

**PROCEEDINGS OF
THE NSF WORKSHOP ON
RELIABLE ENGINEERING COMPUTING**

SEPTEMBER 15-17, 2004 | SAVANNAH, GEORGIA USA

EDITORS

Rafi L. Muhanna
Robert L. Mullen

Uncertainty in Thermal Basin Modeling: An Interval Finite Element Approach

Sebastião C. Pereira

PETROBRAS R&D Center, Rio de Janeiro, RJ, Brazil

Ulisses T. Mello

IBM Thomas J. Watson Research Center, Yorktown Heights, NY 10598, U.S.A.

Nelson M. A. D. Ebecken

COPPE, Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil

Rafi L. Muhanna

Georgia Institute of Technology, USA

Abstract. Uncertainty assessment in basin modeling and reservoir characterization is traditionally treated by geostatistical methods which are normally based on stochastic probabilistic approaches. In this talk, an alternative interval-based approach will be present. A solution for the transient heat conduction in sedimentary basins will be introduced using an interval finite element approach. For this purpose, a novel formulation is developed to deal with both the special interval arithmetic properties and the transient term in the differential equation governing heat transfer. In this formulation, the “stiffness” matrix resulting from the discretization of the heat conduction equation is assembled using an element-by-element technique in which the finite elements are globally independent and lagrange multipliers are used to enforce continuity. This formulation is suggested as an alternative to traditional Monte Carlo method, where repetitive simulations are required to handle uncertainty and worst case system response is underestimated. The newly developed technique is applied to a one-dimensional thermal basin simulation to assess its potential and limitations. Numerical results will be introduced and their quality assessed.

1 - Introduction

Determinist numerical simulations are normally used to predict the behavior of geological systems. The predicted behavior or performance is normally used for risk assessment. A well known limitation of determinist simulations is that they provide a single set of results that do not convey information about the uncertainty associated with input parameters or coefficients. To overcome this limitation, uncertainty assessment is typically coupled with stochastic probabilistic approaches in which the input simulation parameter set is stochastically defined and multiple simulations are executed to estimate the uncertainty associated with a probabilistic distribution of the input parameter set space. While effective, this approach is rather expensive computationally. In addition, in deterministic numerical simulations, such as the traditional finite element approach, all the parameters are assumed to be precisely known. However, frequently in basin modeling this is not the case, since imprecise or fuzzy information may be present in the geometry, age, and material properties of the basin. Stochastic or probabilistic approaches have been developed to account for this kind of uncertainties. However, in these approaches material properties are normally treated as

random variables despite the fact that geological processes are not controlled by random phenomena. These considerations have led us to the consideration of *possibility* rather than *probability* and in this work, we present an alternative to the stochastic probabilistic approaches which is based on the interval mathematics to assess uncertainty. Here, we have applied the newly developed techniques to a one-dimensional thermal basin simulation to assess their potential and limitations.

Interval mathematics is a generalization in which interval numbers replace real, or crisp, numbers, interval arithmetic replaces real arithmetic and interval analysis replaces real analysis (Hansen, 2000). Fuzzy numbers can be represented by confidence intervals and its calculations can be performed through interval mathematics. For an introduction to interval and fuzzy arithmetic we recommend reading Moore (1962), Neumaier (1990) and Kaufman & Gupta (1991). The Appendix A summarizes the most common interval operations and its properties. The numerical solution of partial differential equations (PDEs), governing the heat and fluid transfer in porous media, to be unconditionally stable normally requires that its time discretization is implicit. This stable solution leads to a set of simultaneous linear system of equations. When fuzzy numbers are used to represent material properties such as thermal conductivity, the description of the resulting linear system is no longer crisp, but is ambiguous or imprecise. This requires the linear system to be solved using a non-classic approach and unfortunately, there are few and efficient methods described in the literature to solve these systems. It is noteworthy that the solution of interval linear system is combinatorial in nature and the result is a convex hull bounding all possible solutions for the imprecise input system. The combinatorial method is the most accurate method for solving interval systems of equations. In this method, the system of Equation is solved for all combinations of interval numbers using their upper and lower bounds. Needless to say, that the combinatorial method is extremely expensive and cannot solve large systems. However, it can be used to evaluate the accuracy of the other methods for small systems. A method is said to overestimate the results when they are larger than hull estimated by the combinatorial method.

The classic approaches to solve interval linear systems, such as Gaussian elimination, fails to solve interval systems because of some special properties of interval arithmetic, such as the subcancel property, in which one number minus itself is not zero, and one number divided by itself is not the unit. These properties require extensive modifications in the algorithms to solve the systems. In addition, the overestimation induced by variable repetition in a mathematical expression makes especially difficult to deal with interval numbers. In the literature, several papers have described methods to solve interval linear systems of Equations. For example, Neumaier (1990) proposed a preconditioning technique to Gauss Elimination and Gauss Seidel Method. Unfortunately, these techniques generate overestimation in the solution and they also fail to solve both large problems and systems with large interval widths. Rao (1995) discussed an optimization method using the Powell algorithm to solve interval linear systems. This method is very expensive and frequently generates results in which the range is too tight, underestimating the results. Recently Muhanna (2001) presented an interval-based finite element formulation which makes use of an Element-by-Element (EBE) technique to calculate the solution of steady-state problems in mechanics which avoids most sources of overestimations and computes a very sharp solution hull. In this paper, we extend the EBE technique to handle time dependent problems. In addition, we briefly describe a C++ library that we implemented with the combinatorial, preconditioned Gauss elimination, Gauss Seidel, and the Powel methods to solve interval linear systems of Equations.

