Elastic and Elasto-viscoplastic FFT: basic algorithm and augmented Lagrangian accelerated scheme

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Outline

- The crystal plasticity FFT approach
  - FFT – a brief history until its introduction into mechanics of materials
  - Elastic FFT for modeling heterogeneous materials
  - Elasto-viscoplastic FFT for modeling polycrystals
  - Comparison with FEM

FFT – history

Johann Carl Friedrich Gauß
First concept of fast DFTs
(somewhere in his notebook)

1805

"Nothing" happens

1807

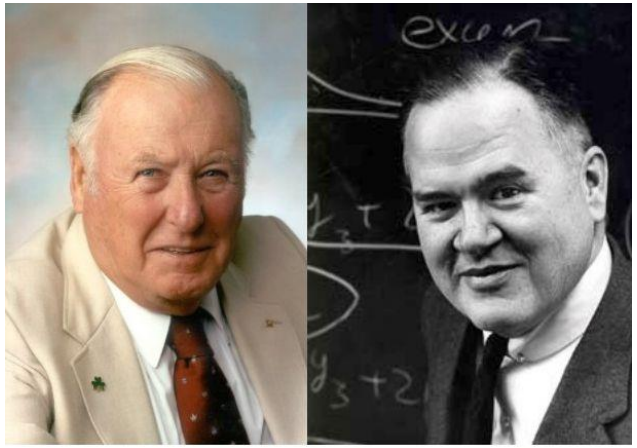
JB Joseph Fourier
presents
harmonic analysis

Danielson &
Lanczos
Propose their
approach

1942

1958

Good
Proposed the prime factor
algorithm



James William Cooley
(1926-)

John Wilder Tukey
(1915-2000)

Popularized the Radix-2
FFT algorithm

1965

Introduced FFT
into mechanics
to study micro-
mechanics of
elastic composites

Hervé
Moulinec

1994

Pierre
Suquet

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A representative volume element (RVE)

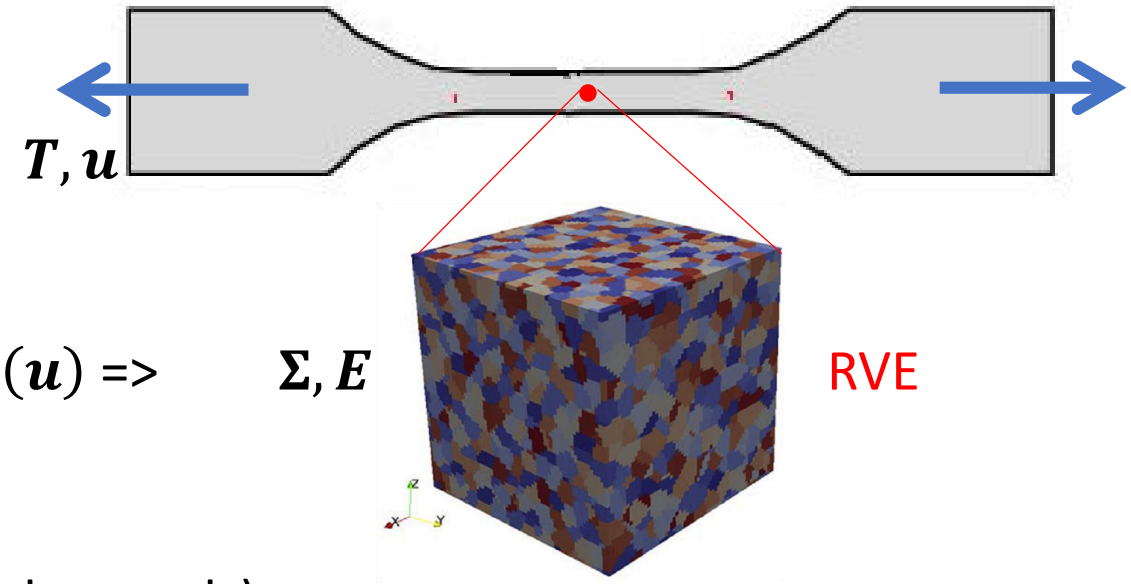
- We are interested in studying the deformation of a multi-phase material that is elastically inhomogeneous subjected to external mechanical loadings.

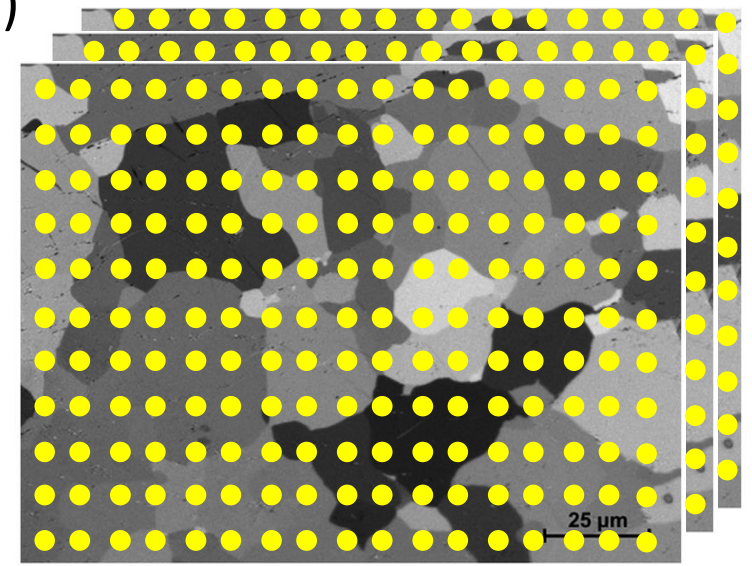
- If these external loadings (force or displacement) are represented in the form of homogenous fields i.e. mechanical stresses and strains, then the effective response of a material can be determined numerically by solving the “local problem” on a representative volume element (RVE) of the microstructure.

