Lecture 14 - Fourier Analysis

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schedule

- 24 Mar - Fourier Analysis, HW 5 Due, Project Abstract Due
- 29 Mar - Method of Cells
- 31 Mar - Workday
- 5 Apr - Damage Theory

outline

- fourier methods
- theoretical basis
- installation

fourier methods

motivation

- Fourier transforms are often used to represent periodic data
- If we have a periodic microstructure, we can formulate the problem in Fourier space
- There are many Fast Fourier Transform (FFT) algorithms available to compute discrete problems very quickly

current implementations

- There are a few different codes (that I am aware of) that use Fourier techniques for modeling micromechanics
- CraFT (I have linked this in the past) link[1] (original FFT for elasticity program)
- Morphhom[2] (another french group)
- MASSIF[3] (modifications made by group at Los Alamos)

[1] http://craft.lma.cnrs-mrs.fr/spip/
[2] http://cmm.ensmp.fr/morphhom/
[3] http://www.icmr.ucsb.edu/programs/3DWorkshop/Rollett-FFT-modeling-method.pdf

uses

- While many Micromechanics tools have been developed around specific applications (such as composites), FFT-based algorithms attempt to be somewhat more general
- Used for polycrystalline materials (metal alloys), grain boundaries, fatigue crack initiation, dislocation stress fields, microcracks, graded microstructures, coatings, etc.
- Requires periodic structure and BC's
- This means it can be used to characterize a material, but cannot solve most structural problems
- Uses image-based inputs (pixels/voxels) which can directly relate to experiments (serial sectioning, 3D X-ray/CT scan), but are a little more difficult to develop conceptually

validation

- Prakash and Lebensohn validated the FFT method against FEM for a rolling simulation.
- link[4]

