Meeting Fracture-based Requirements in the Aerospace Industry

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Abstract

In the aerospace industry, fracture requirements are usually expressed in a document titled "Fracture Control Implementation Plan (FCIP)."

The plan specifies the fracture control criteria and procedures to be implemented on a specific program. The primary objective of these controls is to preclude flaw-induced structural failures that could imperil a mission or a Space Transportation System and its crew.
Meeting the criteria and procedures set in the FCIP is the responsibility of the program system safety engineer (SSE). The SSE maintains close communication with the design and analysis functions, where all structural components are evaluated for fracture criticality. All structural components are fracture critical, unless they fall into one or more of the following categories: fail-safe components, low-release mass components, contained parts, or low-risk parts. Fracture critical components are subjected to tractability, NDE, and safe-life analysis. Safe-life analysis is an expensive analystical requirement, where an engineer must show that a flaw of non-detectable size, oriented in the most critical direction, will not undergo unstable crack growth during its life.

This communication will discuss current analytical procedures used in safe-life analysis, their usage, effectiveness and applicability. The need for the development of new tools based on Greens functions and boundary integral methods is discussed.

A COMPARISON OF THREE METHODS FOR NUMERICALLY COMPUTING THE ANISOTROPIC ELASTIC GREEN'S TENSOR AND ITS DERIVATIVES

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ABSTRACT

At present there exist three methods for the numerical computation of the anisotropic elastic Green's tensor and its first two derivatives. Such numerical data is essential for performing 3-dimensional boundary integral equation calculations and for computing the shapes and interactions of dislocation loops in 3-D simulations of dislocation kinetics and pattern formation. The three methods are (1) a Fourier-transform based reduction which involves a simple numerical integration of real functions on $[0, \pi]$, (2) an iteration technique based on A. N. Stroh's 6 x 6 [N] matrix as suggested by Lothe and Gundersen, and (3) a direct method based on angular derivatives of Stroh's eigenvectors as discussed initially by Malen and Lothe for dislocation energy factors. Here we compare relative computation speeds and accuracy of the methods and discuss storage of these data over the unit sphere of directions for effecting subsequent elastic computations. The method is easily extended to piezoelectric solids.

Building the Green's Functions Digital Library

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This presentation describes the primary components of the **G**reen's Functions **R**esearch and **E**ducation **E**nhancement **N**etwork (GREEN) as part of the NSF National Science, Mathematics, Engineering, Technology Education Digital Library. The GREEN project is a collaboration of the National Institute of Standards and Technology, Kent State University, and Massachusetts Institute of Technology and will include an organized collection of research and educational materials on Green's functions to serve undergraduate, graduate, and professional communities. To meet this end, an information infrastructure has been designed around an Archive, Code Repository, Problem Bank, and Teaching Resources. This presentation discusses on the first phase of the information infrastructure including the metadata repository, the submission process, and the review policy.

Survey of Green's Function Research Related to Transient Heat Conduction

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In our research related to the use of Green's functions in transient heat conduction, many phases have been covered. Recently the motivation is to obtain for three-dimensional bodies extremely accurate numerical values intended for use in verification of complex finite element and control volume codes. Based on Green's functions we have written codes that produce these accurate values and can also be used to obtain certain insights that are more difficult to obtain with approximate numerical methods.

A great many Green's functions (GFs) have been compiled, some of which are cataloged in our book [1] and on our website, BeckEng.com. Because so many GFs have been found, it was expedient to invent a numbering system for conduction solutions for bodies of simple shapes. It builds upon the common terminology of boundary conditions of the first, second and third kinds, which are temperature, heat flux and convective conditions, respectively. A zeroth kind is also proposed for locations where a physical boundary is not present, such as at infinity. An algebra based on this numbering system is possible. This system can be extended to other fields besides heat conduction.

Green's functions have been tabulated for the x-direction in Cartesian coordinates. For parallelepipeds, the 3D GFs are simply the product of three 1D GFs. In most cases two forms of these GFs are given, one coming from the separation of variables and the other from the Laplace transform. A GF can be denoted as $G(x,t|x',t)$ where the point of interest is at x and time t and the impulse is at x' and time t. The Laplace transform type GFs are most efficient for "small" values of $t - t$ and the separation of variable type for "large" values of $t - t$.

