

Mathematical 3D Optimization GNU-Octave with Review of 2D/3D Critical Temperature Optimization Molecular Effect Model in High Temperature Superconductors Thallium Class [$T_c > 0^\circ$] and Superconducting Multifunctional Transmission Line Invent

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ARTICLE INFO	ABSTRACT
Published Online: 24 June 2022	GNU-Octave System software was designed to obtain 3D/2D Graphical Optimization for Molecular Effect Model (MEM) in [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] High Temperature Superconductors (HTSCs) class [exclusively for $T_c > 0^\circ$]. The study results show two parts, namely, GNU-Octave 3D Graphical Optimization and 2D/3D MEM optimization review. Series of 2D MEM GNU-Octave graphs with increasing ILS polynomial degree are developed to demonstrate the equaling of the MEM for this HTSCs class. Comparisons to Matlab solutions from previous contributions were also presented. Results comprise Inverse Tikhonov Regularization algorithms and mathematical methods for this HTSCs class. Solutions prove Numerical/Graphical coincidence between MEM and experimental data is proven. ILS norm-residuals for MEM show be acceptable and low. Electronics Physics applications for Superconductors and HTSCs and optimal T_c selection/constraints are explained. Invention of Superconducting Multifunctional Transmission Line is proposed [Casesnoves, 2021].
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KEYWORDS: Interior Optimization (IO) Methods, Graphical Optimization, Systems of Nonlinear Equations, Inverse Tikhonov Regularization (ITR), Critical temperature [T_c], Inverse Least Squares (ILS), Electronics Superconductors (SC), High-Temperature Superconductors (HTSC), BCS Theory, [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Molecular HTSC Group, Molecular Mass (MO), Molecular Effect Model (MEM), SC-materials (superconductors materials), Superconducting Multifunctional Transmission Line (SCMTS) .	

I. INTRODUCTION

This study continues a series of publications in Superconductors (SCs) and High Temperature Superconductors (HTSCs) for critical temperature [T_c] optimization [1, 4-6, 42, 43]. The model used is Molecular Effect Model (MEM), [Casesnoves, 2020].

In this following contribution, GNU-Octave system is applied to obtain 3D Graphical Optimization and 2D/3D MEM in HTSCs [Ti-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium class. Series of 2D MEM GNU-Octave images with dual-graphs with increasing ILS polynomial degree are developed/improved to demonstrate the matching of the MEM for this HTSCs class. Comparisons to Matlab numerical solutions from previous contributions were also presented.

Sc-materials are the objective/perceivable reality of the physics-chemistry theory. For superconducting effect, there are three critical physical magnitudes, interrelated by an extent number of SC theory formulation [14-16, 26-29, 32-34, 44-46]. These are Critical Temperature, T_c , Critical Current, J , and Critical Magnetic Field. All of them have an important influence on the material superconducting state. MEM, at this stage, is related exclusively to T_c and Molecular Mass (MO) [1, 4-6, 42, 43].

In SCs and HTSCs, the variability related to the physical transition phenomena from normal to superconducting state implies a number of optimal transition-conditions for every superconductor or HTSC [14-16, 26-29, 32-34, 44-46]. One important reason for this optimization is the extensive

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number of sc-materials applications. Sketch 1 shows examples for these selection constraints/conditions. T_C numerical value is obtained from a numerical approximation based on experimental data [14-16, 26-29, 32-34, 44-46]. It depends specifically on every sc-material characteristics. Superconducting effect could appear abruptly, discretely, continuously or in a mixed/undefined way based on those properties [14-16, 26-29, 32-34, 44-46].

New sc-materials are in continuous discovery and improvements. This implies that when any sc-material is required, there are several factors for its desired function/applications, Sketch 1. In other words, there are special sc-material constraints for every sc-material design/manufacturing depending on its functionality, namely internal, external, and operative [14-16, 26-29, 32-34, 44-46]. One important constraint is linked to the optimal required T_C . That is, not only the T_C magnitude itself, but also its demanded transition mode. If the sc-material has got to be using, for example, in a high-precision telecommunications device that has to reach superconducting state almost digitally—speaking in automatic control language, a response-time as short as possible to reach superconducting effect. Or as an alternative, if the sc-material for a medical diagnosis device can get a continuous transition state because the time-interval while setting the patient for exploration is not short [1, 4-6, 42, 43].

