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Low cost surrogate model based evolutionary optimization solvers for inverse heat conduction problem

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1. Introduction

An inverse heat transfer problem is a problem in which the temperatures at some locations inside a domain are known, while one or some of the boundary or initial conditions, or material properties are missing. In this research, our focus will be on the case where we try to find an unknown boundary condition in a heat conduction problem; however, the developed procedures are easily applicable to other cases as well. Because the effects of altering the boundary conditions are generally damped and lagged in the internal sensors, the problem would be characteristically ill-posed, and a high level of sensitivity to the measurement errors is observed. In general, the uniqueness and stability of the solution to an inverse heat conduction problem (IHCP) are not guaranteed [1]. This illposedness is commonly treated by means of one or a mixture of some regularization techniques, e.g. Tikhonov regularization [2], the future information method [1], or the iterative regularization technique [3].

In the last two decades, various numerical algorithms have been developed to obtain a reliable inverse heat transfer solution. The most commonly used methods are the least square regularization method [1], the sequential function specification approach [3], the space marching technique [4], conjugate gradient algorithm [5], steepest descent method [6], the model reduction method [7], genetic algorithms (GA) [8], artificial neural networks [9], and particle swarm optimization [10].

ABSTRACT

Using temperature measurements from inside a solid to determine boundary conditions is a common inverse heat conduction problem. These problems are ill-posed and a robust mathematical solution is not available. Stochastical search algorithms like genetic algorithm (GA) and particle swarm optimization (PSO) have been found to be effective in dealing with these problems. However, they require large population size and do not use the gradient information and, therefore, their computational costs are higher than their gradient based alternatives. This is especially true when using a computationally expensive method like finite element analysis as the direct solver. A computationally cheaper substitute is using surrogate models. They construct an approximation to the direct problem using a set of available data and the underlying physics of the problem. This idea has been employed in this research. The result is a method that has the stability and effectiveness of evolutionary algorithms with a much lower computational cost.

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One major drawback in using the evolutionary algorithms in inverse heat conduction problems is their much higher computational expense compared to the classical gradient-based methods. The problem is especially significant when solving large multi-dimensional problems with transient behavior with many time steps. Several researchers have tried to find remedies for this shortcoming. For example, Tian et al. [11] proposed a hybrid method that combines PSO and conjugate gradient methods to solve the inverse heat conduction problem. Also, the authors [12] tried to modify the basic implementation of PSO to achieve faster convergence in inverse heat conduction applications, especially when multidimensional and transient problems are solved, by using a sequential implementation instead of a whole domain approach and incorporating the concept of future time steps to make it more stable, using a vectorized objective function for the multi-sensor cases, and borrowing the idea of elite members from genetic algorithms. While the resulting algorithm showed better performance than the original implementation, it is still slower compared to the gradient-based algorithms.

Using surrogate models to quickly pre-evaluate the solution is another way to accelerate evolutionary optimization algorithms. If we carefully investigate the contribution of different parts of a stochastical method like GA or PSO to the whole required computational time, it is clear that a major portion of the time is consumed in the solution of the direct problem, in order to obtain the value of the objective function. However, in most cases the exact value of the objective function is not required. In such cases, solving the direct problem using a high-fidelity and expensive simulator like finite element method is not necessary. As a remedy,

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Nomenclature			
C ₀ C ₁ , C ₂ , C ₃	self-confidence parameter in particle swarm method , c_4 acceleration coefficients in particle swarm method	<i>x</i> , <i>y</i> , <i>z</i>	Cartesian coordinates, m
C _p	specific heat, J/kg °C	Greek letters	
ģ	best global solution	α	regularization parameter
h	heat transfer coefficient, W/m °C	β	polynomial coefficients in surrogate modeling
Ι	improvement in a predicted value in surrogate models	Δ	change in a quantity
k	conductivity, W/m °C	ρ	density, kg/m ³
р	best solution of a particle	ψ	radial basis function
r	normally distributed random vector	ω	weights in radial basis function surrogate model
Т	temperature, °C		
t	time, s; student <i>t</i> -test value	Superscripts	
ν	velocity of particles in particle swarm method	calc	calculated
x	position (value) of a particle in particle swarm method	meas	measured

some researchers have recently used surrogate models [13] instead of full direct simulations to lower the computational cost of stochastical search algorithms. For example, Praveen and Duvigneau [13] have used the concept of metamodels and inexact preevaluations to accelerate PSO in the aerodynamic shape optimization application. Also, Bilicz et al. [14] applied this idea to eddy current non-destructive evaluation. The work by Frangos et al. [15] reviews several methods that can be used to reduce the computational complexity of statistical inverse problems, including the use of surrogate models.