Radial and angular cylindrical GFs are also given along with radial spherical GFs. Using transformations it is also possible to give some GFs for solid body flow in Cartesian coordinates. A number of these GFs are available. Care must be taken with the transformations of the boundary conditions with these Green's functions; some unexpected eigenvalues appear.

Another major effort is in the derivation of steady state and transient GFs for a two-layer parallelepiped. These can be challenging from many respects, including imaginary eigenvalues.

Two different procedures have been developed to use the transient GFs for calculating temperature and heat fluxes. We have called the first procedure "time partitioning." In this method two different forms of the GFs are used. Forms of the expressions have been (*contd next page*)

(James Beck's abstract—continued from the previous page)

developed for the GFs evaluated at the boundaries for the various conditions; also integrated over the surface; and derivatives for the heat fluxes. After these results an integration over *t* is needed. Until the partition time, only the short time type (Laplace transform type) is

needed. Beyond that time, both are used. For two- and three-dimensional problems, the integration over *t* for short time GFs is done numerically. The time partitioning procedure is a very powerful method and a computer code called COND3D has been written using it. A great many cases are treated for a homogeneous parallelepiped for various boundary conditions of the 1st, 2nd pr 3rd kinds at each of the six surfaces. A volume energy generation term and nonzero initial temperature are also treated. However, in each of these cases the prescribed boundary temperature (or heat flux or ambient temperature) is a constant with space and time, as is the volume energy generation term. The initial temperature is also treated as a constant. Extremely accurate values are readily obtained, up to 8 or more significant figures.

Currently another program for a homogeneous parallelepiped is being written using the time partitioning method but it also permits certain functional forms of the spatial and temporal dependence of the boundary conditions and volume energy generation term. The same functional forms are allowed in the initial temperature distribution. The functional forms include linear, parabolic and exponential on time and position. All of these features are accommodated using Green's functions. An additional feature is treatment of solid body motion.

We have called the second procedure "spatial partitioning." It was devised to avoid the need of numerical integration over *t*. In this method of partitioning the spatial domain is first made small at the early times and then the spatial domain of interest is gradually increased. A temporal domain is associated with each of these spatial domains; only a small temporal segment is taken at each domain. Superposition of the temperature (or heat flux components) from each of these domains yields the desired numerical values. This concept can be used for homogeneous and nonhomogeneous bodies. A computer code is being written using this concept for a two-layer parallelepiped.

This research has been supported by Sandia National Laboratories at Albuquerque, NM and Dr. Kevin Dowding is the project manager.

Reference

1. J.V. Beck, K.D. Cole, A. Haji-Sheikh and B. Litkouhi, Heat Conduction Using Green's Functions, Hemisphere Press, Washington, D.C., 1992.

Green's functions and applications for steady-state heat transfer in functionally graded and materials.

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Functionally graded materials (FGMs) are designed with spatial variations in elastic, thermal, magnetic, or optical properties for optimal performance. Some examples of FGMs are thermal barrier coatings, bone implants, piezoelectric sensors, and graded optical index components. In this talk, Green's functions will be developed for the steady-state heat transfer problem in FGMs. Both isotropic and anisotropic thermal conductivities will be considered. The developed Green's functions will be used in numerical simulations with the Method of Fundamental Solutions. Results for problems with Dirichlet and Neumann boundary conditions will be presented, and some recent results on an inverse problem in a graded material will be shown.

Steady Heat Conduction in Cartesian Coordinates and a Library of Green's Functions

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In this talk steady heat conduction in Cartesian coordinates is discussed with the method of Green's functions (GF) for the slab, the rectangle, and the parallelepiped. The temperature problem is stated and the solution is given in the form of integrals involving the GF. The commonality among the components of 1-D, 2-D and 3-D GF is emphasized. Although the GF for each geometry is mathematically unique, there are at least two and sometimes several alternative expressions for each GF. Because the numerical convergence behavior of the alternative GF can be very different, an understanding of the alternative GF is important for rapidly-converging numerical evaluation of the GF. An internet site were these GF are available is briefly discussed. This work was supported by Sandia National Laboratory as part of a project to compute high-accuracy values for temperature and heat flux in the parallelepiped for verification of fully-numeric computer codes.