Other factor could be, for instance, the sc-material durability. The T_C has to be steady during all the sc-material functional life. Its most physical and material constants should be approximately invariable for all usage time. If some Electromagnetic-fatigue occurs, let's say, that may change during functional-time the T_C magnitude and/or transition mode. Therefore, in that case it would constitute a physical-design problem. Corrosion, because the O_2 element and free radicals are frequently present in the molecule-lattice of a HTSC [7]. For example, corrosion in aerospace sc-materials exposed to air humidity/pressure. Other number of factors could be the industrial sc-material sources. Not all the new sc-materials designed at laboratory can be produced in the required manufacturing amounts if the zone/country natural, human, or industrial resources do not permit that. Apart from that, new sc-materials require a testing period which is a function of safety/risk applications to make objectively sure that it will get a high functionality standard and safety levels.

In conclusion, critical temperature sc-materials phenomena is rather a complicated subject. Electrical power engineering transmission lines constitute other important application of SCs and HTSCs [44-46]. For their operative constraints, cooling of the SC or HTSc is essential, technically complicated and economically expensive [44-46].

Therefore, this condition justifies the importance of new research for HTSCs design/discovery in order to obtain new sc-materials whose cooling requirements could be easier and economically cheaper, Sketch 1.

OPTIMAL SUPERCONDUCTOR DESIGN FACTORS, EXAMPLES	
INTERNAL FACTOR	CHARACTERISTIC
Critical Temperature	The most important
Critical Magnetic Field	Very Important but not strictly necessary for superconducting effect
Critical Current	Very important
Lattice and Nano-Structure	Very important
EXTERNAL FACTOR	CHARACTERISTIC
Technological Design Supplies	Very Important
Electrical Power Supplies	Very important
Industrial Resources for Manufacturing	Very Important
Natural resource	Very important
OPERATIVE FACTOR	CHARACTERISTIC
Type of application	Very important
Electromagnetic Fatigue	Important
Durability	Very important

Sketch 1.-Examples of constraints for sc-materials related to internal, external, and operational functionality [14-16, 26-29, 32-34, 44-46]

The BCS classical superconductors theory constitutes the extrapolated base for MEM [42,43]. The Isotope Effect model algorithm [1, 4-6, 42, 43], that was implemented in previous publications series, for uni-element superconductors equation, [14-16, 26-29, 32-34, 44-46], reads,

$$\begin{aligned}
 & [M_i]^\alpha T_C - K \cong 0; \\
 & \text{for } i = 1, \dots, n; \\
 & \text{or logarithm - form,} \\
 & \alpha \log[M_i] + \log[T_C] - \log[K] \cong 0; \\
 & \text{for } i = 1, \dots, n;
 \end{aligned}
 \tag{1}$$

where K and α are numerical-experimental constants, M Atomic Element Mass (AMU) of an element with (n) isotopes, T_C is critical temperature (usually Kelvin, in this research Centigrade); (i) is the corresponding isotope for the element. The algorithm can be used in logarithm-form also as it is written in the second formula.

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The Isotope Effect Model, Equation (1), is a simple algorithm with two main optimization parameters [M , T_c] , and two constants [K , α] for experimental-numerical determination. In this contribution, MEM 3D/2D Graphical/Numerical Optimization for HTSCs [TI- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium class is developed with GNU-Octave system, constrained to those compounds whose $T_c > 0^\circ$. A Matlab comparison from previous publications is shown also [1, 4-6, 42, 43]. Specific GNU-Octave software was designed with patterns, loops, and imaging processing subroutines.