- An RVE is the smallest volume that is representative of the properties and response of a material

An RVE of a composite

- RVE = smallest volume that behaves like the whole
  - Deformation of an elastic composite
    - Property: elastic heterogeneity
    - Property: Multi-phase
    - Mechanics: Forces ($\boldsymbol{T}$) and displacements ($\boldsymbol{u}$) => homogeneous stresses ($\boldsymbol{\Sigma}$) and strains ($\boldsymbol{E}$)
- Sources for RVEs:
  - Micrographs (2D/3D SEM, EBSD or 3D XRD – polycrystals)
  - Synthetic (Voronoi tessellations)
- RVEs for FFT
  - Structured grid => Equi-spaced pixels/voxels
  - Periodic boundary conditions





The local problem – Linear elastic case

- Within the RVE (V)
  - Displacements $\boldsymbol{u}(\boldsymbol{x})$ and stresses $\boldsymbol{\sigma}(\boldsymbol{x})$ are piecewise continuous => perfect bonding between material points
  - Equilibrium: $\mathbf{div}\,\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{0}$ or $\sigma_{ij,j}(\boldsymbol{x}) = 0_i; \forall \boldsymbol{x} \in V$
  - Elastic constitutive relationship

    $\boldsymbol{\sigma}(\boldsymbol{x}) = \frac{\partial w(\boldsymbol{\varepsilon}(\boldsymbol{x}))}{\partial \boldsymbol{\varepsilon}(\boldsymbol{x})} = \boldsymbol{C}(\boldsymbol{x}) : \boldsymbol{\varepsilon}(\boldsymbol{x})$ or $\sigma_{ij}(\boldsymbol{x}) = C_{ijkl}(\boldsymbol{x})\varepsilon_{ij}(\boldsymbol{x}); \forall \boldsymbol{x} \in V$

    $w\big(\boldsymbol{\varepsilon}(\boldsymbol{x})\big)$ = elastic strain energy

    Linearity => $w\big(\boldsymbol{\varepsilon}(\boldsymbol{x})\big)$ is quadratic => $\boldsymbol{\sigma}(\boldsymbol{x})$ is a linear function of $\boldsymbol{\varepsilon}(\boldsymbol{x})$

- On RVE surface $(\boldsymbol{S})$
  - $\boldsymbol{u}(\boldsymbol{x})$ and tractions $\boldsymbol{T}(\boldsymbol{x}) = \boldsymbol{\sigma}(\boldsymbol{x}) \cdot \boldsymbol{n}$ undetermined
    => periodic boundary conditions

Splitting the local fields – kinematics

- The local strain field $\boldsymbol{\varepsilon}(\boldsymbol{x})$ is split into its R.V.E. average value $\boldsymbol{E}$ and a fluctuation term $\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})$ such that

$$\boldsymbol{\varepsilon}(\boldsymbol{x}) = \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \boldsymbol{E}$$

- This gives an equivalent relationship for the local displacement $\boldsymbol{u}(\boldsymbol{x})$ in terms of its local fluctuation $\tilde{\boldsymbol{u}}(\boldsymbol{x})$ from the R.V.E. average

$$\boldsymbol{u}(\boldsymbol{x}) = \tilde{\boldsymbol{u}}(\boldsymbol{x}) + \boldsymbol{E} \cdot \boldsymbol{x}$$

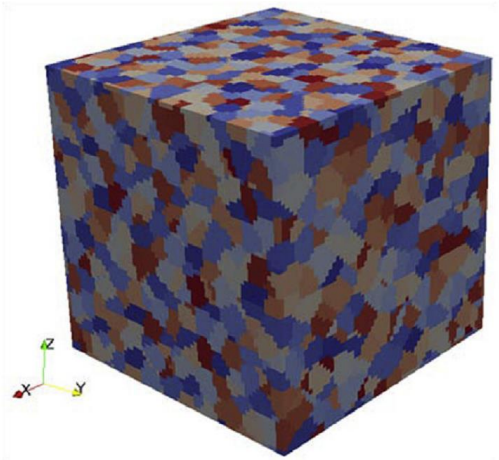
Why?

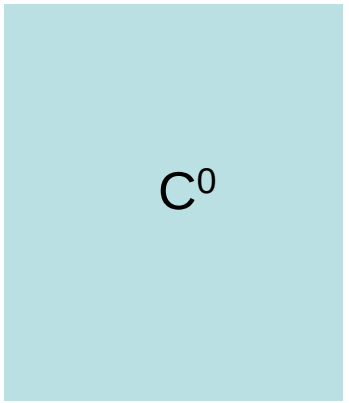
1) Fourier transform of a constant is zero
2) Allows using the Green's function method to solve the local problem

- Periodic boundary conditions ⇒
  - $\tilde{\boldsymbol{u}}(\boldsymbol{x})$ is periodic on $\boldsymbol{S}$ of the RVE; $\forall \boldsymbol{x} \in \boldsymbol{S}$