2 - Heat transfer in sedimentary basins

To illustrate the interval-based uncertainty analysis to basin modeling, we discuss the effect of uncertainty in thermal conductivity of rocks on the predicted temperature evolution of a given basin.

The thermal conductivity of sedimentary rocks is a material property which is well known to vary largely in nature and the impact of its variation can be evaluated with interval mathematics. The thermal conductivity is key parameter in the partial differential equation that governs the heat transfer in compacting porous sediments (Mello, 1994):

$$\left[\frac{\phi}{(1-\phi)} \rho_f c_f + \rho_s c_s \right] \frac{\partial T}{\partial t} = \frac{\partial}{\partial Z} \left[k(1-\phi) \frac{\partial T}{\partial Z} \right] - \rho_f c_f q_f \frac{\partial T}{\partial Z} + \frac{Q_h}{(1-\phi)}, \quad (2.1)$$

where:

ϕ = Sediment porosity;

ρ_f = Pore fluid density, (kg/m^3);

c_f = Pore fluid specific heat, (J/kg);

ρ_s = Solid grain density, (kg/m^3);

c_s = Solid grain specific heat, (J/kg);

T = Temperature, ($^{\circ}C$);

t = Time, (m);

k = Bulk thermal conductivity of sediments, ($W/m^{\circ}C$);

$Z = \int_{z_1}^{z_2} (1-\phi) dz$ = Fully compacted depth (m);

q_f = Darcian fluid velocity, (m/s);

Q_h = Heat source/sink, (J/m).

Equation (2.1) describes the transfer of heat within the sediments via diffusion and advection processes. The bracketed term in the left-hand side of Equation (2.1) is the sediment bulk heat capacity. The first term in the right hand side describes the conduction of heat, the second term represents the advection due to fluid carriage of heat and the final term accounts for the heat gained or lost sources or sinks. The respective essential and natural boundary conditions used to solve Equation (2.1) are:

$$T(S_z) = T_{surf}(t), \quad (2.2)$$

$$k(1-\phi) \frac{\partial T}{\partial Z} \Big|_{z=0} = Q(t), \quad (2.3)$$

where T_{surf} is the temperature at interface water-sediment (S_z) and $Q(t)$ is the basal heat flux entering the basin. This heat flux can be calculated by the degree of crustal and lithospheric mantle thinning as described by McKenzie (1978):

$$Q(t) = \frac{k_a T_m}{a} \left[1 + \frac{\beta}{\pi} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi}{\beta}\right) \exp\left(\frac{-n^2 \pi^2 kt}{a^2}\right) \right], \quad (2.4)$$

where:

k_a = Lithosphere thermal conductivity (W/m°C);

T_m = Mantle temperature (°C);

a = Lithosphere thickness (m);

$k = (k_a / \rho c)$ = Thermal diffusivity (m²/s);

$\tau = (a^2 / \pi^2 k)$ = Thermal decline (s);

β = Lithospheric extension factor.

For deterministic solutions, we have used the data displayed in Table 1 and 2. In Table 1 shows the physical properties for typical sediments are listed and Table 2 presents typical lithospheric parameters.

Lithology	ϕ_0	b	ρ	k	C
Shale	63.0	0.58	2.68	1.5	950.0
Silt	56.0	0.39	2.68	2.0	860.0
Sandstone	50.0	0.50	2.65	3.0	750.0
Limestone	60.0	0.44	2.72	2.5	860.0
Chalk	70.0	0.71	2.67	3.5	800.0
Salt	0.05	0.005	2.20	5.5	854.0
Basalt	5.00	0.0	2.85	2.0	775.0

Table 1 - Physical properties of selected lithologies.

where:

ϕ_0 = Surface porosity;

b = Porosity decay coefficient (1/km);

ρ = Density (g/cm³);

k = Thermal conductivity (W/m°C);

C = Heat capacity (J/kg°C).

Thermal diffusivity	0.008 (m ² /s)
Thermal expansion coefficient	0.000034 (1/°C)
Crustal thickness	31200.0 (m)
Lithosphere thickness	125000.0 (m)
Temperature at the lithosphere base	1333.0 (°C)
Mantle density	3330 (kg/m ³)
Crustal density	2800 (kg/m ³)
Steady-state heat flow	41.84 (mW/m ²)

Table 2 – Lithosphere properties

3 – Traditional finite element formulation for the transient heat conduction

Before we discuss the interval finite element formulation, we briefly review the traditional deterministic Galerkin finite element formulation for solving Equation (2.1). By neglecting the advection term in (2.1), this equation then describes a general diffusion problem which can be stated as an initial-boundary value problem (IBV). It can be expressed in a general form by the following differential equation (Burnett, 1987):

$$\mu(\mathbf{x}) \frac{\partial U(\mathbf{x}, t)}{\partial t} - \frac{\partial}{\partial \mathbf{x}} \left(\alpha(\mathbf{x}) \frac{\partial U(\mathbf{x}, t)}{\partial \mathbf{x}} \right) = f(\mathbf{x}, t). \quad (3.1)$$

When Equation (3.1) is applied to heat conduction, its symbols represent:

$U(\mathbf{x}, t) = T(\mathbf{x}, t)$ = Temperature;

$\mu(\mathbf{x}) = \rho(\mathbf{x})c(\mathbf{x})$ = Heat storage;

$\alpha(\mathbf{x}) = k(\mathbf{x})$ = Thermal conductivity;

$f(\mathbf{x}, t) = Q(\mathbf{x}, t)$ = Heat source;

$\rho(\mathbf{x})$ = Density;

$c(\mathbf{x})$ = Specific heat.