Succintly, the article proves a GNU-Octave 2D/3D Numerical-Graphical optimization research for MEM in HTSCs [TI- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] group. The GNU-Octave software is developed based on SCs and HTSCs previous research series [1, 4-6, 42, 43]. Numerical/graphical results show low errors/residuals. The GNU-Octave model shapes validates clearly sinusoid MEM curves got in [43]. New invention of Superconducting Multifunctional Transmission Line [Casesnoves, 2021] is presented.

II. MATHEMATICAL AND COMPUTATIONAL METHODS

The MEM computational method in terms of experimental database and implemented algorithm is equal in figures and structure than the one presented in [1, 4-6, 42, 43], but in this study all the software is changed/modified specifically for GNU-Octave programming. Optimization algorithm is constructed with Tikhonov Regularization Theory [7,13,31,42,43] . Table 1 shows Numerical Experimental Data for MEM [4-6, 12-15, 32-34, 37, 42, 43].

NUMERICAL OPTIMIZATION DATA [TI-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] CLASS [HT-SUPERCONDUCTORS, [$T_c > 0^\circ$] MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE T_c (CENTIGRADES)
Tl7Sn2Ba2MnCu10O20	2.9531e+03 / 77
Tl7Sn2Ba2TiCu10O20	2.9461e+03 / 65
Tl6Sn2Ba2TiCu9O18	2.6462e+03 / 56
Tl7Sn2Ba2SiCu10O20	2.9263e+03 / 53
Tl6Ba4SiCu9O18	2.6636e+03 / 48
Tl5Ba4SiCu8O16	2.4479e+03 / 44
(Tl5Sn2)Ba2SiCu8O16	2.3264e+03 / 42
(Tl5Pb2)Ba2SiCu8O16	2.5034e+03 / 38
(Tl5Pb2)Ba2Si2.5Cu8.5O17	2.5933e+03 / 35
(Tl5Pb2)Ba2Mg2.5Cu8.5O17	2.5839e+03 / 30
(Tl5Pb2)Ba2Mg2Cu9O18	2.6195e+03 / 28
(Tl5Pb2)Ba2MgCu10O20	2.6907e+03 / 18
(Tl4Pb)Ba2MgCu8O13	2.0401e+03 / 3

Table 1.- The MEM development data, as in [43], for optimization of parameters for Dual-Graphical/Numerical Optimization that is implemented in software. Data nomenclature is equal also than one presented in [42,43].

Continuing with these formulas/algorithms from [4-6, 12-15, 32-34, 37, 42, 43] for MEM but set on GNU-Octave. Equation (2) shows Inverse Tikhonov functional method like [42,43]. The ILS MEM, with a polynomial $p(MO)$ reads,

minimize Tikhonov functional $J(\alpha)$,
with $\alpha_1=0$ and L_2 Norm
 $J_\alpha(u)_{u \in \mathbb{R}^n} = \|Au - p(MO)\|_2^2 + [\alpha 1] J(u);$
Hence minimize
 $\|T_{ci} - p(MO_i)\|_2^2$,
for $i = 1, \dots, n$
subject to ,
 $a \leq MO_i \leq a_1 ;$
 $b \leq T_{ci} \leq b_1 ;$

where, as [1,4-6, 42,43], MO is the molecular mass of the HTSC selected (i) within a HTSC group with (i) elements and [a-b] are constraints intervals. T_{ci} is every critical temperature (Centigrade in this MEM HTSCs class) for each (i) member of HTSCs group. The figure $\alpha 1$ is a specific constant for Inverse Tikhonov Regularization. The constraints, related to T_c and MO values from experimental data, [a-b], are implemented in optimization. Logarithmic-form, like in Equation (1), can also be implemented optionally.