Splitting the local fields – statics

- Split the microstructure
  - Homogeneous effective medium (HEM) with stiffness $\boldsymbol{C^0}$
  - Local perturbations in stiffness: $\boldsymbol{\delta c(x) = c(x) - C^0}$
- Stress polarization
  - $\boldsymbol{\tau(x) = \delta c(x) : \varepsilon(x) = \sigma(x) - C^0 : \varepsilon(x) = \left(c(x) - C^0\right) : (\tilde{\varepsilon}(x) + E); \forall x \in V}$
- Periodic boundary conditions $\Rightarrow \boldsymbol{T(x) = \sigma(x) \cdot n(x)}$ is anti-periodic; $\forall \boldsymbol{x \in S}$





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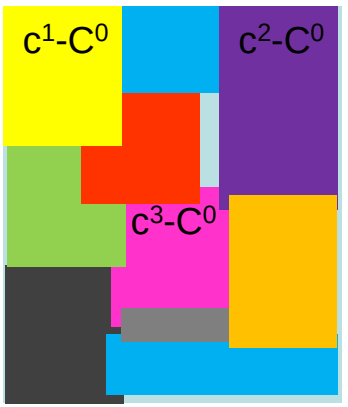

A possibility, $\langle \boldsymbol{c}^i - \boldsymbol{C}^0 \rangle = \langle \boldsymbol{c}^i \rangle - C^0 = 0$

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Local problem – fluctuating fields

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}(\boldsymbol{x}) : (\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \boldsymbol{E}) = \boldsymbol{C^0} : \boldsymbol{\varepsilon}(\boldsymbol{x}) + \boldsymbol{\tau}(\boldsymbol{x}); \forall \boldsymbol{x} \in V$$
$$\mathbf{div}\, \boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{div} \left(\boldsymbol{C^0} : \boldsymbol{\varepsilon}(\boldsymbol{x}) \right) + \mathbf{div}\, \boldsymbol{\tau}(\boldsymbol{x}) = \mathbf{0}; \forall \boldsymbol{x} \in V$$
$$\tilde{\boldsymbol{u}}(periodic), \boldsymbol{\sigma} \cdot \boldsymbol{n}(anti - periodic); \forall \boldsymbol{x} \in \boldsymbol{S}$$

$+ \boldsymbol{\Sigma}, \boldsymbol{E}$

PDE with initial & boundary conditions

How to solve?

- Equilibrium equation

$$\sigma_{ij,j} = C^0_{ijkl} \varepsilon_{kl,j} + \tau_{ij,j} = 0$$

$$C^0_{ijkl} u_{k,lj} + \tau_{ij,j} = 0$$

using continuity condition: $\varepsilon_{kl} = \frac{1}{2}\left(u_{k,l} + u_{l,k}\right)$

Green's function approach

- Equilibrium

$$C^0_{ijkl} u_{k,lj} + \tau_{ij,j} = 0$$

  - Assuming that $\tau_{ij,j}$ is a fictitious body force
  - $G_{km}(\boldsymbol{x} - \boldsymbol{x}')$ = displacement component along x_k direction at point $\boldsymbol{x}$ due to a unit force applied in the x_m direction at the point $\boldsymbol{x}'$

- Then,

$$\tilde{u}_k(\boldsymbol{x}) = \int_V G_{ki}(\boldsymbol{x} - \boldsymbol{x}')\tau_{ij,j}(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}'$$

- After integrating by parts, taking the derivative and symmetrizing:

$$\tilde{\varepsilon}_{ij}(\boldsymbol{x}) = \mathrm{sym}\left(\int_V G_{ik,jl}(\boldsymbol{x} - \boldsymbol{x}')\tau_{kl}(\boldsymbol{x}')\mathrm{d}\boldsymbol{x}' \right)$$

The periodic Lippmann-Schwinger equation

- Calling $\Gamma_{ijkl} = \mathrm{sym}\left(G_{ij,kl}\right)$, and noting that "$*$" means a convolution integral, we get

$$\varepsilon_{ij}(\boldsymbol{x}) = \underbrace{\left(\Gamma_{ijkl} * \tau_{kl}\right)(\boldsymbol{x})}_{\tilde{\varepsilon}_{ij}(\boldsymbol{x})} + E_{ij}$$

Periodic Lippmann-Schwinger equation

- Fourier transform of $\boldsymbol{\varepsilon}(\boldsymbol{x})$ gives

$$\hat{\varepsilon}_{ij}(\boldsymbol{\xi}) = \hat{\tilde{\varepsilon}}_{ij}(\boldsymbol{\xi}) = \hat{\Gamma}_{ijkl}(\boldsymbol{\xi})\hat{\tau}_{kl}(\boldsymbol{\xi})$$

Modified Green's function

- Compute $\Gamma_{ijkl}(\boldsymbol{x})$ in Fourier space $\hat{\Gamma}_{ijkl}(\boldsymbol{\xi})$
- Recall equilibrium equation in real space: $C^0_{ijkl} G_{km,lj}(\boldsymbol{x} - \boldsymbol{x}') + \delta_{im}\delta(\boldsymbol{x} - \boldsymbol{x}') = 0$
- Fourier transform the equilibrium equation

$$\Rightarrow C^0_{ijkl}\xi_l\xi_j\hat{G}_{km}(\boldsymbol{\xi}) = \delta_{im}$$

$$\Rightarrow \hat{G}_{ki}(\boldsymbol{\xi}) = \left[C^0_{ijkl}\xi_l\xi_j\right]^{-1} \text{ and}$$

$$\Rightarrow \hat{\Gamma}_{ijkl}(\boldsymbol{\xi}) = -\frac{1}{2}\left(\xi_j\xi_l\hat{G}_{ki}(\boldsymbol{\xi}) + \xi_j\xi_l\hat{G}_{ik}(\boldsymbol{\xi})\right)$$

The periodic Lippmann-Schwinger equation in Fourier space

- $\hat{\Gamma}_{ijkl}(\boldsymbol{\xi})$ can be calculated at any frequency except at the origin in the Fourier space i.e. $\boldsymbol{\xi} = \mathbf{0}$ where the value of $\hat{\hat{\boldsymbol{\varepsilon}}}$ is already given directly by $\hat{\hat{\boldsymbol{\varepsilon}}}|_{\boldsymbol{\xi}=\mathbf{0}} = 0$ i.e. the average value of the strain fluctuations in the real space vanishes in the Fourier space.

