# NON-DESTRUCTIVE ESTIMATION OF SPATIALLY VARYING MATERIAL PROPERTIES AND INCLUSIONS IN 3D OBJECTS

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In many practical problems, physical properties of the material of an arbitrarily shaped three-dimensional object varies spatially, that is, throughout that object. Non-destructive methods that require strictly boundary measurements of the field variables to determine parameters defining the spatial distribution of the physical property of the material within the domain are needed. A methodology for non-destructive, accelerated inverse estimation of spatially varying material properties using only boundary measurements is presented. With advances in additive manufacturing, it is now possible to create three-dimensional objects that feature spatially varying thermo-physical properties. For example, when applied to the thermal diffusion problems, it can be stated as: For a specified temperature/heat flux distribution on the boundaries of a solid object, what should be the spatial variation of thermal conductivity in this domain that will create such temperature/heat flux distribution at the boundaries?

The spatial distribution of diffusion coefficient in 3D solid object is determined by minimizing the sum of the least-squares difference between measured and calculated values. The forward problem is solved using the finite volume and finite element methods, both of which were compared against analytical solution. The inverse problem was solved using an optimization technique to minimize the normalized sum of the least-square errors. The non-destructive estimation was accelerated by the use of surrogate models to solve the forward problem. The presented methodology is applied to measurements containing varying levels of noise. In addition, this inverse method can be used to detect the location, size and shape of a subdomain within a solid object and material property of the subdomain material.

The material properties such as thermal conductivity, electric permittivity, magnetic permeability, and concentration diffusivity, influence the spatial variation of the field quantities such as temperature, electric field potential, magnetic field potential, diffusion of non-reacting particles in a solid. These field problems can be modeled by an elliptic partial differential equation governing the steady-state diffusion of the field variable $\phi = \phi(x,y,z)$ where $\lambda = \lambda(x,y,z)$ is the diffusion coefficient. Using this mathematical model, the question to answer becomes: Using the boundary values of the field function, $\phi$, or its normal derivatives on the boundary of the solid, how can the spatial distribution of the diffusion coefficient $\lambda$ be determined throughout the arbitrarily shaped solid object?

Forward or analysis problem can be numerically integrated inside the arbitrarily shaped three-dimensional object using finite element or finite volume methods for a known distribution of $\lambda$ and Dirichlet or Neumann boundary conditions.

In the case of an inverse problem, the spatial distribution of $\lambda$ is not known and is to be determined iteratively. Non-destructive determination of the diffusion coefficient requires measured boundary values of $\phi = \phi(x,y,z)$ or the measured values of the normal derivative of $\phi = \phi(x,y,z)$ on the boundary of the solid object. The easiest and the most versatile method for solving this inverse problem is minimization of the properly scaled sum of differences between the computed $\phi$ or $\partial\phi / \partial n$ values on the boundaries subject to chosen values of the parameters in an analytic model for the spatial distribution of $\lambda$, and the measured $\phi$ or $\partial\phi / \partial n$ values on the boundaries. In this case, these unknown parameters need to be iteratively optimized to give an accurate match between the calculated and the measured boundary values of $\phi$ or $\partial\phi / \partial n$.

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# DEVELOPMENT OF HYBRID RESPONSE SURFACE ALGORITHMS AND HYBRID MULTI-OBJECTIVE OPTIMIZATION ALGORITHMS

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The FIU Multi-Objective Hybrid Optimizer (MOHO) is a High Level Relay Hybrid metaheuristic optimization algorithm. In its current version, three different evolutionary multi-objective search algorithms are coordinated and applied in order to expedite the search for a Pareto front. Like many other evolutionary algorithms, MOHO runs in steps of population generations. At each generation the algorithm that is selected creates a new generation using any or all of the information provided to it: the last generation's population and the latest non-dominated set. Then, the MOHO algorithm combines the new generation and the latest non-dominated set to create a new non-dominated set. MOHO keeps track of this process to detect five possible improvements to the dominated set (the Pareto approximation). If the particular search algorithm can achieve at least two of any of the five improvements, this algorithm is allowed to create the next generation.

If the search algorithm in question is not able to achieve at least two improvements, or it has consecutively run for the user-specified limiting number of iterations, the latest population and non-dominated set are passed to the next search algorithm. MOHO runs until the maximum number of function evaluations is performed. All optimization run parameters are specified by the user in an external input file.