III. 2D/3D GNU-OCTAVE MEM OPTIMIZATION RESULTS

The results are presented in three subsections. First one is 3D MEM graphical implementation which is shown in GNU-Octave Figures 1,2. Those graphs confirm Matlab results obtained in [43]. Second group is a series of 2D Graphical Optimization to demonstrate how the method is getting the optimal MEM polynomial degree/structure, Figures 3-8. These ones begin with the best 3 and 4 degree ILS MEM single-charts, and continue with comparative dual-curves charts to corroborate the algorithm evolution towards the best fitness. Namely, optimal MEM corresponds to Figures 7,8, where it is proven the 3,4,5 degree finest MEM. Finally, a review of the most important MEM numerical equations from [43] is presented, with a Matlab

chart, Figure 9 from [43], that also validates GNU-Octave Figures 1,2 results. Definitely, MEM sinusoid shape is demonstrated for this HTSCs group, in contrast with parabolic curves for MEM of [Sn-Sb-Te-Ba-Mn-Cu-O] class [42,43].

3D GNU-Octave Graphical Optimization

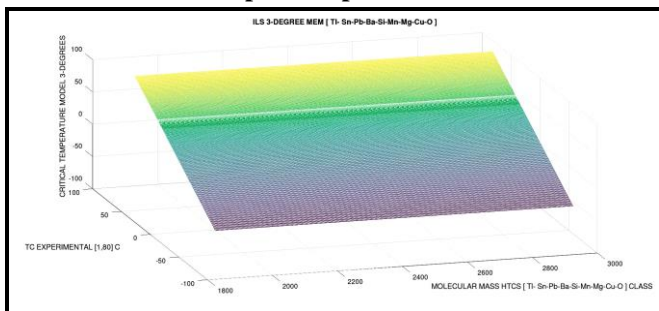


Figure 1.- 3-Degree GNU-Octave polynomial MEM 3D graph showing model T_c prediction and 3D experimental data. Note the darker zone at surface that means the separation between negative and positive T_c for the MEM. Running time is approximately 10 seconds longer than Matlab [42,43]. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are $\approx [350 \times 350]$.

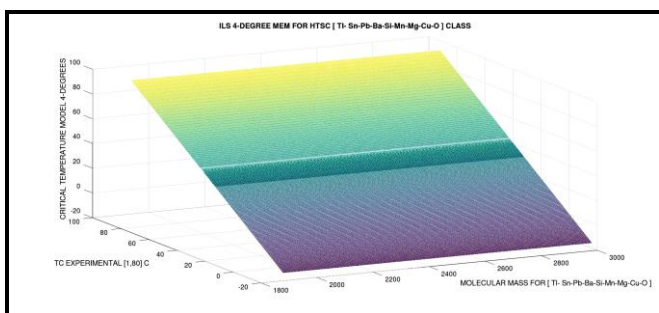


Figure 2.- 4-Degree GNU-Octave polynomial MEM 3D graph showing model T_c prediction and 3D experimental data. Note the darker zone at surface that means the separation between negative and positive T_c for the MEM. Running time is approximately 10-12 seconds longer than Matlab [42,43]. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are $\approx [350 \times 350]$.

2D/3D GNU-Octave with Dual Numerical-Graphical Algorithm Sequences

The sinusoid-like shape of this MEM was shown in [43]. Here, with GNU-Octave, the numerical evolution of the algorithm is developed from 1 to 5 Degree ILS charts. The aim is to prove how the MEM go forwards this optimal shape while increasing the MEM polynomial-degree. First, single charts are shown Figures 3,4. Secondly, comparative-dual graphs are presented, Figures 5-8. Running time is

approximately 8-12 seconds longer than Matlab [42,43] in all the graphics.

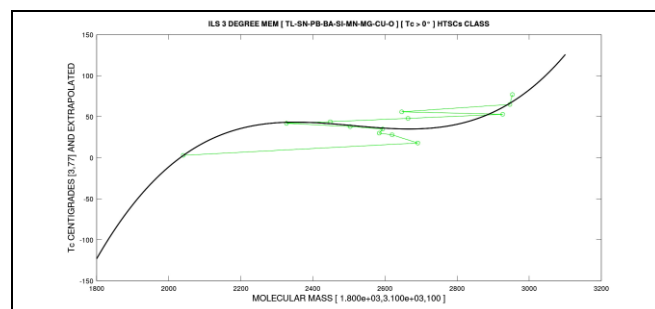


Figure 3.- GNU-Octave programming with 3-degree ILS MEM polynomial optimization for [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. GNU-Octave modelled curve (black) and experimental data (green). Imaging processing quality is acceptable. MEM results to confirm a sinusoid-shape curve, like in [43], approximately. Since this HTSCs class has a number of compounds with $T_c < 0^\circ$, MEM validates that trend.