- The derivations in the Fourier space shown so far can be used to compute the accurate solution of the local strain field (accuracy depends on the domain discretization) if the transformed perturbation field $\hat{\tau}_{ij}$ is known.

- **But $\hat{\tau}_{ij}$ is *a priori* unknown !! Solution?**
  Use an iterative procedure

Elastic FFT – Iterative procedure

- Prior to proceeding with the numerical procedure, we need to note that the R.V.E. under consideration is finite sized and if it is discretised into $N_1 \times N_2$ equispaced pixels in 2D or $N_1 \times N_2 \times N_3$ equispaced voxels in 3D then the **continuous Fourier transform** that appeared before can be replaced by a **discrete Fourier transform** which can be computed using the **Fast Fourier Transform (FFT)** approach as discussed in the slides *FFT: a brief review* on my website.

Elastic FFT – Fixed point algorithm (Basic Scheme)

- Initialization: $\boldsymbol{\varepsilon^0(x) = E}$

$$\boldsymbol{\sigma^0(x) = c(x) : \varepsilon^0(x)}$$

- Iteration $i+1$ ($\boldsymbol{\varepsilon^i}$ and $\boldsymbol{\sigma^i}$ are knowns)

1. $\boldsymbol{\hat{\sigma}^i = FFT(\sigma^i)}$
2. $err = \dfrac{\left(\left\langle \left|\left|\mathbf{div}\,\sigma^i\right|\right|^2 \right\rangle\right)^{\frac{1}{2}}}{\left|\left|\langle \sigma^i \rangle\right|\right|} = \dfrac{\left(\left\langle \left|\left|\xi \cdot \hat{\sigma}^i(\xi)\right|\right|^2 \right\rangle\right)^{\frac{1}{2}}}{\left|\left|\hat{\sigma}^i(\mathbf{0})\right|\right|}$ (if converged then stop)
3. $\boldsymbol{\tau^i = \sigma^i - C^0 : \varepsilon^i}$
4. $\boldsymbol{\hat{\tau}^i = FFT(\tau^i)}$
5. Calculate $\Gamma_{ijkl}(\boldsymbol{\xi})\ \forall\ \boldsymbol{\xi \neq 0}$
6. $\hat{\tilde{\varepsilon}}^{i+1} = \hat{\boldsymbol{\Gamma}} : \hat{\tau}^i$ with $\hat{\tilde{\varepsilon}}^{i+1}|_{(\xi=\overline{0})} = 0$
7. $\tilde{\varepsilon}^{i+1} = FFT^{-1}\left(\hat{\tilde{\varepsilon}}^{i+1}\right)$ and $\boldsymbol{\sigma}^{i+1} = \boldsymbol{c} : \left(\boldsymbol{E} + \tilde{\varepsilon}^{i+1}\right)$
8. Repeat from 1

Slow convergence for high contrast or non-linear materials

(Note that $\boldsymbol{x} \in \{\boldsymbol{x_d}\}$ where x_d is the appropriate discretization for FFT to be applied)

Need for an accelerated scheme

- Adapted from Michel et al. (2000, 2001)
- The rate of convergence of the FFT method varies with the contrast between the phases (for linear composites) and can be very slow for composites with high contrast (typically above 10^4) and is even not ensured for composites with infinite contrast (typically materials containing voids or rigid inclusions). New schemes have to be developed for these extreme situations.
- Another motivation for proposing alternative schemes comes for non-linear problems. Although the method has been successfully applied to linear elastic and elastic–plastic composites in Moulinec and Suquet [2], it cannot be straightforwardly extended to all non-linear material behaviours, such as power-law stress-strain relations which occurs for visco-plastic materials. With such materials, the initial moduli (which can be the secant moduli for instance) are very large. In addition, these moduli are very contrasted in zones undergoing inhomogeneous deformations. Therefore, a non-linear composite with power-law phases behaves as a linear composite with many different and highly contrasted phases. This bring us back to the problem of highly contrasted phases.
- Finally, there is a theoretical interest in the non-linear properties of power-law materials containing voids or rigid inclusions. These materials provide good tests to assess the accuracy of non-linear bounds and estimates. In this case both difficulties (high contrast stemming from the non-linearity and infinite contrast stemming from the inclusion phase) are present.

Effective behavior – a minimization problem

- The effective behavior of the composite also results from an effective strain-energy W^{hom}, which can be characterized by the variational property (Suquet, 1987; Ponte-Castaneda & Suquet, 1998):

$$W^{hom}(\boldsymbol{E}) = \min_{\boldsymbol{u} \in \boldsymbol{K}(\boldsymbol{E})} \langle w(\boldsymbol{\varepsilon}(\boldsymbol{u})) \rangle$$

where $\langle . \rangle$ denotes the spatial average over volume V, and $\boldsymbol{K}(\boldsymbol{E}) = \{\boldsymbol{u} \text{ such that } \boldsymbol{\varepsilon}(\boldsymbol{u}) = \boldsymbol{E} + \boldsymbol{\varepsilon}(\tilde{\boldsymbol{u}}), \tilde{\boldsymbol{u}} \text{ is periodic}\}$ is the set of displacement fields that are kinematically admissible with the average strain $\boldsymbol{E}$.