IBV problems consists of finding $U = U(\mathbf{x})$ satisfying (3.1) $\forall \mathbf{x} \in \Omega$ and the prescribed boundary conditions (BCs) which are assumed take the form:

$$U(\mathbf{x}) = g(\mathbf{x}) \quad \forall \mathbf{x} \in \Gamma_g \quad (3.2)$$

$$\alpha \frac{\partial U}{\partial \mathbf{x}} = h(\mathbf{x}) \quad \forall \mathbf{x} \in \Gamma_h \quad (3.3)$$

where Ω is the domain and Γ the boundary, g and h are given functions, g is the essential, or Dirichlet BC, and h is the natural, or Newman BC.

Approximating $U = Na$ and solving (3.1) by the Galerkin method using the implicit time method results into the following element equations:

$$[k_{eff}] \{a\}_n = \{f_{eff}\} \quad (3.4)$$

where:

$$[k_{eff}] = \frac{1}{\Delta t_n} [c] + [k]; \quad (3.5)$$

$$\{f_{eff}\} = + \{f\}_n + \left(\frac{1}{\Delta t_n} [c] \right) \{a\}_{n-1}; \quad (3.6)$$

Δt_n = time step n;

$\{a\}_{n-1}$ = solution for the time-step n-1;

N = shape functions.

The coefficients of the element “stiffness” (k) and accumulation (c) matrices are given by:

$$k = \begin{bmatrix} \frac{\alpha}{L} & -\frac{\alpha}{L} \\ -\frac{\alpha}{L} & \frac{\alpha}{L} \end{bmatrix} \quad c = \begin{bmatrix} \frac{1}{3}\mu L & \frac{1}{6}\mu L \\ \frac{1}{6}\mu L & \frac{1}{3}\mu L \end{bmatrix} \quad (3.7)$$

where L is the length of 1D finite element. In the steady-state heat conduction problem, the element ‘stiffness’ is only composed by the k matrix. In a transient heat conduction problem, an additional accumulation matrix c is added to form the effective element “stiffness” k_{eff} . The accumulation matrix represents the element heat storage capacity, μ . For the global solution of the IBV problem, the elements are assembled in a global stiffness K_{eff} and in a global F_{eff} vector. Then a linear system of equations is solved for the primary variable a :

$$[K_{eff}] \{a\}_n = \{F_{eff}\} \quad , \quad (3.8)$$

$$[K_{eff}] = \underset{e=1}{\overset{nel}{A}} k_{eff} \quad , \quad \{F_{eff}\} = \underset{e=1}{\overset{nel}{A}} f_{eff} \quad ,$$

symbol A represents the assembly operation.

4 – The Element-by-Element (EBE) Formulation with Element Overlap

A straightforward way to transform the traditional finite element formulation into a interval finite element formulation is to replace the real “stiffness” matrix by an interval, or fuzzy, stiffness matrix and solve the resulting interval linear system. Unfortunately, the direct solution of this linear system of Equations can produce overestimated results and arithmetic operations problems (Kulpa, 1998). This occurs due to the large number of arithmetic operations and the width of the intervals numbers during the solution process. Muhanna (2001) proposed an EBE finite element method for steady-state problems that avoids a great number of these operations. In his method, the assembly operation is modified by keeping the elements effectively disconnected and enforcing continuity in the mesh by using Lagrangian constraints. Using this approach, the stiffness matrix can be factored in two matrices: one interval diagonal matrix and another real banded matrix. The inversion of these matrices is done separately and involves very few interval arithmetic operations because the inversion of the diagonal matrix requires a single interval division per row. In spite of this advance, this method is not directly applied to transient problems in which the stiffness matrix has the contribution of the heat capacity term (C matrix). In this case, the resulting stiffness matrix cannot be factored using the same algorithm that was described for steady-state case.

In the sequence, we discuss a new formulation to extent the EBE formulation to solve interval transient heat conduction problems. The goal of this formulation is the same of the steady-state formulation described previously, that is, to factor the global stiffness matrix into two matrices, one interval diagonal and another banded real to reduce the number of arithmetic operations involving interval numbers during the solution of the linear system.

Figure 1 illustrates the EBE formulation using a one-dimensional thermal basin modeling example. In this example, there are three stratigraphic horizons ($H_i, i = 1 \dots 3$) and two layers

($C_i, i = \dots 2$) represented by the traditional finite element mesh with three nodes (horizons) and two elements (layers). The heat flux is specified (natural condition) at bottom ($Q(t)$) and the surface temperature specified (essential boundary) at the top (T_{surf}). Each layer i , has its physical properties: conductivity (α_i), heat capacity (μ_i) and its thickness (L_i).

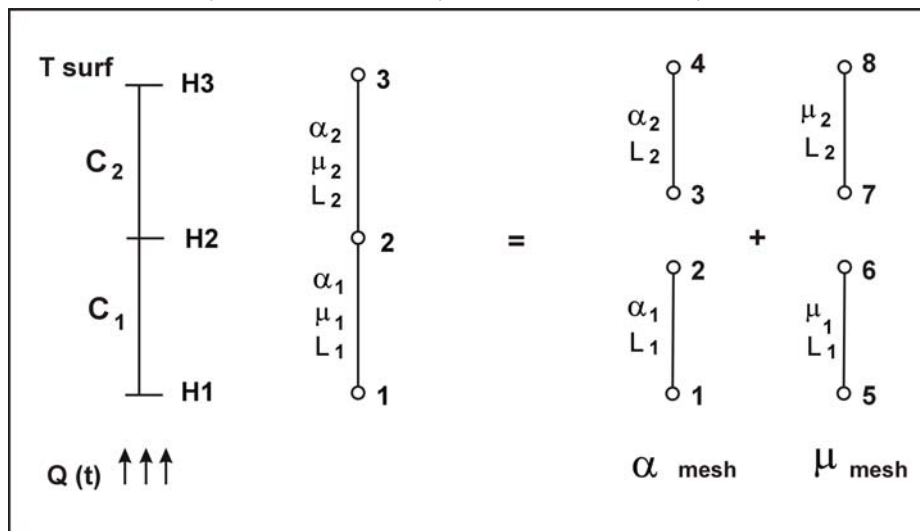


Figure 1 – EBE scheme for a mesh with 2 elements. The nodes are split and renumbered producing 4 overlaps elements.