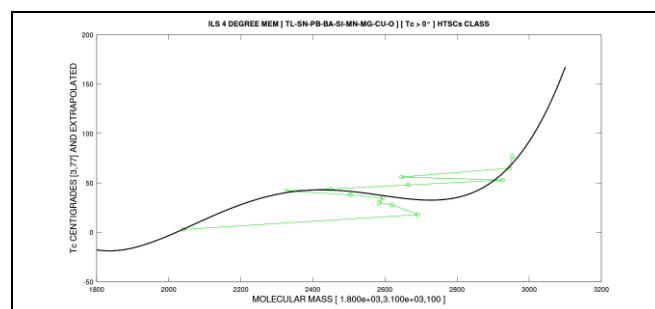


Figure 4.- GNU-Octave programming with 4-degree ILS MEM polynomial optimization for [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. GNU-Octave modelled curve (black) and experimental data (green). Imaging processing quality is acceptable. In the following Figures 5-8, this optimal shape is verified. MEM results to confirm a sinusoid-shape curve, like in [43], approximately. Since this HTSCs class has a number of compounds with $T_c < 0^\circ$, MEM validates that trend.

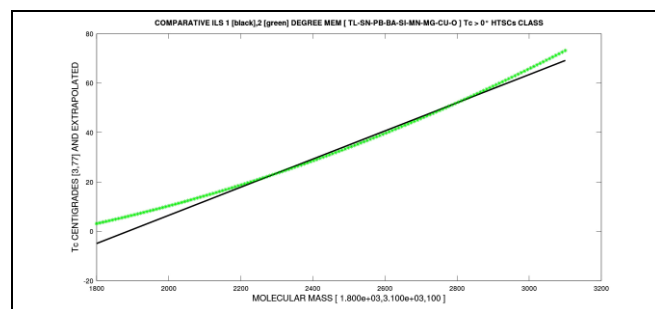


Figure 5.- 1-2 Degree comparative dual-approach, GNU-Octave, with 1,2-degree ILS MEM polynomial optimization for [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. 1-Degree (black) is linear, and it is seen how when passing on 2-Degree (green) polynomial the curve begins to take

sinusoid analytic geometry shape. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0^\circ$, MEM starts to confirm that affinity.

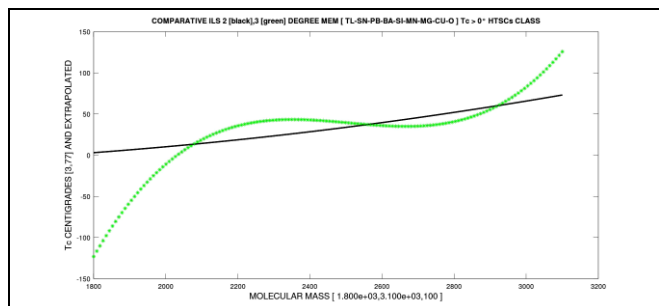


Figure 6.- 2-3 Degree comparative dual-approach, GNU-Octave, with 2,3-Degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. 2-Degree (black) is linear, and it is seen how when passing on 3-Degree (green) polynomial the curve begins to take sinusoid-like shape. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0^\circ$, MEM starts to confirm clearly that affinity with the green 3-Degree shape.