The above equation can be reformulated as a minimization problem

$$\min_{\boldsymbol{e}} \left\{ \min_{\boldsymbol{u} \in \boldsymbol{K}(\boldsymbol{E})} \langle w(\boldsymbol{e}) \rangle \right\}$$

Under the constraint (compatibility condition)

$$\boldsymbol{\varepsilon}(\boldsymbol{u}(\boldsymbol{x})) - \boldsymbol{e}(\boldsymbol{x}) = \boldsymbol{0} \qquad \forall \boldsymbol{x} \in V$$

Accelerated scheme – Augmented Lagrangian

- The above equation is a **constrained minimization problem** that can be solved using the **Augmented Lagrangian** technique.

NOTE: The augmented Lagrangian technique is a modification of the **penalty method**. The latter converts a constrained minimization problem into an unconstrained minimization problem. For instance, if we are trying to solve

$$\min f(\boldsymbol{x})$$

$$\text{Subject to } c_i(\boldsymbol{x}) \leq 0 \; \forall i \in I$$

Then using the penalty method, it can be converted to the following unconstrainted problem

$$\min \phi_k(\boldsymbol{x}) = f(\boldsymbol{x}) + \mu_k \sum_{i \in I} g\big(c_i(\boldsymbol{x})\big); \text{ where } g\big(c_i(\boldsymbol{x})\big) = \max\big(0, c_i(\boldsymbol{x})\big)^2$$

Here $g\big(c_i(\boldsymbol{x})\big)$ is the external penalty function and μ_k are the penalty coefficients. At each iteration k, the penalty method solves the above unconstrained problem by increasing the penalty coefficient μ_k with respect to the previous coefficient and uses the solution as an initial guess for the next iteration $k+1$. Solutions of the successive unconstrained problems will eventually converge to the solution of the original constrained problem.

The **augmented Lagrangian** method, in its general form, uses the following unconstrained objective

$$\min \phi_k(\boldsymbol{x}) = f(\boldsymbol{x}) + \frac{\mu_k}{2} \sum_{i \in I} g\big(c_i(\boldsymbol{x})\big) - \sum_{i \in I} \lambda_i c_i(\boldsymbol{x})$$

After each iteration, in addition to updating μ_k, the variable λ is also updated according to the rule

$\lambda_i \leftarrow \lambda_i - \mu_k c_i(\boldsymbol{x}_k)$ where λ is Lagrange multiplier and $\boldsymbol{x}_k$ is the solution to the unconstrainted problem at the kth step. The main advantage of this method is that unlike the penalty method, it is not necessary to take $\mu \to \infty$ in order to solve the original constrained problem. Instead because of the presence of the Lagrange multiplier , μ can stay much smaller, thus avoiding ill-conditioning.

Accelerated scheme – Augmented Lagrangian

- Coming back to our constrained minimization problem

$$\min_{\boldsymbol{e}} \left\{ \min_{\boldsymbol{u} \in \boldsymbol{K}(\boldsymbol{E})} \langle w(\boldsymbol{e}) \rangle \right\}$$

Under the constraint (compatibility condition)

$$\boldsymbol{\varepsilon}\big(\boldsymbol{u}(\boldsymbol{x})\big) - \boldsymbol{e}(\boldsymbol{x}) = \boldsymbol{0} \qquad \forall \boldsymbol{x} \in V$$

- Let $\lambda(\boldsymbol{x})$ denote the Lagrange multiplier associated with the compatibility condition mentioned in the previous slide. Then the "**augmented Lagrangian**" can be written as

$$L_{\boldsymbol{c}_0} = (\varepsilon(\boldsymbol{u}), \boldsymbol{e}, \lambda) = \langle w(\boldsymbol{e}) \rangle + \langle \lambda : (\varepsilon(\boldsymbol{u}) - \boldsymbol{e}) \rangle + \frac{1}{2} \langle (\varepsilon(\boldsymbol{u}) - \boldsymbol{e}) : \boldsymbol{c}_o : (\varepsilon(\boldsymbol{u}) - \boldsymbol{e}) \rangle$$

$\boldsymbol{c}_0$ possess the same order and symmetries that are characteristic of a stiffness tensor. It is chosen depending on the problem under consideration.

Our constrained problem has now turned into an unconstrained saddle point problem for $L_{\boldsymbol{c}_0}$. The saddle point can be reached with the help of Uzawa's algorithm (Glowinski and Le Tallec, 1989; Licht and Suquet, 1986).