NSDL and Its "Core Integration" Effort

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The National Science Digital Library (NSDL) is a distributed network of resources that--through a "Core Integration" effort--function as a single, well-organized library. The NSDL purpose is to catalyze and support continual improvements in science, technology, engineering, and mathematics education, at all levels of instruction in all settings, formal and informal. This talk outlines the Core Integration project, led by the University Corporation for Atmospheric Research, Cornell University, and Columbia University, touching on the transformative potential of an effectively integrated NSDL.

Possible Applications for Green's Functions in Simulation Software

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The use of computer programs to solve field equations for temperatures, stresses, fluid velocities and other data becomes a more wide spread part of the industrial design process every year. Simulation programs most often use finite element, finite volume, or boundary element-based techniques. Improvement of the performance of simulation computer programs by using Green's functions as part of the field equation solution is an intriguing possibility.

As an example, the 3-D boundary element code *Lanis,* developed by Pan, Yang and Yuan uses multi-layered Green's functions as part of structural analysis of joints made with composite materials.

Another possible application for Green's Functions is in the simulation of the electric fields in integrated circuit (IC) devices. Maintaining signal integrity is vitally important to IC designers. Ideally, a solution of the 3-D Maxwell's Equations for the electric field (*E*) and magnetic field (*B*) in the devices would be used to calculate parasitic losses and to test how well a design maintains signal integrity. However, computing times for conventional finite element solution of the wave equations based on the Ritz or Galerkin methods are beyond what can be tolerated in a rapid design cycle. A solution based on based on a Green's function could have the potential to be more rapid and therefore be more practical.

Unfortunately, the Green's function solutions that are widely known seem to be for unbounded domains. IC packages are made up of multiple layers, each layer of different materials.

Of particular interest would be a Green's Function solutions for a layered domain using a continuity boundary condition between layers. Continuity boundary condition is used to mean the specification that the components of the fields tangential to the layer boundary are equal on both sides of the layer, and the normal flux obeys the condition:

$$E_{n1} \cdot \boldsymbol{e}_a = E_{n2} \cdot \boldsymbol{e}_2$$

$$\frac{B_{1t}}{B_{2t}} = \frac{\mu_1}{\mu_2}$$

where å is the dielectric constant, and μ is the permeability.

Direct Evaluation of 3D Hypersingular Integrals

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Direct algorithms for evaluating hypersingular integrals arising in a three-dimensional Galerkin boundary element analysis are presented. By integrating two of the four dimensions analytically, the coincident singular integral (defined as a limit to the boundary) is shown to be divergent. However, the divergent terms can be explicitly calculated and shown to cancel with corresponding singularities in the adjacent edge integrals. A single analytic integration is employed for the edge and vertex integrations. This is sufficient to display the divergent term in the edge-adjacent integral and to demonstrate that the vertex integral is finite. By explicitly identifying the divergent quantities, hypersingular integrals can be computed without recourse to Stokes' Theorem or Hadamard Finite Part. The algorithms are discussed in the context of the Laplace equation; however, the extension to more complicated Green's functions (e.g., anisotropic elasticity) will be mentioned. Finally, this direct method leads to a highly efficient and accurate algorithm for computing tangential derivatives. This post-processing step is often required for "moving boundary" simulations, and several examples of industrial interest will be given.

What Online Mathematical Content Could be Useful to Commercial Software Development?

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There is abundant online mathematical material that is potentially useful for commerical software developers. Unfortunately, transfer from into working code is primarily an intellectual, rather than computerized, activity. Journal papers (for instance pdf files) contain high level information, but a task such as "give me an implementation of equation 1 in language A with coding convention B" is purely an intellectual activity even though the steps are highly technical and repetetive. Computer source codes initially appear to much more structured, but in practice the combination of language, coding conventions, and operating system issues has resulted in usefulness of online source taking on "all or nothing" characteristics.

This talk will consider properties that would allow online content to be more useful as starting material for a highly automated transfer into commercial software environments. The basic assumption is that online content is to be read and processed by a compterized, rather than human reader. Facilitating this automated access and transformation requires consideration of (a) granularity, (b) syntactic properties, and (c) semantic content, and (d) software tools.

The world of Green's function analysis may appear to be quite distant from these issues. However, the complexity of BEM kernel expressions provides an unusually high opportunity for payback from ubiquitous automation of the process.