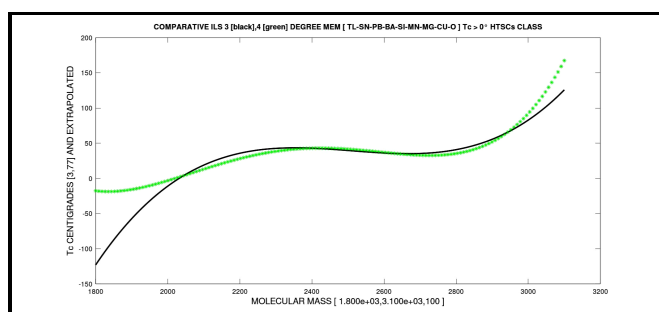


Figure 7.- 3-4 Degree comparative dual-approach, GNU-Octave, with 3,4-Degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. 3-Degree (black) is linear, and it is seen how when passing on 4-Degree (green) polynomial the curve begins to take sinusoid shape. Overlap is almost complete along the experimental data line, which proves the fit correctness. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0^\circ$, MEM confirms clearly that affinity with the green 3,4-Degree shape. Enhanced in Appendix.

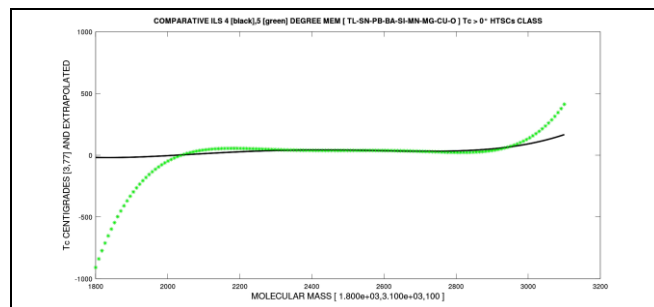


Figure 8.- 4-5 Degree comparative dual-approach, GNU-Octave, with 4,5-Degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. 4-Degree (black) is linear, and it is seen how when passing on 5-Degree (green) polynomial the curve begins to take analytic geometry sinusoid shape. Overlap is almost complete along the experimental data line, almost linear, which proves the fit correctness. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0^\circ$, MEM confirms clearly that affinity with the green 4,5-Degree shape.

Review GNU-Octave Algorithm Numerical-Equations with a Matlab Comparison

In the following, GNU-Octave equations for 3-Degree ILS Optimization is shown, Table 2. This equation matches almost exactly the results obtained in [43]. A comparative MEM 3D Graphical Optimization chart from [43] with Matlab system is presented in Figure 9.

GNU-OCTAVE ILS MEM [3-DEGREE]	
COEFFICIENT	VARIABLE X SELECTED
-8.2906e+003	CONSTANT
10.0383e+000	X
-4.0163e-003	X ²
533.5328e-009	X ³
RESIDUAL = 5.8316e+000	
MODEL EQUATION	
$T_c = [-8.2906e+003] + \dots$ $\dots + [10.0383e+000] MO + \dots$ $\dots + [-4.0163e-003] MO^2 + \dots$ $\dots + [533.5328e-009] MO^3$	

Table 2.- First 3-degree ILS polynomial optimization of Molecular Effect Model Equation. Approximations were not numerically possible since there are not coefficients very high with negative powers. IMPORTANT NOTE: In previous publication with Matlab, [43], a printing mistake in polynomial constant is the default of negative sign. The

correct value is [-8.2906e+03], and NOT like in [43], [+8.2906e+03]

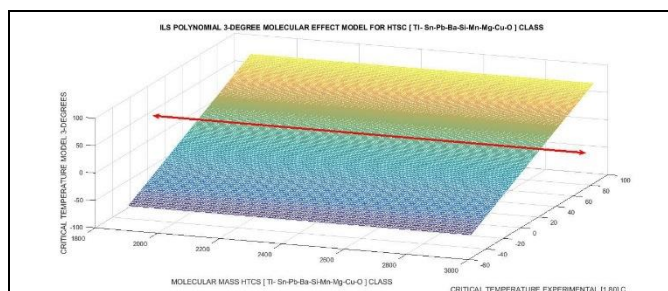


Figure 9.- A Matlab system perspective from [43], for 3-Degree polynomial MEM 3D graph showing model T_C prediction and 3D experimental data which are approximately equal to GNU-Octave results in Figures 1,2 . Note, as in GNU-Octave, the dark zone at surface over the red arrow that means the transition between negative and positive T_C for the MEM. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are [300 x 300].