Accelerated scheme – Augmented Lagrangian

- Uzawa's algorithm for our constrained problem (adapted from Michel et al., 2000, 2001)

  Iteration i: given $\boldsymbol{e}^{i-1}$ and λ^{i-1}

  (1) compute $\boldsymbol{\varepsilon}(\boldsymbol{u}^i)$ solution of the problem:

$$\min_{\boldsymbol{u}\in\boldsymbol{K}(\boldsymbol{E})} L_{\boldsymbol{c}_0}\left(\boldsymbol{\varepsilon}(\boldsymbol{u}), \boldsymbol{e}^{i-1}, \lambda^{i-1}\right)$$

  (2) compute $\boldsymbol{e}^i$ solution of the nonlinear equation (at each point $\boldsymbol{x}$):

$$\frac{\partial w}{\partial \boldsymbol{e}}\left(\boldsymbol{x}, \boldsymbol{e}^i\right) + \boldsymbol{c}_0 : \boldsymbol{e}^i(\boldsymbol{x}) = \boldsymbol{c}_0 : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^{\boldsymbol{i}}(\boldsymbol{x})\right) + \lambda^{i-1}(\boldsymbol{x})$$

  (3) update λ^i:

$$\lambda^i(\boldsymbol{x}) = \lambda^{i-1}(\boldsymbol{x}) + \boldsymbol{d}_0 : \left(\boldsymbol{\varepsilon}\left(\boldsymbol{u}^i(\boldsymbol{x})\right) - \boldsymbol{e}^i(\boldsymbol{x})\right)$$

$\boldsymbol{d}_0$ is a fourth order tensor which serves to give the descent direction in Uzawa's algorithm. Once we achieve convergence, $\boldsymbol{e}$ coincides with $\boldsymbol{\varepsilon}(\boldsymbol{u})$ and $\boldsymbol{\lambda}$ is the stress $\partial w\left(\boldsymbol{\varepsilon}(\boldsymbol{u})\right)/\partial\boldsymbol{\varepsilon}$.

In the following slides we will discuss in more detail the above algorithm.

Accelerated scheme – Augmented Lagrangian

(1) Step 1: Auxiliary problem

The minimization problem $\min_{\boldsymbol{u}\in\boldsymbol{K}(\boldsymbol{E})} L_{\boldsymbol{c}_0}\left(\boldsymbol{\varepsilon}(\boldsymbol{u}), \boldsymbol{e}^{i-1}, \lambda^{i-1}\right)$ is a classic elasticity problem for a homogeneous, linear elastic medium with stiffness moduli $\boldsymbol{c}_0$. This homogeneous material will be referred to here as the reference medium. Recalling the local problem associated with the above equation:

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c}^{\boldsymbol{0}}\colon \boldsymbol{\varepsilon}(\boldsymbol{x}) + \boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{c}^{\boldsymbol{0}}\colon \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \boldsymbol{c}^{\boldsymbol{0}}\colon \boldsymbol{E} + \boldsymbol{\tau}(\boldsymbol{x});\ \boldsymbol{x} \in V$$

$$\mathbf{div}\,\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{div}\left(\boldsymbol{c}^{\boldsymbol{0}}\colon \tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})\right) + \mathbf{div}\,\boldsymbol{\tau}(\boldsymbol{x}) = \mathbf{0}; \forall \boldsymbol{x} \in V$$

$$\tilde{\boldsymbol{u}}(periodic), \boldsymbol{\sigma}\cdot\boldsymbol{n}(anti-periodic)\ on\ \boldsymbol{S}$$

Where the periodic polarization field is

$$\boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{\lambda}^{i-1}(\boldsymbol{x}) - c_0\colon \boldsymbol{e}^{i-1}(\boldsymbol{x})$$

The solution to the local problem is obtained by the Green's function method as seen earlier

- Real space: $\tilde{\varepsilon}_{ij}(\boldsymbol{x}) = \left(\Gamma_{ijkl} * \tau_{kl}\right)(\boldsymbol{x});\ \forall \boldsymbol{x} \in V$
- Fourier space: $\hat{\tilde{\varepsilon}}_{ij}(\boldsymbol{\xi}) = \hat{\Gamma}_{ijkl}(\boldsymbol{\xi})\hat{\tau}_{kl}(\boldsymbol{\xi}); \forall \boldsymbol{\xi} \neq \mathbf{0}, \hat{\tilde{\boldsymbol{\varepsilon}}}(\mathbf{0}) = \mathbf{0}.$

Accelerated scheme – Augmented Lagrangian

2) Step 2: Nonlinear equation

The equation $\frac{\partial w}{\partial \boldsymbol{e}}\left(\boldsymbol{x}, \boldsymbol{e}^i\right) + \boldsymbol{c}_0 : \boldsymbol{e}^i(\boldsymbol{x}) = \boldsymbol{c}_0 : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^{\boldsymbol{i}}(\boldsymbol{x})\right) + \lambda^{i-1}(\boldsymbol{x})$ is a tensorial nonlinear equation. When w is convex i.e. $\partial w/\partial \varepsilon$ is a monotonic function, this equation admits a unique solution which can be reached using any classical method (Newton's method, substitution method, etc.). There are some particular cases that can be interesting, one of which is a nonhomogeneous linear material with stiffness $\boldsymbol{c}(\boldsymbol{x})$

The above equation reduces to $\boldsymbol{e}^i = \boldsymbol{\varepsilon}\left(\boldsymbol{u}^i\right) + (\boldsymbol{c_0} + \boldsymbol{c})^{-1}\left(\boldsymbol{\lambda}^{i-1} - \boldsymbol{c} : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^i\right)\right)$

3) Step 3: Updating the Lagrange multiplier

In the equation $\lambda^i(\boldsymbol{x}) = \lambda^{i-1}(\boldsymbol{x}) + \boldsymbol{d}_0 : \left(\boldsymbol{\varepsilon}\left(\boldsymbol{u}^i(\boldsymbol{x})\right) - \boldsymbol{e}^i(\boldsymbol{x})\right)$, there are several possibilities for choosing $\boldsymbol{d}_0$. One of the simplest choices is $\boldsymbol{d}_0 = \boldsymbol{c}_0$ which also has some advantages. In the particular case of voided materials (linear or nonlinear), it can be checked that it leads to $\boldsymbol{\lambda}^i = 0$ in the voids. Equilibrium is then satisfied everywhere, including the voids.