The overlapping elements are in the right (Fig. 1), there is essentially one mesh for the conductivity (α mesh) overlapping with another one for the heat capacity (μ mesh). The thermal conductivity and the heat capacity are intervals numbers represented by $\alpha = [\underline{\alpha}, \bar{\alpha}]$ and the $\mu = [\underline{\mu}, \bar{\mu}]$. In the interval notation, the underscore and overscore symbols represent the interval lower bound and upper bound respectively. After the mesh split, the nodes are duplicated, node 1 becomes 1 and 5; node 2 becomes 2, 3, 6, 7; and node 3 becomes 4, 8. The mesh compatibility, or the result continuity, has to be enforced and thus constraining equations must be satisfied: $T_1 = T_5$; $T_2 = T_3 = T_6 = T_7$; $T_4 = T_8$, where T is temperature.

The global linear system of equations with the node compatibilities using the EBE formulation with overlap for this mesh is:

$$\mathbf{DRT} = \mathbf{P} - \mathbf{C}^T \boldsymbol{\lambda} \quad (4.10)$$

Finally, the temperature solution vector can be obtained from (4.10) by:

$$\mathbf{T} = \mathbf{R}^{-1} \mathbf{D}^{-1} (\mathbf{P} - \mathbf{C}^T \boldsymbol{\lambda}) \quad (4.11)$$

This Equation can be further simplified by defining the vector:

$$\mathbf{p} = (\mathbf{P} - \mathbf{C}^T \boldsymbol{\lambda}) = \{p_1, p_2, p_3, p_4, p_5, p_6, p_7, p_8\}^T, \quad (4.12)$$

then Equation (4.11) becomes:

$$\mathbf{T} = \mathbf{R}^{-1} \mathbf{M} \boldsymbol{\delta}, \quad (4.13)$$

where:

$$\mathbf{M} = \begin{bmatrix} p_1 & 0 & 0 & 0 \\ p_2 & 0 & 0 & 0 \\ 0 & p_3 & 0 & 0 \\ 0 & p_4 & 0 & 0 \\ 0 & 0 & p_5 & 0 \\ 0 & 0 & p_6 & 0 \\ 0 & 0 & 0 & p_7 \\ 0 & 0 & 0 & p_8 \end{bmatrix} \quad \text{and} \quad \boldsymbol{\delta} = \left\{ \begin{array}{l} \frac{L_1}{\alpha_1} \\ \frac{L_2}{\alpha_2} \\ \frac{\Delta t}{\mu_1 L_1} \\ \frac{\Delta t}{\mu_2 L_2} \end{array} \right\} \quad (4.14)$$

The matrix \mathbf{M} has dimensions $(4 \times \text{number of elements}) \times (2 \times \text{number of elements})$ and the vector $\boldsymbol{\delta}$ has dimensions $2 \times \text{number of elements}$. The rows of the vector $\boldsymbol{\delta}$ are essentially the diagonal values of \mathbf{D}^{-1} . Because the interval numbers occur only once in this vector, we avoid interval operation repetition with the same number. The matrix sizes are twice as large as the EBE for steady-state formulation because of the mesh duplication and this is the cost to reduce the number of interval operations.

5 - Details of the Implementation

Because no library was readily available to us to solve interval linear systems of equations, we have implemented one using Object-Oriented (OO) technologies in C++. By making use of templates and traits techniques we have been able to develop a library that can solve a linear systems of equations for distinct types of numbers such as real, interval and fuzzy using the same implementation. This library also can handle different matrix storage structures such as dense, banded, and tridiagonal. In this library, we have implemented the following methods: (1) preconditioned Gauss-Seidel (Kulpa, 1998); (2) Preconditioned Gaussian elimination (Kulpa, 1998); (3) Optimization using Powell's method (Rao, 1998) ; and (4) the combinatorial method (Muhanna,2000). Figure 2, a graphical

representation of a fuzzy linear system of equations with triangle numbers, shows that a fuzzy system can be solved by α -cuts planes of interval linear system of equations.

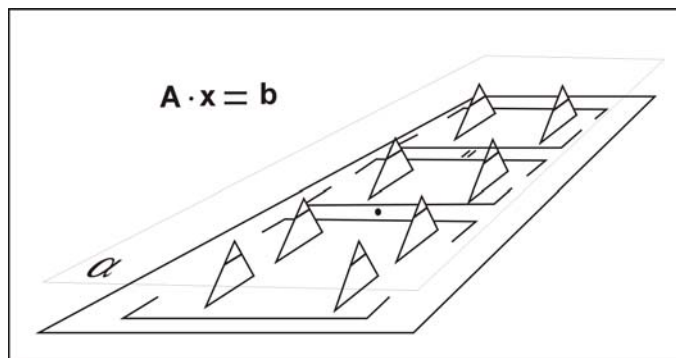


Figure 2 – Fuzzy linear system of equations.

In Figure 3, we display the class derivation scheme for numbers and matrices, as well as the main algorithm classes for solution of linear systems. Following the OO approach, each class number is responsible by its operations (addition, subtraction, multiplication, division, absolute value, etc). This data encapsulation approach is also applied to each matrix class which is responsible by its own matrix operations (LU decomposition, multiply by vector, inverse, determinant, rank etc). We used the classes implemented by Deodato (1995) for interval and fuzzy number operations. In his implementation, the fuzzy number is subdivided in α -cuts confidence intervals. We made extensive use of operator overload, inlining, and templates in our implementation.