We propose to develop robust and computationally efficient general purpose algorithmic systems using Bayesian statistics, hybrid response surface algorithms and hybrid multi-objective optimization algorithms:

1. Make use of a Bayesian approach based on Monte Carlo Markov Chain (MCMC) method based on the Metropolis-Hastings algorithm. This work deals with the use of radial basis functions (RBF) for the interpolation of the likelihood function in parameter estimation problems. We have successfully applied the proposed interpolation of the likelihood function to test cases of inverse problems in heat and mass transfer, solved with the Metropolis-Hastings algorithm. The use of the interpolated likelihood function reduces significantly the computational cost associated with the implementation of such MCMC method without loss of accuracy in the estimated parameters.
2. Use our method involving the fittest radial basis function polynomial for generation of multi-dimensional response surfaces. We have developed and successfully tested a preliminary version of this method that is offering superior accuracy of fitting multi-dimensional objective function topologies while requiring an order of magnitude less computing time than a number of other candidate methods currently in use by commercial software vendors.
3. Use our hybrid self-organizing multi-dimensional response surfaces generation method that uses locally optimized basis functions to fit arbitrary topologies of multi-dimensional discrete values of objective functions. We have developed and tested a preliminary version of this algorithm that automatically chooses among linear, quadratic, cubic, quartic and RBF polynomials as local basis functions to perform the most robust and accurate fits of response surfaces.
4. Use our robust hybrid multi-objective evolutionary optimization algorithm (with automatic switching among strength-Pareto evolutionary algorithm, particle swarm algorithm, non-sorting differential evolution algorithm) augmented with the addition of predator-prey algorithm thus further improving robustness and convergence to the Pareto front of this complex multi-objective optimization algorithm. The switching algorithm is designed to favor those search algorithms that quickly improve the Pareto approximation and grades improvements using five criteria.

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# INTERACTING HIGH FREQUENCY AND HIGH POWER ELECTRO-MAGNETO-HYDRO-DYNAMICS AND HEAT TRANSFER

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It is well known that simultaneously externally applied electric and magnetic fields can influence flow pattern of a moving liquid and convection heat transfer in a process known as Electro-Magneto-Hydro-Dynamics (EMHD) [1-3]. This paper analyzes computationally the high frequency, high intensity electric and magnetic fields combined with a strong convection/conduction (conjugate) heat transfer in the flowing liquid and the container walls. It also offers an answer to the intriguing question: Is it possible for cooling fluid and its flow-field and temperature field to influence high frequency and high intensity electric and magnetic fields. This “reverse EMHD” effect has been proven analytically to exist when physical properties vary significantly with temperature [4,5]. Numerical simulations were performed using a modified version of COMSOL software to explore possible back-influence of liquid flow on the high frequency (10MHz to 10GHz) electric and magnetic fields, while accounting for physical properties of liquid that depend on temperature and frequency of the applied fields.

Recently, the “reverse EMHD” effect was confirmed numerically [6] for cases of very weak, high frequency (10MHz to 10GHz) electric and magnetic fields in case of pure water and strong heat transfer (heat flux as high as 1000 W $cm^{-2}$) typical of integrated cooling of high power microelectronics. The objective of this work is to examine if such “reverse EMHD” effect is significant also in cases of very strong high frequency electric fields applied to strong conjugate heat transfer. Moreover, since the “reverse EMHD” effect was not noticeable in the case of very weak high frequency magnetic fields [6], it is of interest if this effect is important in case of very strong high frequency electric and magnetic fields applied together with strong conjugate heat transfer. All simulations were fully three-dimensional, fluids were pure water and sea water, and flow was steady and laminar. Electric conductivity was treated as a function of temperature, while real and imaginary parts of the electric permittivity were treated as dependent on frequency, temperature and salinity of the cooling liquid.

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# MULTI-OBJECTIVE DESIGN OPTIMIZATION OF CHEMISTRY OF ALLOYS

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A novel approach is presented here for creating a work plan for efficiently using a set of computational tools for the design of alloy chemistry and multi-objective optimization of desired macroscopic properties of various alloys. This approach combines information from limited experimental databases with focus on stability of critical phases/structures while utilizing a number of numerical design optimization algorithms. These algorithms are based on several concepts from artificial intelligence including supervised and unsupervised machine learning algorithms.

We selected eight alloying elements and set their concentration bounds after literature review. Composition of the initial batch of 80 alloys was predicted by Sobol's quasi-random sequences generation algorithm. These alloys were screened on the basis of phase equilibrium using Thermocalc and Factsage software. A recent work from the developers of this software demonstrates the importance of phase transition diagrams and we have also reported it in our recent works. We performed a few *ab-initio* based calculations to estimate the stable structures through open source database, Materials Project that has been categorized on the basis of magnetic ordering and stability. Both *ab-initio* calculations and phase transformation diagrams through CALPHAD approach are effective for predicting properties of alloys with up to four alloying elements. A combined experimental-computational methodology for accelerated design of AlNiCo type permanent magnetic alloys is presented with the objective of simultaneously extremizing several magnetic properties. Chemical concentrations of eight alloying elements were initially generated using a quasi-random number generator so as to achieve a uniform distribution in the design variable space. It was followed by manufacture and experimental evaluation of these alloys using an identical thermo-magnetic protocol. This experimental data was used to develop meta-models capable of directly relating the chemical composition with desired macroscopic properties of the alloys. These properties were simultaneously optimized to predict chemical compositions that result in improvement of properties.

