employed for the rod. Since the problem is symmetrical, there is no heat flux in the circumferential direction, allowing the modelling of only a sector of the disk. It was chosen to model a fraction of 11.25 degrees.

The temperature distribution calculated by INSANE can be seen on Fig. 9 - (b), and the comparison between the analytical and numerical results is shown in Fig. 9 - (c). The numerical solution calculated by the software converged to the analytical result.

4.2.3 Solution using three dimension elements - Heat transfer in a hollow sphere

In Fig. 6 we can see a hollow sphere that was modeled using 306 three dimensional hexahedral elements of eight nodes as depicted in Fig. 10. The temperature prescribed on the inner surface was 0 °C and on the outer surface 1000°C. Since the problem is symmetrical, as was also the case of the disk, there is no heat flux neither in the circumferential nor in the azimuthal directions. We chose to model only a fraction of 5.625 degrees of the sphere. The thermal conductivity is $k(T) = 20 + T$, the same used for the rod and for the disk.

Figures 11 - (a) and 11 - (b) exhibit, respectively, the temperature distribution in the sphere calculated by INSANE and the comparison between the analytical and the numerical analyses. The results obtained validated the solution for the three dimensional case, since they presented good agreement.

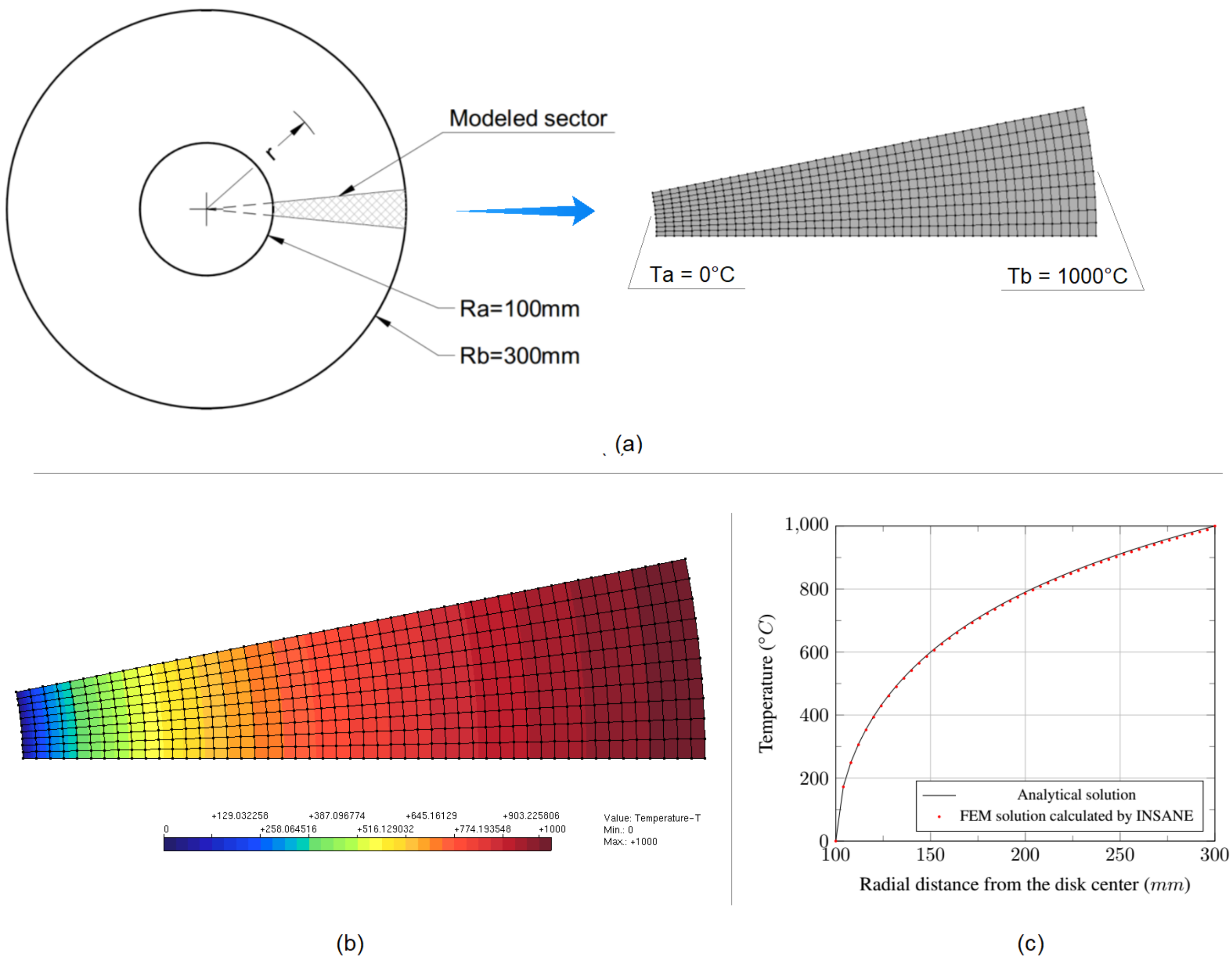


Figure 9. Analysis of the disk. FEM Model (a) - Temperature Distribution (b) - Results comparison (c)