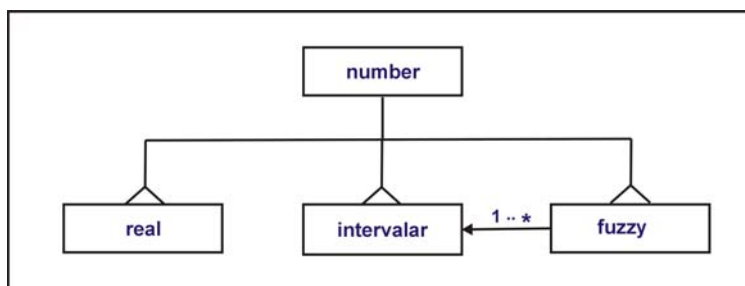


Figura 3 – Derivation class for number types.

Using templates and the generic programming approach (Mello & Khabibrakhmanov, 2003), there is a single implementation for the solution of the system ($Ax = y$), independently of the number type and matrix structure. The matrix and number types are template parameters implemented by the template specialization techniques.

This is a definitive advantage of generic programming, the algorithm does not need to know the details of the data structures used as long a common interface is provided for each number or matrix type. Then, the numbers and matrices operations are responsibility of the numbers and the matrix classes respectively. Consequently, the same algorithm works regardless the type of the matrix or number provided.

In order to apply the concepts discussed so far in this paper, we modified a one-dimensional basin modeling software denominated GEOFEM - *Geological applications Of the Finite Element Method* – (Mello, 1994) which was originally written in C language, to C++ (GEOFEM++) to perform interval and fuzzy operations. A specific EBE assembly operation was added to this software to obtain the global stiffness matrix. We have adapted GEOFEM++ to perform Monte Carlo simulations with uniform, triangular, normal, and exponential density distributions.

6 - Application and Discussion

In this section, we apply the techniques discussed in this paper and we compare its performance with more traditional methods to assess uncertainty. For this discussion, we have used a synthetic well, in which we consider the thermal conductivity of shale and sandstone uncertain as described in Table 3. The lower and upper bounds of the interval value are obtained by the medium subtracting and adding the standard deviation respectively.

Lithology	Minimum	Maximum	Medium	Standard Deviation	Interval Value
Shale	1.3	1.7	1.50	0.05	[1.45, 1.55]
Sandstone	2.90	3.10	3.00	0.10	[2.90, 3.10]

Table 3 – Thermal conductivity values for shale and sandstone (W/mK)

For the sake of simplicity, we discuss initially a very simple example to evaluate the algorithm efficiency in relation to the size of the mesh and the width of the interval numbers. In Figure 4, we display a one-dimensional mesh representing the present-day column of sediments with 4 elements (layer) and 5 nodes (horizons).

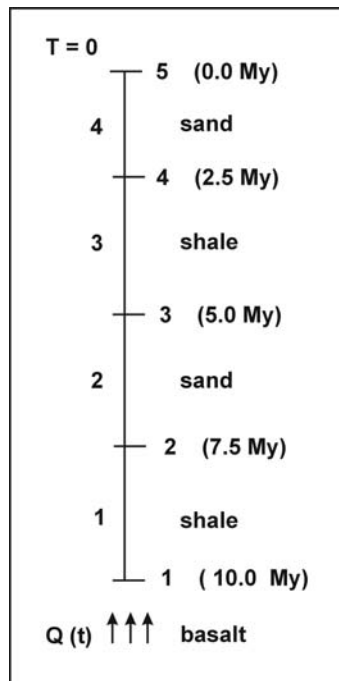


Figure 4 – The elements in the mesh represent geological layers and the nodes the horizons. The respective age, million of years (My), of each horizon is shown on the right of the node numbers.

We calculated the evolution of this mesh over the time, the results for a single node of the mesh at present-day time are shown in Table 4. The value (15.86 °C) is the result of a traditional deterministic simulation using real numbers (Crisp solution) for the thermal conductivity (center value in Table 3). In the sequence, the Monte Carlo (MC) method was applied with 1000 experiments using a uniform distribution, and the results provide a range of uncertainty to the temperature between 14.95 to 16.85 °C. For the uniform distribution, the average value is the same as the crisp solution. Note that an uncertainty of 13 to 17% in the thermal conductivity of the sediments induced a lower than 7% uncertainty in the temperature. The combinatorial methods, which provides an accurate hull for the solution, resulted in a range, [15.43 16.50], close to the MC method but with a little tighter interval. The Preconditioned Gaussian elimination and Gauss-Seidel results are clearly overestimated, whereas the Powell method generated a much tighter solution. Clearly, a poor selection of the interval solution method can provide inaccurate solutions. The EBE method provided a good solution close to the combinatorial method. This shows the advantages and limitations of the interval methods. In our opinion, the EBE method and MC method were able to assess the uncertainty accurately in this simple case.

Method	Temperature
Crisp	15.86
Monte Carlo (MC)	[14.95, 15.86, 16.85]
Preconditioned Gauss Elimination	[12.38, 15.86, 21.80]
Preconditioned Gauss-Seidel	[10.77, 15.86, 27.35]
Combinatorial	[15.43, 15.86, 16.50]
Powell	[15.83, 15.86, 16.01]
EBE	[15.58, 15.86, 16.30]

Table 4 – Comparison among different solution methods for node 3 for the mesh displayed in Figure 4.