The augmented Lagrangian FFT algorithm

An iteration of Uzawa's algorithm shown above reads (adapted from Michel et al. 2000) :

Iteration i: given $\boldsymbol{e}^{i-1}$ and $\boldsymbol{\lambda}^{i-1}$,

a) $\boldsymbol{\tau}^{i-1}(\boldsymbol{x}) = \boldsymbol{\lambda}^{i-1}(\boldsymbol{x}) - \boldsymbol{c}_0 : \boldsymbol{e}^{i-1}(\boldsymbol{x})$

b) $\hat{\boldsymbol{\tau}}^{i-1}(\boldsymbol{\xi}) = FFT\left(\boldsymbol{\tau}^{i-1}\right)$

c) $\hat{\hat{\boldsymbol{\varepsilon}}}^{i}(\boldsymbol{\xi}) = \hat{\Gamma}(\boldsymbol{\xi}) : \hat{\boldsymbol{\tau}}^{i-1}(\boldsymbol{\xi}); \forall \boldsymbol{\xi} \neq \boldsymbol{0}, \hat{\boldsymbol{\varepsilon}}^{i}(\boldsymbol{0}) = \boldsymbol{E}$

d) $\tilde{\boldsymbol{\varepsilon}}^{\boldsymbol{i}}(\boldsymbol{x}) = FFT^{-1}\left(\hat{\varepsilon}^{i}(\boldsymbol{\xi})\right)$

e) (**A***) Solve $\frac{\partial w}{\partial \boldsymbol{e}}\left(\boldsymbol{x}, \boldsymbol{e}^{i}\right) + \boldsymbol{c}_0 : \boldsymbol{e}^{i}(\boldsymbol{x}) = \boldsymbol{c}_0 : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^{\boldsymbol{i}}(\boldsymbol{x})\right) + \lambda^{i-1}(\boldsymbol{x})$ for $\boldsymbol{e}^{i}(\boldsymbol{x})$

f) $\boldsymbol{\lambda}^{i}(\boldsymbol{x}) = \boldsymbol{\lambda}^{i-1}(\boldsymbol{x}) + \boldsymbol{c}_0 : \left(\boldsymbol{\varepsilon}^{i}(\boldsymbol{x}) - \boldsymbol{e}^{i}(\boldsymbol{x})\right)$

g) (**B***) Convergence test

In the following, we will discuss **A*** and **B***.

A* - Newton approach for the elastic problem

We want to solve the nonlinear equation:

$$\frac{\partial w}{\partial \boldsymbol{e}}\left(\boldsymbol{x}, \boldsymbol{e}^i\right) + \boldsymbol{c}_0 : \boldsymbol{e}^i(\boldsymbol{x}) = \boldsymbol{c}_0 : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^i(\boldsymbol{x})\right) + \boldsymbol{\lambda}^{i-1}(\boldsymbol{x})$$

To do this we can use the Newton approach. In this approach, the problem reduces to nullifying the residual

$$\boldsymbol{R}\left(\frac{\partial w}{\partial \boldsymbol{\varepsilon}}\left(\boldsymbol{\varepsilon}^i\right)\right) = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}\left(\boldsymbol{\varepsilon}^i\right) + \boldsymbol{c}_0 : \boldsymbol{e}^i(\boldsymbol{x}) - \boldsymbol{\lambda}^{i-1}(\boldsymbol{x}) - \boldsymbol{c}_0 : \boldsymbol{\varepsilon}\left(\boldsymbol{u}^i(\boldsymbol{x})\right) = \boldsymbol{0}$$

Let $\boldsymbol{S}^i = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}\left(\boldsymbol{\varepsilon}^i\right)$ then

$$\boldsymbol{S}^{i,j} = \boldsymbol{S}^{i,j-1} - \left(\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{S}}\right|_{\boldsymbol{S}^{i,j-1}}\right) : \boldsymbol{R}\left(\boldsymbol{S}^{i,j-1}\right)$$

Gives the $(j+1)$ guess for $\boldsymbol{S}^i$. The Jacobian reads

$$\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{S}}\right|_{\boldsymbol{S}^{i,j-1}} = \boldsymbol{I} + \boldsymbol{c}_0 : \boldsymbol{c}^{-1}$$

Once convergence is achieved on $\boldsymbol{S}^i$ then we can compute $\boldsymbol{\lambda}^i(\boldsymbol{x})$ in step (f) on the previous slide.

B* - Convergence criterion

The convergence test focuses on the compatibility equations and the stress-strain relations. If we defined the following norm of a second order tensor

$$\|\boldsymbol{a}\| = \max_{\boldsymbol{x}} \sqrt{\boldsymbol{a}(\boldsymbol{x}) : \boldsymbol{a}(\boldsymbol{x})}$$

Then the iterative procedure is stopped when

$$\max\left(\frac{\|\boldsymbol{\varepsilon}^i - \boldsymbol{e}^i\|}{\|\boldsymbol{E}\|}, \frac{\left\|\boldsymbol{\lambda}^i - \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}^i)\right\|}{\left\|\left\langle \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{E}) \right\rangle\right\|} \right) \leq \eta$$

Where typically $\eta \leq 10^{-5}$

At the end of the iterative loop, one gets a compatible strain field that is constitutively related to an equilibrated stress field.