IV. SUPERCONDUCTING MULTIFUNCTIONAL TRANSMISSION LINE ELECTRONICS PHYSICS APPLICATIONS [CASESNOVES, 2021]

A Superconducting Multifunctional Transmission Line (SCMETS) is defined as a multi-operative transmission line that is adaptable on power energy supplies and demands optimization in function of environmental/artificial temperatures and electrical power engineering parameters [Casesnoves, 2021].

Its cylinder-shaped structure is provided with several encircled layers of conducting and superconducting materials. It could be coaxial also. The innermost layer is formed by a conventional conductor—for standard option power transmission. From inner to outwards, series of stratum of separated and independent superconducting circular layers/covers are set. If necessary, cooling layers stratum are set between any subsequent types of superconductors or HTSCs. From inner to outwards, the specific magnitude of T_C is decreasing. In such a way, the most external superconductor layer has the maximum T_C . Other orders are possible. According to power engineering demands optimization, one or several superconducting layers can be used for power transmission, or the conventional inner conductor exclusively if physical-thermodynamical and/or environmental energy constraints require that choice. Magnetic fields created by the superconductors and/or HTSCs layers while power conducting could be synergic also and increase the efficiency by decreasing the T_C magnitude.

V. DISCUSSION AND CONCLUSIONS

The first objective of this study was to get a comparative GNU-Octave 3D/2D Graphical/Numerical Optimization MEM for [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class constrained to $T_C > 0^\circ$ C. Secondly, to set an analytic geometry proof of the MEM for this HTSCs class. That is, to develop software series of comparative-degree 2D graphs to demonstrate the increasing correctness of the MEM fitness.

Although GNU-Octave software gives acceptable imaging processing quality, running time is longer than Matlab. The programming for dual-charts with GNU-Octave required modifications in patterns, loops, and subroutines. It is sharply proven the step-by-step sequences along increasing ILS polynomial degree till reaching the best fit at 3,4,and 5 degrees.

T_C MEM based on experimental data for [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group were extrapolated with GNU-Octave, as in [43] with Matlab, for values under/above 0° C . That extrapolation matches approximately the experimental figures for this HTSCs class along all experimental critical temperature intervals.

With this theoretical groundwork, the invent proposal of Superconducting Multifunctional Transmission Lines [Casesnoves, 2021], is shown concisely.

In Brief, GNU-Octave comparative-software for 3D Graphical and Numerical Optimization and 2D ILS dual-method Graphical Optimization for HTSCs [Ti- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] were approached with adequate solutions. Applications in Electronics Physics could be guessed from the 3D/2D Numerical/Graphical complementary analysis results.

VI. SCIENTIFIC ETHICS STANDARDS

IMPORTANT NOTE: In previous publication with Matlab, [43], a printing mistake in polynomial constant is the default of negative sign. The correct value is [-8.2906e+03], and NOT like in [43], [+8.2906e+03]. Superconducting Multifunctional Transmission Line (SCMETS) was invented by Dr Casesnoves in 2021, and it is an invent original proposal. This article comprises original GNU-Octave software-variation related to previous publications series [1, 4-6, 42, 43]. 2D/3D Graphical Optimization Methods were created by Dr Francisco Casesnoves in 3rd November 2016, and Interior Optimization Methods in 2019. 2D/3D/4D Graphical and Interior Optimization Methods were created by Dr Francisco Casesnoves in 2020. This article has previous papers information, whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in GNU-Octave constitutes a software engineering improvement from previous contributions [1,4-6,42,43]. The 2D/3D/4D Interior Optimization method is

original from the author (August 2020-1). This study was carried out, and their contents are done according to the European Union Technology and Science Ethics. Reference, ‘European Textbook on Ethics in Research’. European Commission, Directorate-General for Research. Unit L3. Governance and Ethics. European Research Area. Science and Society. EUR 24452 EN [38-41]. And based on ‘The European Code of Conduct for Research Integrity’. Revised Edition. ALLEA. 2017. This research was completely done by the author, the computational-software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the author. When a mathematical statement, proposition or theorem is presented, demonstration is always included. The article is exclusively scientific, without any commercial, institutional, academic, religious, religious-similar, non-scientific theories, personal opinions, political ideas, or economical influences. When anything is taken from a source, it is adequately recognized. Ideas and some text expressions/sentences from previous publications were emphasized due to a clarification aim [38-41].