In the next experiment, we doubled the number of elements in the mesh as shown in Figure 5, the results for the node 5 are presented in Table 5.

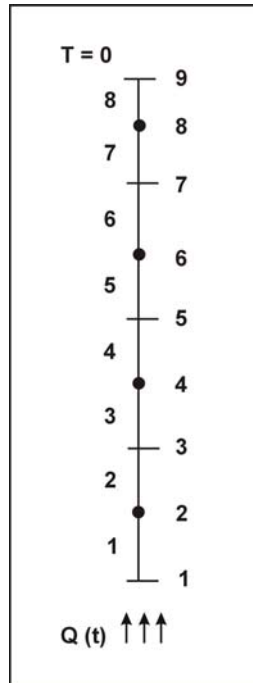


Figure 5 – Mesh with 8 elements.

Method	Temperature (°C)
Crisp	15.66
Monte Carlo (MC)	[14.83, 15.66, 16.73]
Preconditioned Gauss Elimination	<i>Failed</i>
Preconditioned Gauss-Seidel	[7.07, 15.66, 60.33]
Combinatorial	[15.22, 15.66, 16.34]
Powell	[15.66, 15.66, 15.73]
EBE	[15.14, 15.66, 16.22]

Table 5 – Results for the node 5 of the mesh shown in Figure 5.

When the number of the elements increases, the number of operations to invert the interval global stiffness matrix also increases, leading to potential problems such as excessive overestimation. This can be verified in Table 5, especially for the Preconditioned Gauss-Seidel method. For this case, the preconditioned Gauss elimination failed. This failure occurred due the large number of operations with interval number during the pivoting phase of the Gaussian elimination. The large number of operation tends to increase the width of interval number. This width may include zero in the range, making the interval division underdetermined. Similarly to the previous case, the Powell method results were again too tight, and the MC and EBE methods provided good results.

To evaluate the effect o wider range of uncertainty, we multiplied the standard deviation of the thermal conductivity by two (Table 6). The results of the application of the selected methods are shown in Table 7 for this experiment. We used the same four-element mesh as displayed in Figure 4.

Lithology	Minimum	Maximum	Medium	Standard Deviation	Interval Value
Shale	1.30	1.70	1.50	0.10	[1.40, 1.60]
Sandstone	2.90	3.10	3.00	0.20	[2.80, 3.20]

Table 6 – Thermal conductivity for shale and sand (W/mK).

Method	Temperature (°C)
Crisp	15.66
Preconditioned Gauss Elimination	<i>Failed</i>
Preconditioned Gauss-Seidel	<i>Failed</i>
Combinatorial	[14.58, 15.66, 17.34]
Powell	<i>Failed</i>
Monte Carlo (MC)	[14.95, 15.90, 16.92]
EBE	[15.01, 15.66, 16.87]

Table 7 – Results increasing the thermal conductivity width of the shale and sand as shown in Table 6.

The increase in the range of uncertainty caused further deterioration in the quality of some solution methods. In this case, the preconditioned Gauss Elimination and Gauss-Seidel failed to converge. The Powell method converged to an incorrect result. The EBE is the only interval method that provided results with good quality. It is interesting to note that the MC method resulted in slight tighter result when compared with the solution hull. This result could be even tighter if one included a density distribution with a shape different from the box distribution we selected.

As the last evaluation case, we applied the EBE, MC and Combinatorial methods to a well with real data. The stratigraphy is described in Table 8. In the first line, sandstone is the lithology between the horizons 1 and 2. Table 9 shows the lithology conductivity uncertainty used in this case.

Horizon	Age (My)	Depth (m)	Lithology
1	0.0	0.0	Sandstone
2	14.4	438.0	Silt
3	25.0	973.0	Sandstone
4	32.5	1698.0	Shale
5	42.0	3018.0	Limestone
6	64.70	3681.0	Shale
7	83.0	4050.0	Sandstone
8	98.8	4243.0	Silt
9	110.8	4719.0	Shale
10	114.0	4873.0	Silt
11	120.0	6448.0	-----

Table 8 – Stratigraphy for the well used in our analysis.

Lithology	Minimum	Maximum	Medium	Standard Deviation	Interval Value
Shale	1.30	1.70	1.50	0.20	[1.30, 1.50]
Sandstone	2.50	3.50	3.00	0.50	[2.50, 3.50]
Limestone	2.00	2.50	3.00	0.50	[2.00, 3.00]
Silt	1.50	2.00	2.50	0.50	[1.50, 2.50]

Table 9 – Conductivities used in the 22 elements mesh (W/mK).

For this analysis we assumed no variation in the paleobathymetry and sea-level over time. We built a finite element mesh with 22 elements to represent the stratigraphy listed in Table 8, with two elements for each layer. For this modeling, we used the approach described in Mello et al. (1994a) and Mello & Karner (1996), which make use of a fully compacted coordinate system, to eliminate mesh deformation over time. Figure 6 summarizes the temperature calculation at present-day time.

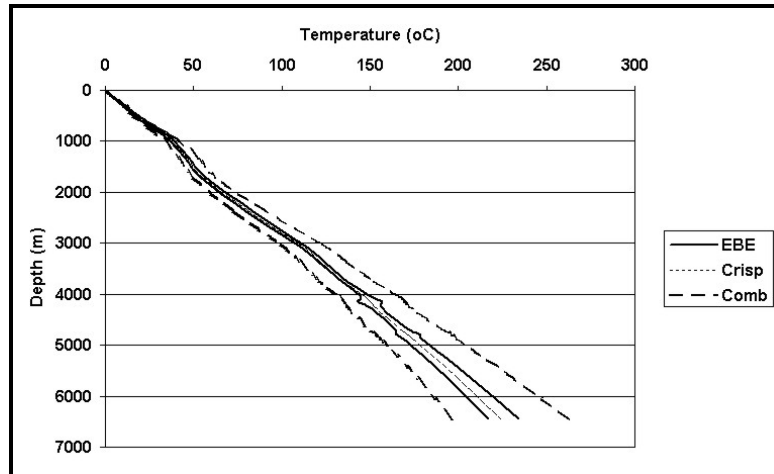


Figure 6 – Temperature versus depth for the data of Table 8.