On Green's function for a three-dimensional exponentially-graded elastic solid

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The problem of a point force acting in an unbounded, three-dimensional, isotropic elastic solid is considered. Kelvin solved this problem for homogeneous materials. Here, the material is inhomogeneous; it is `functionally graded'. Specifically, the solid is `exponentially graded', which means that the Lam\'e moduli vary exponentially in a given fixed direction. The solution for the Green's function is obtained by Fourier transforms, and consists of a singular part, given by the Kelvin solution, plus a non-singular remainder. This grading term is not obtained in simple closed form, but as the sum of single integrals over finite intervals of modified Bessel functions, and double integrals over finite regions of elementary functions. Knowledge of this new fundamental solution for graded materials permits the development of boundary-integral methods for these technologically important inhomogeneous solids.

The talk describes joint work with Joe Richardson, Len Gray and John Berger. A paper with the same title as the talk has been accepted for publication in the Proceedings of the Royal Society A.

Application of BEM in Dislocation Dynamics and other problems in Micro- and Nano-Scale

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The evolution of the flow stress for grain sizes ranging from about 16 micro-meter to 2 micro-meter under shear deformation is simulated by using two-dimensional discrete dislocation dynamics. The edge dislocations are modeled as line defects in an elastic medium. A superposition technique coupled with BEM is used to obtain the dynamics of dislocation microstructure. The long range interactions of dislocations are modeled by using a Multi-Pole Algorithm instead of an artificial cut-off radius. A set of constitutive rules is used to model nucleation and annihilation of the dislocations. The flow stress values for different grain sizes are expressed as a function of the dislocation density normalized by the grain size.

Boundary Element Analysis Usage in Caterpillar

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Abstract

Boundary Element Analysis has been in use in Caterpillar since late 70's. It is used extensively in the analysis of parts with complicated geometries or with a lot of details such as engine components, transmission components and vehicle components. A lot of work has been done to the analysis software to satisfy needs from designers and analysts within Caterpillar. The proprietary software—EZBEA/EZBEA+ solves structural and heat transfer analysis problems from a description of the model surface only. Boundary Element Analysis helped to increase reliability, reduce design time and save costs for Caterpillar machines

The presentation gives an overview of the Boundary Element Analysis usage in Caterpillar. The time saving and modeling ease of BEA are illustrated with specific examples. A brief description of software capabilities is given along with a demonstration of the software. The strength and challengers for applications of Boundary Element Analysis to engineering design is discussed.

Calculation of properties of defects in semiconductors

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Chalcopyrites and related compounds are key materials for devices generating high power mid-infrared radiation. For example, zinc germanium phosphide (ZGP) is one of the most promising members and has been proposed for 2.05 μm-pumped type-I oscillators. However, the presence of an absorption band near the pump wavelength limits the effectiveness of this material for device applications. This absorption band in the spectral region of 1-2 μm has been attributed to photo-ionization of a highly compensated deep native acceptor center.

Significant understanding of theoretical and practical aspects of chalcopyrites has been developed, but much remains to be done before chalcopyrites achieve their full potential in device applications. In this talk, we will describe a quasichemical formalism to make quantitative predictions of the native point defect densities in chalcopyrites. The electronic contribution to the defect formation free energy will be calculated using the self-consistent first principles LCAO method in the framework of the density functional theory. A Green's function approach based on a valence force field plus a point Coulomb model will be used to calculate the vibrational contributions to the defect free energy.

Integrating Domain Specific Content and Document Description Markup With Collection Metadata in a Green's Functions Digital Library

Gregory M. Shreve
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This paper discusses the relationship between resource level metadata description and domain-specific content markup languages in the context of the GREEN (Green's Functions Research and Education Enhancement Network) digital library. The paper argues that definitions of library resources cannot stop arbitrarily at the "natural" boundaries of the existing resource. Attempts must be made to use markup languages and new approaches to information discovery such as corpus linguistics to extend the library's information access to objects contained within resources.

Instead of supporting the parallel evolution of resource markup and content markup, we seek convergence. Using the GREEN collection of mathematical and materials science resources, we will explore when, where, how, and why LOM metadata and MatML content markup should be integrated to make the GREEN digital library more useful as a research and education tool for the materials science community. This integration should also support other uses of the collection, as for instance, document assembly, computer-assisted authoring, ontology extraction, and data mining.