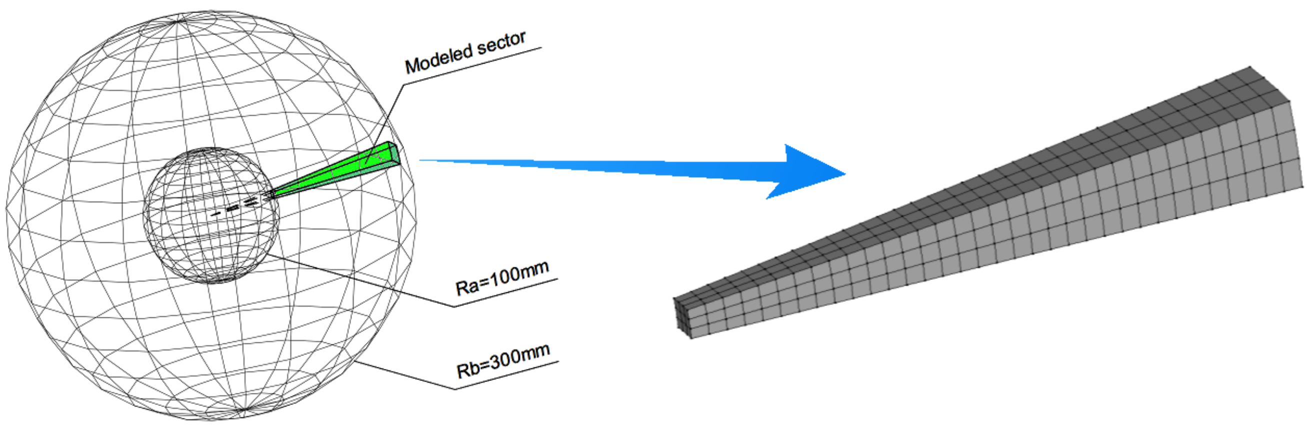
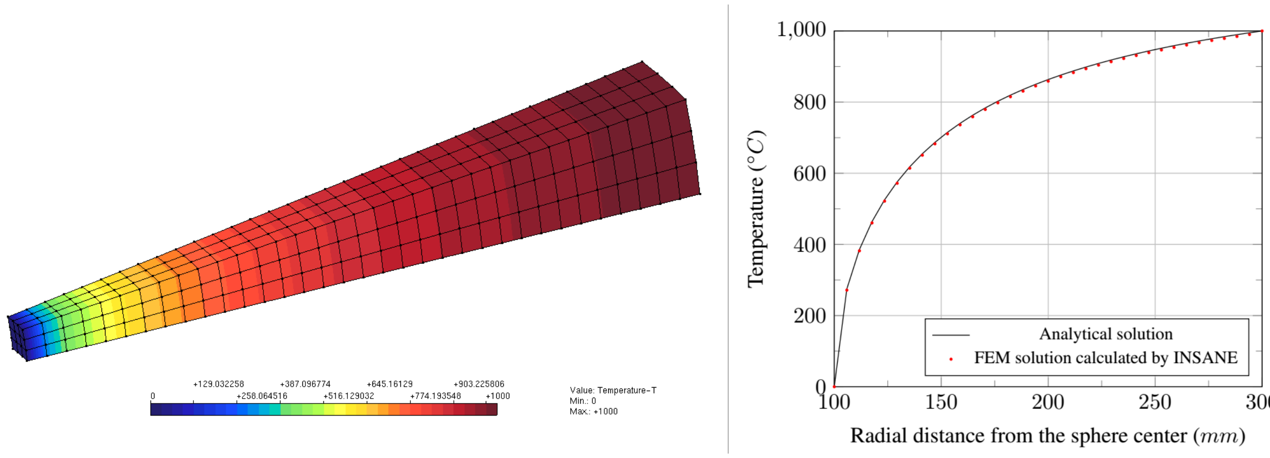


Figure 10. Finite Element Model of the sphere.

5. CONCLUSIONS

Classes for managing and solving physically non-linear heat transfer problems were implemented into INSANE's numerical core. These classes were supported by the existing source code and they were introduced in the software with minimum impact on the generality and modularity. Once the inheritance mechanism was used, only the particularities associated to the non-linear heat transfer problem had to be described.



(a) (b)

Figure 11. Temperature distribution on the sphere and comparison.

Since the solution algorithm focused on the parametric formulation of the Finite Element Method, the classes written were able to analyze models containing parametric elements of any type: line, plane and solid elements.

Reference problems whose analytical solutions are readily known were modeled and solved by INSANE and the results validated the implementation presented in this paper.

6. ACKNOWLEDGEMENTS

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