In this figure, we display the results for Crisp, Combinatorial and EBE methods. The other methods failed for this case. The uncertainty increases with the depth due to the transient numerical solution. Note that, the EBE results were confined within the hull of the solution as defined by the combinatorial method. Although the MC result is not displayed in Figure 6, it was close to the EBE result (Table 10). This table shows the comparison of the MC method with the EBE and Combinatorial methods at the selected depth of 4146 m. For the MC simulations, it was used a uniform distribution of the thermal conductivity, 1000 events, 15 histogram classes, and a cut-off of 5%.

Method	Temperature (°C)
Crisp	150
Combinatorial	[134, 169]
Monte Carlo	[143, 156]
EBE	[143, 157]

Tabela 10 – Temperature estimation at the depth 4146 m in Figure 6.

The EBE simulation took approximately 6 seconds and the MC took 35 minutes in a Intel P4 machine with 1,7GHZ and 1GB of RAM. The good quality of the EBE result was only achievable due to the EBE formulation which reduce the number of interval operations significantly.

7- Conclusions

In this work we evaluated the potential and limitations of an interval possibilistic approach to assess uncertainty in basin modeling. The interval arithmetic approach is an alternative to traditional probabilistic stochastic methodology. We extended the interval finite element EBE formulation to transient heat transport Equation. This formulation proved to present good results within the hull of possible solutions with a quality similar to the Monte Carlo method. However, the EBE formulation has the advantage to perform the uncertainty analysis with a single simulation, requiring much less computational resources.

Here we compared the EBE formulation with more traditional solutions for interval systems of Equations and the EBE has proved to be the most robust. The Preconditioned Gaussian elimination and Gauss-Seidel methods did not performed well with large meshes by either being excessively overestimated or failing to converge. In addition, these methods also had problems to deal relatively wide numbers.

The optimization Powel method algorithm may produce incorrect or too tight results in basin modeling. The Combinatorial method, which provides the exact convex hull of the possible solutions, cannot be used in practical problems since it requires 2^n operation and becomes rapidly unviable when the number of interval variables grows.

The Monte Carlo method gives adequate results to uncertainty analysis when there is sufficient statistical information about the variables. The MC method has the advantage of allow analysis of multiple uncertain variables simultaneously without the need to change simulation applications. The major problem with MC method is the computational cost and the randomness assumption for geological processes that are in general not random.

The EBE with element overlap seems to be a viable alternative for one-dimensional basin modeling due to the quality of its results. However more studies are necessary to analyze its possible applications to multidimensional basin modeling. In higher dimensions, the size of the EBE global matrices may become too large to be solved efficiently.

8 – Acknowledgments

This paper has benefited greatly by the critically reviewing made by Andrew Conn.

References

1. Burnett, D. S., 1987, *Finite Element Analysis from Concepts to Applications*. Addison-Wesley Publishing Company, Whippany NJ, USA, and ISBN: 0-201-10806-2.
2. Deodato, S., Anile, A. M., Privitera, G., 1995, "Implementing fuzzy arithmetic", *Fuzzy Sets and Systems*, v. 72, pp. 239-250.
3. Hansen E. R., 2000, "The Hull of Preconditioned Interval Linear Equations *Reliable Computing*", v.6, n.2, pp. 95-103.
4. Hanss, M., 1999, "On the Implementation of Fuzzy Arithmetical Operations for Engineering Problems", *Proceedings of the 8th International Conference of the North American Fuzzy Information Processing Society - NAFIPS 99*, New York, NY, pp. 462-466.
5. Kulpa Z., Pownuk A., Skalna I., 1998, "Analysis of Linear Mechanical Structures with Uncertainties by Means of Interval Methods", *Computer Assisted Mechanics and Engineering Sciences*, v. 5, pp. 443-477.
6. McKenzie D., 1978, "Some remarks on the development of sedimentary basins", *Earth Planet. Sci. Lett.*, v. 40, pp. 25-32.
7. Mello, U. T. and Karner, G. D. -1996- Development of sediment overpressure and its effect on thermal maturation: Application to the Gulf of Mexico basin. *American Association of Petroleum Geologists Bulletin*, v.80(9):1367-1396.
8. Mello, U. T. and Khabibrakhmanov, I., 2003, On the Reusability and Numeric Efficiency of C++ Packages in Scientific Computing. *Proceeding of the ClusterWorld Conference and Expo*, June 23-26, 2003 in San Jose, California.
9. Mello, U. T., 1994, *Thermal and Mechanical History of Sediments in Extensional Basins*. Ph.D. dissertation, Columbia University, USA.
10. Mello, U. T.; Karner, G. D. and Anderson, R. N. -1994a- A physical explanation for the positioning of the depth to the top of overpressure in shale-dominated sequences in the Gulf Coast basin, United States. *Journal of Geophysical Research*, v.99, p. 2775-2789.
11. Moore, R. E., 1962, *Interval Arithmetic and Automatic Error Analysis in Digital Computing*. PhD dissertation, Stanford University, USA.
12. Muhanna, R. L., Mullen, R. L., 1995, "Development of Interval Based Methods for Fuzziness in Continuum Mechanics", *Proc., ISUMA-NAFIPS'95*, September 17-20, pp. 145-150.
13. Muhanna, R. L., Mullen, R. L., 1999, "Formulation of Fuzzy Finite Element Methods for Mechanics Problems", *Computer-Aided Civil and Infrastructure Engineering (previously Microcomputers in Civil Engineering)*, v. 14, pp. 107-117.
14. Muhanna, R. L., Mullen, R. L., 2000, "Sharp Enclosure for Material Uncertainty in Solid and Structural Mechanics-Interval Based Approach, Part I, *Proceedings of the Eighth ASCE Joint Specialty Conference on Probabilistic Mechanics and Structural Reliability*, University of Notre Dame, Notre Dame, Indiana, pp. 24-26.
15. Muhanna, R. L., Mullen, R. L., 2001, "Treatment of Geometric Tolerances In Finite Element Analysis," *International Journal of Advanced Manufacturing Systems*, v. 4, n. 1, pp. 143-162.
16. Muhanna, R. L., Mullen, R. L., 2001, "Uncertainty in Mechanics Problems - Interval-Based Approach", *Journal of Engineering Mechanics, ASCE*, v. 127, n. 6, pp. 557-566.
17. Muhanna, R., Ballarini, R., R. Mullen, 1998, "Calculation of Stress Intensity Factors with Fuzzy Loading, *Proceedings of the 4-th International Conference on Stochastic Structural Dynamics*, University of Notre Dame, Notre Dame, IN, USA, pp. 6-8.
18. Mullen, R. L., Muhanna, R. L. 1999, "Bounds of Structural Response for All Possible Loadings", *Journal of Structural Engineering, ASCE*, v. 125, n. 1, pp 98-106.

