Office of Science
U.S. DEPARTMENT OF ENERGY

Advanced Scientific Computing Research
FY 2004 Accomplishment

Evaluation of Function Derivatives in Boundary Integral Analysis

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Summary

A fast and accurate boundary integral method for evaluating first and second order function derivatives has been developed. This is a key step in many boundary integral applications, most notably for computing surface velocities in moving boundary simulations, and for developing a Hermite interpolation algorithm.

Boundary integral equations are particularly well suited for an important class of applications known as “moving boundary problems”. The goal in these simulations is to track the evolution of a surface, and the boundary integral approach only requires remeshing of the new surface; this is significantly easier than remeshing the entire volume. Example applications are void growth in computer chip interconnects (electromigration), propagation of water waves, crystallization of solids, etc. The key task in these calculations is an accurate determination of the surface velocity function, and this generally requires knowing all first order function derivatives, e.g. gradient of potential or complete stress tensor, on the surface.

These derivatives can be expressed as boundary integrals of known quantities, but there are two main difficulties in their numerical evaluation. The first is that the integrals involve highly singular functions, termed hypersingular. As a consequence the integrals do not exist unless conditions are placed on the numerical approximations, and these conditions are very difficult to enforce. The second problem is that the expressions for the derivatives involve a complete integration over the boundary, and this is computationally very expensive.

A previously developed first-order derivative evaluation algorithm [1] was able to eliminate these difficulties. This was achieved by recasting the integral expressions using a weighted average (Galerkin) formulation and employing a boundary limit analysis to evaluate the hypersingular integrals [2]. As a consequence, instead of the full double boundary integration, only a few integrals over the local neighborhood of each point need to be computed.

An added benefit of this new algorithm is accuracy. The calculation is limited to local integrals that are evaluated partly analytically, eliminating many sources of error (numerical quadrature, function interpolation). As a result, test calculations indicate that the method is superconvergent: a linear element approximation achieves quadratic convergence.
A technologically important example of a moving boundary problem is the simulation of crystal growth. In order to follow the crystal evolution, an accurate determination of the interface velocity is essential. The

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recrystallization of amorphous silicon (see in Fig 1), which has significant implications for electronic device fabrication, is one such application.

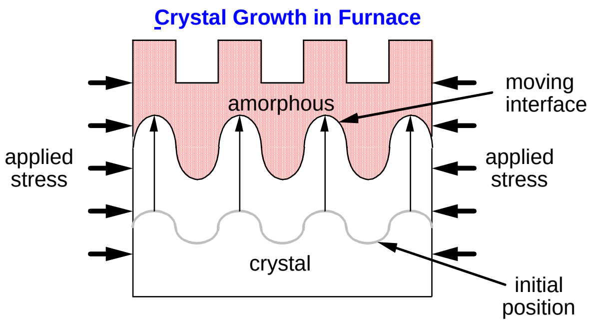

Fig 1. Experimental set up for the recrystallization of amorphous silicon. This is an example of an experiment in which the surface derivative technique will be employed to calculate the interface velocity.

We have now extended this work to the evaluation of ***second order function derivatives*** on the boundary. Although the singular integrals are now *worse* than hypersingular, the interior and exterior limit analysis succeeds in producing a well defined finite value. As with first order, second order derivatives can be evaluated without a complete boundary integration, only local integrations are required. One important consequence of this work is that a complete cubic Hermite approximation, suitable for use in moving boundary simulations, can now be developed.

[1] L .J. Gray, A.-V. Phan, and T. Kaplan, "Boundary Integral Evaluation of Surface Derivatives," *SIAM J. Scientific Computing* (in press)

[2] L. J. Gray, J. M. Glaeser, and T. Kaplan, "Direct Evaluation of Hypersingular Galerkin Surface Integrals," *SIAM J. Scientific Computing* **25**, pp. 1534-1556 (2004).

[3] M. N. Moore, L. J. Gray, and T. Kaplan, “Evaluation of Second Order Derivatives in the Boundary Element Method,” (in preparation)

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