Considering the success of surrogate models in other areas of inverse problems, they would be expected to be equally beneficial in inverse heat conduction problems. Reviewing the literature indicates that there has been limited work in this area [16], and there is a certain need to explore and examine different variations of surrogate models in solving real-world inverse heat conduction problems. In this research, we try to utilize the idea of inexact pre-evaluations using surrogate models to speed up our developed GA and PSO algorithm in solving the inverse heat conduction problem.

2. Direct and inverse formulation

In this study, the finite element method is used to solve the direct (forward) heat conduction problem. First, a brief description of the direct heat conduction equations and the discretized finite element equations is given below for completeness. More detailed account may be found in Refs. [17,18]. Then, the inverse heat conduction problem is defined in the form of an objective function.

2.1. Governing equation and boundary conditions

The general governing equation for the 3D conduction heat transfer problem can be written as

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) + q^b = c_p \rho \frac{\partial T}{\partial t} \tag{1}$$

where *T* is the temperature, °C; q^b is the heat generation per unit volume, W/m³; k_x , k_y , and k_z are the conductivities in the *x*-, *y*-, and *z*-directions, respectively, W/m °C; ρ is the density, kg/m³; c_p is the specific heat, J/kg °C; *t* is the time, s; and *x*, *y*, and *z* are the Cartesian coordinates of a point.

The boundary conditions may be one or a combination of the followings cases: Prescribed temperature $(T = T_s(x,y,z,t))$, prescribed heat flux $\left(-\left(k_x \frac{\partial T}{\partial x} + k_y \frac{\partial T}{\partial y} + k_z \frac{\partial T}{\partial z}\right) = q_s(x,y,z,t)\right)$, convective

heat exchange $\left(-\left(k_x\frac{\partial T}{\partial x}+k_y\frac{\partial T}{\partial y}+k_z\frac{\partial T}{\partial z}\right)=h(T_s-T_f)\right)$, and/or radiation $\left(-\left(k_x\frac{\partial T}{\partial x}+k_y\frac{\partial T}{\partial y}+k_z\frac{\partial T}{\partial z}\right)=\varepsilon\sigma\left[T_{sr}^4-T_r^4\right]\right)$.

2.2. Finite element formulation

We assume an approximation function for the temperature given by

$$T(\mathbf{x}) = N_i(\mathbf{x})T_i \tag{2}$$

where $N_i(\mathbf{x})$ is the shape function with *i* varying from one to the number of nodes per element, the vector \mathbf{x} has the components *x*, *y* and *z*, and T_i are the nodal temperatures. Using a weighted residual Galerkin procedure, the final finite element equations may be written as follows:

$$\begin{split} & [C] \cdot \{\tilde{T}^e\} + ([K_c] + [K_h] + [K_r]) \cdot \{T^e\} \\ & = \{Q\}^b + \{Q\}^s + \{Q\}^h + \{Q\}^r \end{split}$$
(3)

where *C* is the equivalent heat capacity matrix; *K* is the equivalent heat conductivity matrix; *T* and \dot{T} are vectors of the nodal temperature and its derivative with respect to time, respectively; and *Q* is the equivalent load vector. Detailed expressions of these matrices can be found in the literature [17,18], and will not be repeated here.

2.3. Inverse formulation

The boundary inverse heat conduction problem can be formulated as an optimization problem in which we try to minimize the norm of difference between the measured temperatures obtained from an experiment or a simulated experiment and the calculated temperatures obtained from a direct solution of the problem with some guessed boundary conditions. In order to damp the oscillations in the solution, and make the algorithm more stable in dealing with noisy measurement data, it is very common to include more variables in the objective function. A common choice in inverse heat transfer problems is to use a scalar quantity based on the boundary heat fluxes, with a weighting parameter α , which is normally called the regularization parameter. The regularization term can be related to the values of heat flux, or their first or second derivatives with respect to time or space. Based on the previous experience [18], as well as our own trial of different regularization terms, we choose to use the heat flux values (zeroth-order regularization). The objective function then will be

$$f(q) = \sum_{j=1}^{J} \left(\sum_{i=1}^{N} \left(T_j^{i,meas} - T_j^{i,calc} \right)^2 + \alpha \sum_{i=1}^{N} \left(q_j^i \right)^2 \right)$$
(4)

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