19. Mullen, R. L., Muhanna, R. L., 1996, "Structural Analysis with Fuzzy-Based Load Uncertainty", *Proc, 7th ASCE EMD/STD Joint Specialty Conference on Probabilistic Mechanics and Structural Reliability*, WPI, MA, pp. 310-313.
20. Mullen, R. L., Muhanna, R. L., 1998, "Interval Based Finite Element Methods ", *Proceedings of the 4-th International Conference, NMA'98, Recent Advances in Numerical Methods and Applications II*, Aug. 19-23, editors, Iliev, O. P., Kaschiev, M. S., etc., World Scientific, pp. 362-371.
21. Mullen, R. L., Muhanna, R., L., 1999, "Interval-Based Geometric and Material Uncertainty for Mechanics Problems," *Proceedings of the 13th ASCE Engineering Mechanics Division Conference*. The Johns Hopkins University, Baltimore, MD, pp. 13-16.
22. Mullen, R. L., Muhanna, R., L., 2000, "Sharp Interval Estimates for Finite Element Solutions with Fuzzy Material Properties, "*Proceedings of the 14th ASCE Engineering Mechanics Conference*, The University of Texas at Austin, pp. 21-24.
23. Nakagiri, S., Suzuki, K., 1999, "Finite Element Interval Analysis of External Loads Identified by Displacement Input Uncertainty", *Comput. Methods Appl. Mech. Engrg.* 168, pp. 63-72.
24. Neumaier, A., 1990, *Interval methods for systems of Equations*, Cambridge University Press, New York.
25. Neumaier. A., 1987, "Overestimation in Linear Interval Equations", *SIAM J. Numerical Analysis*, v. 24, n. 1, pp. 207-214.
26. Rao, S. S., Berke, L., 1997, "Analysis of Uncertain Structural Systems Using Interval Analysis", *AIAA Journal*, v. 35, n. 4, pp. 727-735.
27. Rao, S. S., Li Chen, 1998, "Numerical Solution of Fuzzy Linear Equations In Engineering Analysis, "*Int. J. Numer. Meth. Eng.* v. 43, pp. 391-408.
28. Rao, S. S., Sawyer, P., 1995, "Fuzzy Finite Element Approach for Analysis of Imprecisely Defined Systems", *AIAA Journal*, v. 33, n. 12, pp. 2364-2370.
29. Rump S. M., 1990, "Rigorous sensitive analysis for systems of linear and nonlinear Equations", *Math. Of Computations*, v. 54, n. 90, pp. 721-736.

APPENDIX - INTERVAL ARITHMETIC OPERATIONS

An interval number x is represented by:

$$x = [\underline{x}, \bar{x}]$$

where:

\underline{x} = lower bound

\bar{x} = upper bound

\tilde{x} = is a real number that belongs to the interval number $x = [\underline{x}, \bar{x}]$

\tilde{x} = is the real number midpoint of x

wid $x = \bar{x} - \underline{x}$, is the width of interval number x

- Operations:

$$x + y = [\underline{x} + \underline{y}, \bar{x} + \bar{y}] = [\underline{x} + \underline{y}, \bar{x} + \bar{y}]$$

$$x - y = [\underline{x} - \bar{y}, \bar{x} - \underline{y}]$$

$$x \times y = [\min \{ \underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y} \}, \max \{ \underline{x}\underline{y}, \underline{x}\bar{y}, \bar{x}\underline{y}, \bar{x}\bar{y} \}]$$

$$\frac{1}{x} = \left[\frac{1}{\bar{x}}, \frac{1}{\underline{x}} \right], \text{ if } \underline{x} \times \bar{x} > 0$$

- Properties:

$$x(y \pm z) \subseteq xy \pm xz, \text{ para } x, y, z \in IR$$

$$x - y \subseteq (x + z) - (y + z)$$

$$x/y \subseteq (xz)/yz$$

$$x - x \neq 0, \quad 0 \in (x - x)$$

$$x/x \neq 1, \quad 1 \in x/x$$

Note that when there is a repetition of a variable in a mathematical expression we get an overestimated result.