[4] http://iopscience.iop.org/article/10.1088/0965-0393/17/6/064010/meta

RVE

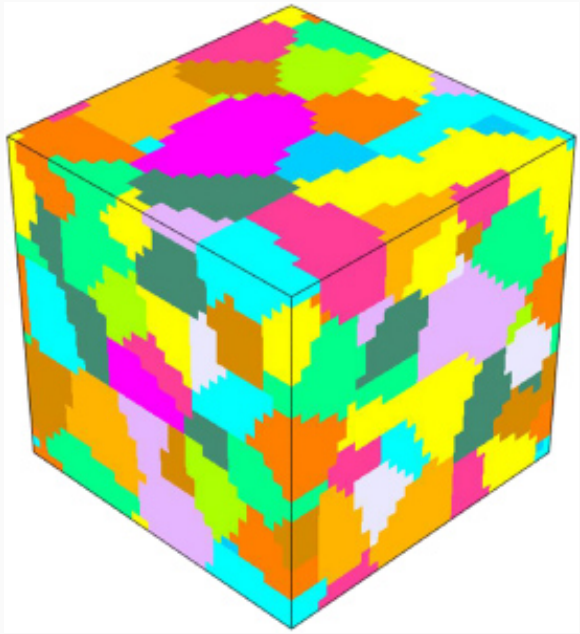

Figure 1: image

deformed

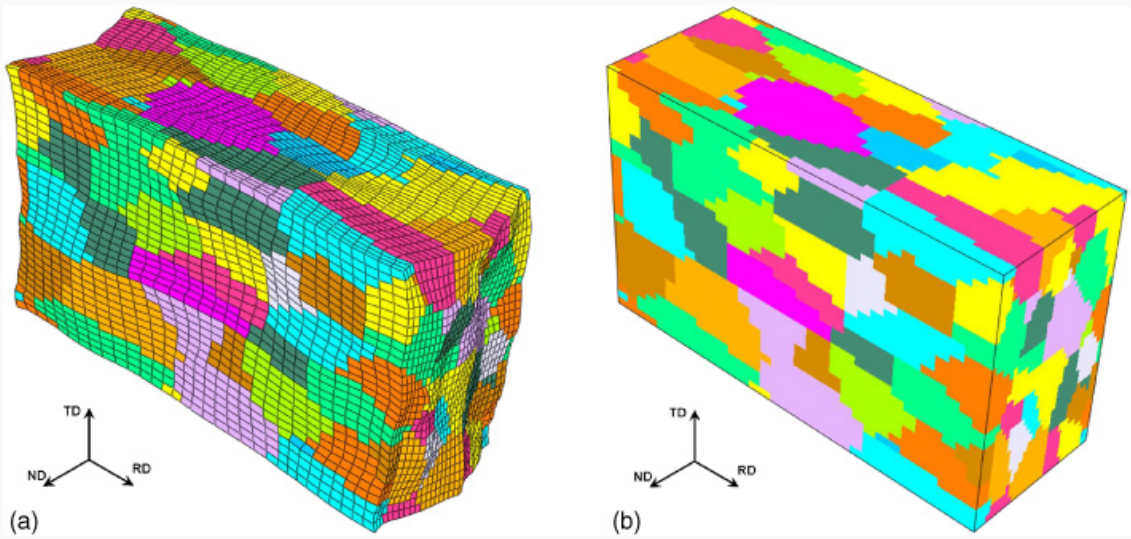

Figure 2: image

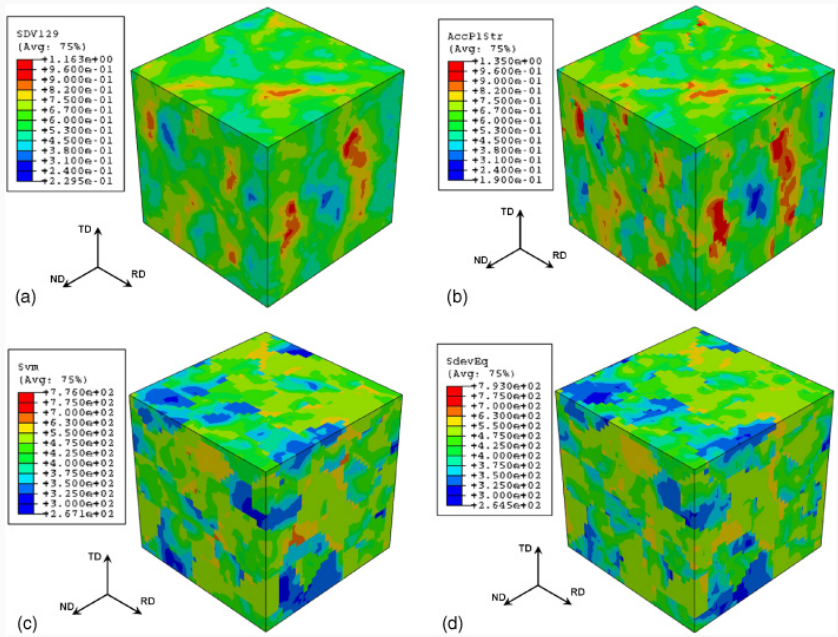

Figure 3: image

theoretical basis

references

- Textbook chapter 11 (pp 419-431) discusses Fourier methods for periodic structural homogenization
- There are also many papers on the subject, link[5] (Fourier-based schemes for computing the mechanical response of composites with accurate local fields by Francois Willot) is a good review

[5] https://arxiv.org/pdf/1412.8398.pdf

linear elasticity

- All Fourier schemes begin with the standard equations of linear elasticity

$$\begin{aligned} \sigma_{ij}(x) &= C_{ijkl}\epsilon_{kl}(x) \\ \sigma_{ij,j}(x) &= 0 \\ \epsilon_{ij}(x) &= \frac{1}{2}(u_{i,j}(x) + u_{j,i}(x)) \end{aligned}$$

- While we have listed material properties as functions of x, we usually have only 2-3 phases of material, and thus these functions will be piecewise, simply differentiating between the phases

lippmann-schwinger equations

- Fourier Methds are based on the Lippmann-Schwinger equations where we define the polarization field as

$$\tau_{ij} = \sigma_{ij}(x) - C^0_{ijkl}\epsilon_{kl}(x)$$

- We also use the Green operator, which is given (in the Fourier space) as

$$G_{ijkl}(q) = q_i \left[q_m C_{mjkn^0 q_n}\right]^{-1} q_l$$

- and the strain field can be expressed as

$$\epsilon_{ij}(x) = \bar{\epsilon}_{ij} - \int_{x'} d^d x' G_{ijkl}(x' - x)\tau_{kl}(x')$$

direct scheme

- These equations are generally solved iteratively, with different assumptions used to arrive at the solution
- The "direct" scheme solves the problem iteratively using

$$\epsilon^{k=0} = \bar{\epsilon}$$
$$\epsilon^{k+1} = \bar{\epsilon} - G(\sigma - C^0 : \epsilon^k)$$

- Where each iteration is solved in the Fourier space (where the convolution integral is an algebraic product)
- The convergence of this method is quite slow when there is high contrast between the two phases

accelerated schemes

- There are many methods to accelerate the convergence for high contrast materials
- One is referred to as the "acclerated scheme" another is known as the "augmented lagrangian"
- In the accelerated scheme the strain is calculated as

$$\epsilon^{k+1} = \epsilon^k + 2(C + C^0)^{-1} : C^0 : [\bar{\epsilon} - \epsilon^k - G(C : \epsilon^k - C^0 : \epsilon^k)]$$

- C^0 is a reference stiffness, and while it is arbitrary, the choice of C^0 does affect the convergence, and for isotropic materials the optimal C^0 is given by

$$k^0 = \sqrt{k^1 k^2} \qquad \mu^0 = \sqrt{\mu^1 \mu^2}$$

installation

installation

- For now, CraFT is the only FFT program I have tried, although I have contacted other authors so we may possibly be able to use those in the future as well
- It must be compiled from source on Linux, I will provide information on how to do this on a Windows machine
- First, you need to emulate linux, I use virtualbox[6] but there are other virtual machines
- Next, you need to download and install a Linux distribution to install in Virtualbox (or your virtual machine), I used ubuntu[7]
- There are many tutorials on the internet if you wish to use a different Linux distribution, you may have to modify some commands slightly

[6] https://www.virtualbox.org/wiki/Downloads

[7] https://www.ubuntu.com/download

compiling

- Next you need to obtain and compile the source for CraFT. I have the source code and will share it with you if you do not want to contact the authors directly
- To build the source code, first you need to obtain some standard libraries, as well as the FFT library used in CraFT
- In ubuntu type into the command line `sudo apt-get install build-essential gfortran libfftw3-dev`
- Navigate to the directory with CraFT and unpack it using `tar xvfz craft-1.0.12g.tgz`
- Navigate to the CraFT directory `cd craft-1.0.12g`
- Type `make` and the program will compile

post processing

- CraFT includes some basic pre-processing, but no post-processing
- It saves output files in the vtk format, there are multiple programs that can view these files
- I used paraview which can be installed using `sudo apt-get install paraview`