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Computational Modeling of Functionally Graded Materials via a Parallel Domain Decomposition Algorithm

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Summary

The grading of material properties to optimize their performance for specific applications is a relatively new area of materials research having many potential energy related applications. Most commonly, a graded material is constructed so that the shear modulus of the solid varies in one direction; for example, a graded material could behave as a metal on one side of a cube, a ceramic on the opposite end, and transition continuously between the two. The goal of this work is to develop advanced computational tools for modeling this class of non-homogeneous materials. A domain decomposition algorithm based upon singular integral equations has been developed and implemented for parallel computers. This computational method is therefore capable of analyzing real world situations involving complex geometries wherein the grading changes with position.

A specific energy-related application that has stimulated the research and development of Functionally Graded Materials (FGMs) involves *thermal barrier coatings*. In electric power generation (or aircraft engines), thin ceramic coatings are employed to protect the metal turbine blades from heat, hopefully allowing the turbine to run at higher temperatures. The turbine is more efficient at higher temperatures, and even a small increase in efficiency can result in large economic savings.

Unfortunately, the sharp transition from metal turbine blade to ceramic coating leads to high stress concentrations near the interface of the two materials. As a consequence, the coating will often fracture and fall off, and the turbine must be run at lower temperatures to avoid damaging the blades. The simple idea of a graded material is to try to transition continuously from the base metal to the ceramic, thereby creating a coating that avoids a sharp interface. Without the stress concentration, this coating should be much stronger and less prone to failure.

Numerical methods for elasticity based upon singular integral equations have been very successful, particularly for fracture mechanics. However, almost all of this work has been for homogeneous materials. The goal of this work has been to extend these techniques to the much more difficult non-homogeneous graded material. The primary challenge is that the integral equation approach is based upon a *fundamental solution* (Green's function), and the FGM function is significantly more

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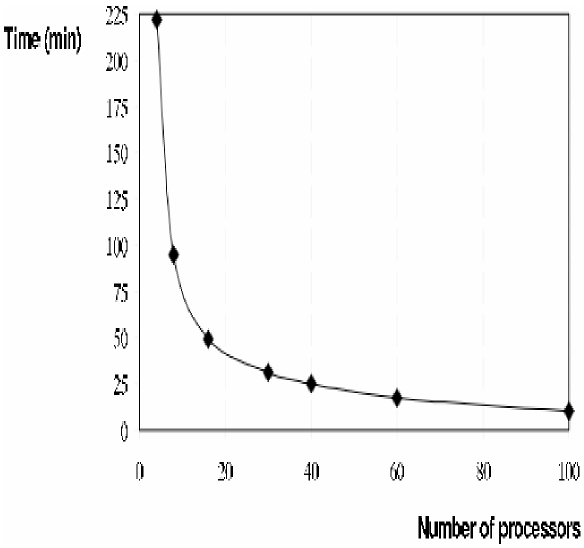
complicated than that for a homogeneous material.

We have now developed a computational simulation of an FGM that employs a domain decomposition method for solving the integral equations. The full geometry is decomposed into small sub-domains, and while the grading direction is constant in each small piece, its value can vary depending upon the sub-domain. This allows the analysis of complicated geometries, such as the turbine blade. Domain decomposition, particularly for thin coating geometries, also reduces the computational effort, as the integrations are carried out over smaller surfaces.

Nevertheless, the computational effort required is significant, as the evaluation of the FGM fundamental solution is quite time-consuming. We have therefore implemented the algorithm for parallel computing, and as indicated in the figure, the total computation time scales very well with the number of processors.

In addition to thermal barrier coatings, FGMs have been studied for, applications in bio-medicine (bone and dental implants), defense (vehicle and personal body armor), electromagnetic sensors, and optics.



Computation time versus number of processors for an FGM calculation.

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