This data was further utilized to discover various correlations within the experimental dataset by using concepts of artificial intelligence. In this work, an unsupervised neural network known as Self Organizing Maps (SOMs), was used to discover various patterns reported in the literature. These maps were also used to screen the composition of the next set of alloys to be manufactured and tested in the next iterative cycle. Several of these Pareto-optimized predictions out-performed the initial batch of alloys. This approach helps significantly reducing the time and the number of alloys needed in the alloy development process.

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# MULTI-SCALE INVERSE ANALYSIS AND DESIGN OF MICROFIBER AND NANO-PARTICLE LADEN MATERIALS

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It is well known that defects in short fiber composites are often due to uncontrolled fiber orientation and concentration during composites manufacturing. These defects can significantly reduce the functionality of the composite material. Also, in many applications it would be highly desirable to have directional dependence of physical properties of the material, that is, to have strongly non-isotropic materials. This implies that it would be of interest to perform curing of the resin in such a way that the local concentration and orientation of the fibers is fully controlled. During a controlled solidification process from a melt, it is important to understand the process of solid phase formation. The accumulated solid phase effectively reduces and deforms the cross sectional area of the passages and causes significant local variations in pressure and melt flow-field shear stresses. During the solidification process, melt flow is generated due to strong thermal buoyancy forces. This process cannot be effectively controlled in the case of strong heat transfer, except if influenced by a global body force. One such body force is the general electromagnetic Lorentz force that is created in any electrically conducting fluid when either a magnetic field or an electric field is applied.

The objective of this work is to explore the feasibility of manufacturing specialty metal matrix and polymer composite materials that will have specified (desired) locally directional variation of bulk physical properties like thermal and electrical conductivity, modulus of elasticity, thermal expansion coefficient, etc. The fundamental concept is based on specifying a desired pattern of orientations and spacing of micro fibers or particles in the final composite material product. Then, the task is to determine the proper strengths, locations, and orientations of magnets and/or electrodes that will have to be placed along the boundaries of the curing composite, so that the resulting magnetic field or electric field lines of force will coincide with the specified (desired) pattern of the matrix distribution. The basic idea is that the fibers will align with the local magnetic or electric lines of force.

This project deals with the development of an appropriate software package for the numerical solution of the partial differential equation system governing electro-magneto-hydro-dynamics (EMHD) involving combined fluid flow, electric and magnetic fields, as well as heat transfer that includes liquid-solid phase change. It also uses constrained optimization software that is capable of automatically determining the correct strengths, locations, and orientations of a finite number of magnets that will produce the electric/magnetic field force pattern which coincides with the desired and specified fiber/particle concentration and orientation pattern in the curing composite material part. A crucial aspect for achieving this goal relies on developing consistent links between macro and micro levels, through multi-scale modeling, such as homogenization techniques. Homogenization, considering stochastically and periodically distributed heterogeneities will be considered in order to determine the effective thermal and mechanical properties of the composites, which shall be compared to the target properties, during the solution of the inverse design problem.

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# NON-DESTRUCTIVE EVALUATION OF UNSTEADY ULTRA-HIGH HEAT FLUXES

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The objective of this project is to develop a new class of robust inverse algorithms capable of reliably determining ultra-high (of the order of tens of kilowats per square centimeter) unsteady heat fluxes applied on inaccessible surfaces and perform these calculations in real time.

Identification of high magnitude heat fluxes in real time is a challenging problem, since most of the currently available algorithms require large computing times in comparison with the time scale of the real physical problem. Furthermore, the existing inverse determination algorithms suffer from problems of numerical stability, thus requiring sophisticated regularization techniques which consume additional computing time and allow for only relatively small errors in the measurement data. This proposal presents a methodology that promises to allow for quantifying the locations and magnitudes of multiple unsteady high heat fluxes (hot spots) and their corresponding extremely fast rising temperatures in real time by developing new inverse algorithms based on variants of Steady-State Kalman Filter.

The novel concepts used in the proposed work include development of reduced models for non-linear heat conduction in 3D arbitrarily shaped solid objects utilizing classical lumped analysis and an improved lumped analysis. The inverse analysis of estimating the heat flux $q(x,y,t)$ by using measurements of the temperature $T(x,y,0,t)$ is recast in the form of a state estimation problem within the Bayesian framework. Thus, the problem is modeled in the form of the evolution-observation model. The estimation of the state vector with measurements that are related to the state vector by the observation model can be efficiently solved by the technique known as the Steady-State Kalman Filter. The name *Steady-State* refers to the time-invariant values of certain matrices, although the system is highly dynamic. This algorithm is a very attractive choice, because of the significant reduction of the number of operations in comparison with the classic Kalman Filter method. Preliminary results presented in this proposal already demonstrate the ability of the basic version of the proposed inverse determination algorithms to predict multiple suddenly imposed very high heat fluxes in less than two seconds of computing time. This is more than one order of magnitude shorter time than required by the currently used methods.