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APPENDIX

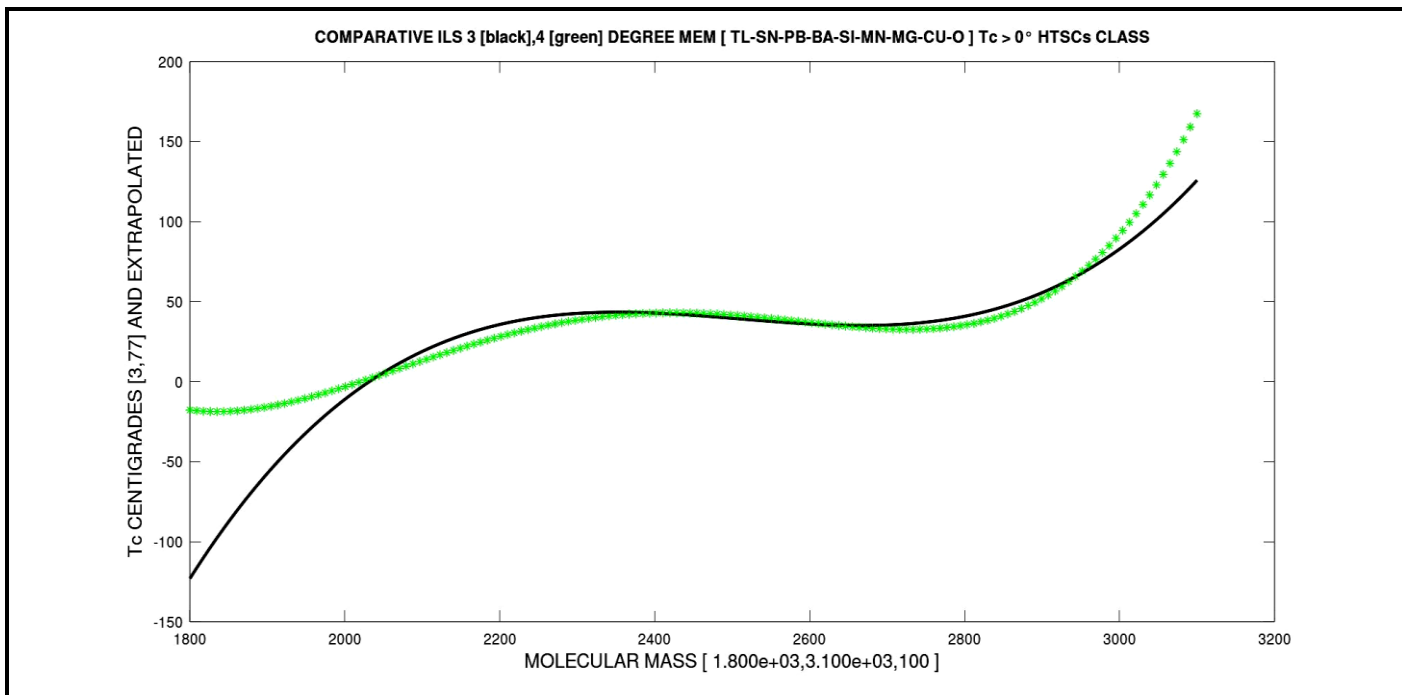


Figure 7. [Enhanced]- 3-4 Degree comparative dual-approach, GNU-Octave, with 3,4-Degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. 3-Degree (black) is linear, and it is seen how when passing on 4-Degree (green) polynomial the curve begins to take sinusoid shape. Overlap is almost complete along the experimental data line, which proves the fit correctness. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0^\circ$, MEM confirms clearly that affinity with the green 3,4-Degree shape. Enhanced in Appendix.