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FAST FOURIER METHODS APPLIED TO PERTURBATION-BASED HOMOGENIZATION RELATIONS

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ABSTRACT

Relationships between microstructure, local properties, and effective (global) properties of a material are often achieved through perturbation expansions [1, 2]. These may be written in the form of an infinite series of integrals involving correlation functions of increasing order. One major drawback of these series is the amount of computational effort required to include higher order terms. Hence they are often terminated at the first order (or less frequently, second order) terms. A common form of perturbation expansion for elastic properties, sometimes referred to as the weak contrast solution, is as follows [3]:

$$\mathbf{C}^{*} = P^{h}\mathbf{C}^{h} - P^{h}\left(\tilde{\mathbf{C}}^{h}\right)\mathbf{E}\left(\tilde{\mathbf{C}}^{h}\right) + \int_{R(\Omega),r\neq 0}\left\{P^{hh'}(\mathbf{r}) - P^{h}P^{h'}\right\}\left(\tilde{\mathbf{C}}^{h}\right)\boldsymbol{\Phi}(\mathbf{r})\left(\tilde{\mathbf{C}}^{h'}\right)d\mathbf{r} + \ldots \quad (1)$$

where $\mathbf{C}$ indicates the stiffness tensor, $\mathbf{E}$ and $\boldsymbol{\Phi}$ are components of the isotropic Green's function, and $P^{h}, P^{hh'}, \ldots$ are correlation functions of increasing order for material with local states h, h', etc. This has formed the basis for various studies in material design using inverse methods (e.g. [4]), hampered mainly by the intense computational requirements.

A more robust formulation may be derived from the work of Brown [5] and Torquato [6], and is referred to as the strong contrast formulation, due to the absolutely convergent integrals, and it's stability when applied to materials of higher contrast (in properties) between the phases. This formulation has recently been extended to enable its application to anisotropic polycrystalline materials [3]. A key element in the resulting framework is the introduction of a spectral framework, and the use of Fast Fourier transforms (FFTs) to enable rapid calculation of the higher order terms in the series. For example, by exploiting the convolution theory the third order correlation function may be efficiently calculated as:

$$P^{hh'h''}_{n_1 n_2} = \frac{1}{N}\Im^{-1}\left[\left(\Im\left(M_t^{\,h}\right)\right)^{*}_{k_1}\Im\left(M_t^{\,h'}\right)_{k_1-k_2}\Im\left(M_t^{\,h''}\right)_{k_2}\right] \quad (2)$$

where $M_t^{\,h}$ is the local structure function for the material, defined on a grid with positions, *t*, and local states, *h*; $P^{hh'h''}_{n_1 n_2}$ is the 3-point correlation function in this digital space; N is the total number of points on the grid; and $\Im$ indicates FFT. The final form of the efficient FFT framework for both the weak and strong contrast formulations is given in [3].

The integrals in Eq. (1) are typically evaluated between an infinitesimally small sphere about the origin, and a large sphere that is well beyond the correlation length. However, a significant error may arise from estimating an integral on a sphere using a rectangular grid. The isotropic Green's function has natural symmetry on the sphere which is poorly captured using a rectangular grid – especially in the region of the origin. This is a particularly critical region of integration due to the singularity at the origin. Recent analysis using accurate monte-carlo integration indicates the potential for large errors in this region using the grid-based integrals typical of several previous works. These errors have masked the increased accuracy that should result from adding higher order terms to the series.

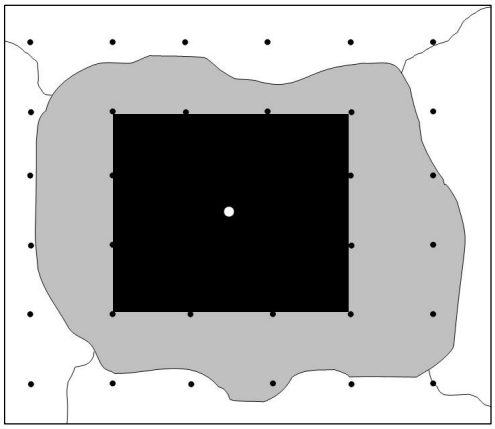

Fig. 1. Material of a single state is shown about the origin as grey. The integral is evaluated on a grid outside a cube about the origin. The remaining integral (shown in black) is evaluated using a single constant correction term.

However, the issue can be resolved to good accuracy by exploiting the fact that the integral that includes the Green's function is identically zero in an annulus that contains material in a single local state. Similarly, the integral over a region between a sphere and a cube which contains material in a single state is a constant value – independent of their relative sizes. Thus, the tactic is to integrate over the grid used to define the FFTs, outside a cubic region that surrounds the origin, and within which lies a single material state. Then a single (constant) correction term is required to adjust for the remaining integral between an infinitesimal sphere and the cube (see Fig. 1).

A similar correction can be made for the region between the outer bounds of the rectangular grid, and a sphere that encompasses it.

These issues are amongst those that will be discussed in this presentation, along with an evaluation of the benefits obtained from exploiting the FFT framework – including the application to material design in the areas of both composites and polycrystals..

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