Multiscale modeling of point defects near interfaces and free surfaces in thin films

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Many physical properties of thin films depend upon the presence of point defects such as vacancies and interstitials and their elastic interactions with the interface between the film and the substrate and the free surfaces. Whereas the macroscopic continuum model can be applied to calculate the strain field due to extended defects such as the interfaces and free surfaces, a model for point defects must account for the discrete atomistic structure of the crystal lattice. A Green's function method is described for multiscale modeling of point defects at the atomistic level and free surfaces and interfaces at the macroscopic level in a common formalism. We use the lattice static Green's function for atomistic modeling of a point defect and the continuum Green's function model for free surfaces and interfaces. The advantage of the lattice static Green's function is that it is semi-analytic and can model a large crystallite containing about a million atoms with no excessive CPU requirement. The lattice static Green's function reduces asymptotically to macroscopic continuum Green's functions which we use to model free surfaces and interfaces. We use the virtual force method along with the asymptotic limit of the lattice static Green function to satisfy the continuity conditions at the interface and the zero traction boundary condition at the free surface. The resulting Green's function has the discrete atomistic behavior near the point defects and the macroscopic continuum behavior near the interface and the free surface. The method is applied to calculate the lattice distortion and strains in thin films of metallic and semiconductor crystals containing vacancies and also the elastic interaction between a vacancy, the interface and the free surface.

Recent Advances on Green's Functions

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Since a list of Green's functions was compiled two year ago on a Web site (www.ctcms.nist.gov/gf/references.php3), there have been activities on research on Green's functions. This is particular the case for three-dimensional problems. Some of them gave new and better solutions to the existing Green's functions. Others presented Green's functions for new geometries such as strips, wedges, layered materials, layered half-space etc., or more complicated materials such as piezoelectric, magneto-electric and poroelastic materials. The main contributors are K. C. Wu, Chien-Ching Ma, E. Pan, Z. Q. Yue and their collaborators. The highlights of their contributions are presented.

Integrating Research and Education in the NSF NSDL: the Green's Functions Research and Education Enhancement Network

Summary prepared by Laura Bartolo

The National Science Foundation has launched the National Science, Mathematics, Engineering, and Technology Education Digital Library (NSDL) program to stimulate and sustain continual improvements in the quality of science, mathematics, engineering, and technology education. The NSDL Program is a major digital library initiative and the Green's Functions Research and Education Enhancement Network" (GREEN) Project is a collaboration of the National Institute of Standards and Technology (NIST) Materials Science and Engineering Laboratory and the Center for Theoretical and Computational Materials Science, Kent State University, and the Massachusetts Institute of Technology. Building upon the efforts of the NIST Green's Functions Working Group, the GREEN Project seeks to integrate research, education, and application of Green's functions at the national level for undergraduate, graduate and professional communities.

In 2001, the NSF NSDL program received one hundred and nine proposals, of which grants were awarded to thirty-five projects. These individual digital library projects comprising the NSDL program are engaged in a collective effort to build a national digital library to support the needs of learners and researchers, and to facilitate the integration of research and education in formal and informal settings. Envisioned as the premier portal to current and future high-quality research and educational content, the NSDL virtual facility will enable seamless access to a rich array of interactive materials and resources, distinguished by the depth and breadth of the subject matter addressed, and valued for its authority and reliability. The GREEN Project is building the information infrastructure in Green's functions and materials science content for the NSDL.

The GREEN project has two primary research objectives: (1), to transform and expand the existing digital resources of the NIST Green's Functions Working Group as part of the NSF NSDL Digital Library Program; and (2) to enhance the educational and research value of the library by applying an education-oriented metadata schema (IEEE Learning Object Metadata schema) and a content-oriented markup language (NIST MatML) to the collection.

In partnership with NIST, the GREEN project seeks to bring together a consortium of experts from university, industry, and government to contribute to the NSF GREEN Digital Library, to advise its development, and to serve as an editorial board for evaluating contributions from other participants. The Editorial Board of the GREEN Project would select, provide, and encourage contributions by colleagues of high quality research and education Green's functions resources:

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1. Problem Bank: A bank of available problems, introduced by industrial members of the consortium and the community at large.
2. Code Bank: Working code for solved Green's functions routines.
3. Literature Bank: A list of citations to relevant literature, and published / unpublished works subject to copyright restrictions, with links elsewhere for additional information.
4. Teaching Bank: A collection of lecture / course notes from existing university courses, as well as providing a form for discussion of approaches to teaching this material.