Note that for a time dependent loading, this iterative loop has to be embedded in a time loop.

Elasto-viscoplastic FFT – the local problem

- The algorithm was presented in the work of Lebensohn et al. (2012) in small small strain framework.
- Part of the local problem is still written as

$$\boldsymbol{\sigma}(\boldsymbol{x}) = \boldsymbol{c^0}:\boldsymbol{\varepsilon}(\boldsymbol{x}) + \boldsymbol{\tau}(\boldsymbol{x}) = \boldsymbol{c^0}:\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x}) + \boldsymbol{c^0}:\boldsymbol{E} + \boldsymbol{\tau}(\boldsymbol{x});\ \boldsymbol{x} \in V$$

$$\mathbf{div}\,\boldsymbol{\sigma}(\boldsymbol{x}) = \mathbf{div}\left(\boldsymbol{c^0}:\tilde{\boldsymbol{\varepsilon}}(\boldsymbol{x})\right) + \mathbf{div}\,\boldsymbol{\tau}(\boldsymbol{x}) = \mathbf{0}; \forall \boldsymbol{x} \in V$$

$$\tilde{\boldsymbol{u}}(periodic), \boldsymbol{\sigma}\cdot\boldsymbol{n}(anti-periodic)\ on\ \boldsymbol{S}$$

- Now, in addition, we have visco-plastic deformation whose contribution can be mathematically accounted for via the rate-dependent power law relationship between the plastic strain rate ($\dot{\varepsilon}^{vp}$), the shear rate per slip system s ($\dot{\gamma}_s$) and the Cauchy stress (Hutchinson 1976, Pan & Rice 1983, Asaro & Needleman 1985)

$$\dot{\varepsilon}^{vp} = \sum_{s=1}^{N} \dot{\gamma}_s m_s = \sum_{s=1}^{N} \dot{\gamma}_0^s \left(\frac{\boldsymbol{\sigma}:\boldsymbol{m}_s}{\tau_s^c}\right)^n \mathrm{sgn}\,(\boldsymbol{\sigma}:\boldsymbol{m}_s)$$

Here, $\boldsymbol{\sigma}:\boldsymbol{m}_s$ is the resolved shear stress on each slip system, τ_s^c is the critical resolved shear stress, $\dot{\gamma}_0^s$ is the reference shear rate and n is the power law exponent which is the inverse of the rate sensitivity parameter. The elastic strain is related to the total and plastic strains as $\boldsymbol{\varepsilon}^e = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{vp}$

EVPFFT augemented Lagrangian algorithm

- The algorithm remains the same as the one presented for the elastic case with the only difference comes into the Newton-Raphson approach where the Jacobian is computed as:

$$\left.\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\sigma}}\right|_{\boldsymbol{\sigma}^{i,j-1}} = \boldsymbol{I} + \boldsymbol{c}_0 : \boldsymbol{c}^{-1} + \Delta t \left(\boldsymbol{c}^0 : \left.\frac{\partial \dot{\boldsymbol{\varepsilon}}^{vp}}{\partial \boldsymbol{\sigma}}\right|_{\boldsymbol{\sigma}^{i,j-1}} \right)$$

- Note here that $\boldsymbol{\sigma} = \boldsymbol{S}$
- The derivative on the right is the tangent compliance of the viscoplastic relationship $\dot{\varepsilon}^{vp} = \sum_{s=1}^{N} \dot{\gamma}_s m_s = \sum_{s=1}^{N} \dot{\gamma}_0^s \left(\frac{\boldsymbol{\sigma} : \boldsymbol{m}_s}{\tau_s^c} \right)^n \operatorname{sgn}(\boldsymbol{\sigma} : \boldsymbol{m}_s)$

FFT vs FEM

Criteria	FFT	FEM
Computational time	**O ($N\log_2 N$)**	O(N^2)
Mesh	**No**	Yes
Spatial arrangement of material points	**Structured grid**	Depends on mesh (affects convergence)
Boundary conditions	Homogeneous stress or strain rate (force and displacement now possible via non-periodic FFTs)	**Forces and displacements**
Domain	Periodic RVE (although efficient non-periodic FFTs exist)	**Any shape and size**
Interfaces	Not well defined (has its advantages/disadvantages)	Well-defined (has its advantages/disadvantages)
Dimensions	**2D/3D full field**	**2D/3D full field**
Large deformations	Computations done in reference configuration	**Computations in reference and current configurations**

Further reading

- H Moulinec, P Suquet, (1998) “A numerical method for computing the overall response of nonlinear composites with complex microstructure”, *Computer methods in applied mechanics and engineering* 157 (1-2), 69-94
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- JC Michel, H Moulinec, P Suquet, (2000) “A computational method based on augmented Lagrangians and fast Fourier transforms for composites with high contrast”, *CMES(Computer Modelling in Engineering & Sciences)* 1 (2), 79-88
- JC Michel, H Moulinec, P Suquet, (2001) “A computational scheme for linear and non-linear composites with arbitrary phase contrast”, *International Journal for Numerical Methods in Engineering* 52 (1-2), 139-160
- RA Lebensohn, AK Kanjarla, P Eisenlohr, (2012), “An elasto-viscoplastic formulation based on fast Fourier transforms for the prediction of micromechanical fields in polycrystalline materials”, *International Journal of Plasticity*, 32–33, 59-69