In many practical problems it is highly desirable to computationally predict an unsteady process in order to effectively control it when only indirect measurements are available. When this analysis is performed in "whole-domain", *i.e.,* all experimental measurements are processed at once, the inverse problem is solved off-line and limitations in computation time are not so restrictive. However, when this estimation process is performed sequentially, where each measurement is processed at the moment that it is acquired, the computations take more time than the measurements. One example of how recursive estimation can still be a computationally challenging problem is identifying locally applied unsteady high magnitude heat fluxes in a three dimensional heat conduction problem. In this problem, the heat flux applied on one boundary of a given geometry is estimated by taking temperature measurements on another boundary. For example, detecting locations and magnitudes of the rapidly growing heat fluxes (and corresponding temperatures) at multiple hot spots on inaccessible surfaces and performing this prediction in real time is of significant importance to designers of high power density electronic circuitry. The same inverse problems solution is also highly pertinent in biomedical engineering when performing laser ablation of living tissues. In the era of the growing importance of various directed energy weapons, it is the matter of essential survival to detect the location and the magnitude of the ultra-high heat flux at the impact of such an energy beam and to do this detection within a second so that an evasive maneuver can be performed to avoid an explosive growth of temperature at a hot spot.

# MULTI-OBJECTIVE OPTIMIZATION OF LIQUID FUEL MIXTURES

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We propose to solve the problem of developing superior liquid fuel mixtures for marine combustion engines by utilizing a combination of experimental data, computational combustion results, and a hybrid constrained evolutionary multi-objective optimization strategy. Fuel compositions will be developed and optimized by performing combustion and deposit tests in an experimental facility fully instrumented and utilizing a multi-objective multidimensional response surface hybrid optimizer to indicate possible fuel candidates to achieve more efficient and lean combustion. This iterative interaction between numerical and experimental work will reduce the cost and time needed for the experimental evaluation of the fuels, while maintaining a good accuracy of the numerical prediction analysis and optimization.

Regarding the Cetane number, that measures the quality of fuels used in Diesel engines, it is well known that the type of C-H chains used to produce the fuel affects considerably the quality of the ignition. Hydrocarbons with long non-cyclic single-bound chains, such as the Paraffins usually have better combustion characteristics for Diesel engines than double-bounded chains (e.g. Olefins) or ring structure hydrocarbons such as the Cycloparaffins and the Aromatics.

On the other hand, for Otto engines, where the quality of combustion is measured by the Octane number, the situation is inverted. Since Diesel and gasoline fuels are actually made of a mixture of different C-H chains, whose manufacturing process is very dependent on the type of crude oil used and also on certain economic factors, the optimization of such blends is also of utmost relevance to obtain more efficient fuels. Concerning Diesel engines, the optimization of ternary mixtures of Diesel-biodiesel-ethanol has been considered for several years as a way to decrease the particulate matter by the addition of the biodiesel and also keep the NOx emissions low by the use of hydrous ethanol. The use of biodiesel as an additive to Diesel fuel has several advantages. One of the most important advantages is the fact that such additives provide extra lubricity to the fuel, a factor that usually is lost when the level of sulfur in Diesel fuel is decreased to meet the emissions regulations. Objectives of fuel mixtures optimization are:

It is evident that there is a strong need to optimize fuel compositions in order to:

(i) Meet the gaseous and particulate matter emission regulations;
(ii) Increase the power of engines;
(iii) Avoid fouling of fuel injectors;
(iv) Promote fuel stability and lubricity;
(v) Do not alter current engine materials.

This cannot be achieved without a proper design of experiments and a multi-objective constrained optimization process. Also, since the carbon-hydrogen chains can vary with time due to economic and logistic reasons, the use of a rational response surface methodology is crucial to avoid an excessive use of very expensive and time-consuming experimentation.

**We propose to use our hybrid constrained multi-objective evolutionary optimization algorithms and multi-dimensional response surface generation algorithms in conjunction with experimental data provided by the UFRJ-Brazilian subcontractor team and with numerical analysis of combustion data and multi-objective optimization performed at Florida International University.**

Objectives are to obtain fuel mixtures with the following characteristics:

- High values of lower heating values,
- Low gaseous and particulate matter emissions,
- Low fouling tendency, and
- Low corrosion tendency.