A Piecewise Polynomial Approximation Scheme Based on the Hashin-Shtrikman Variational Principle of Polycrystals

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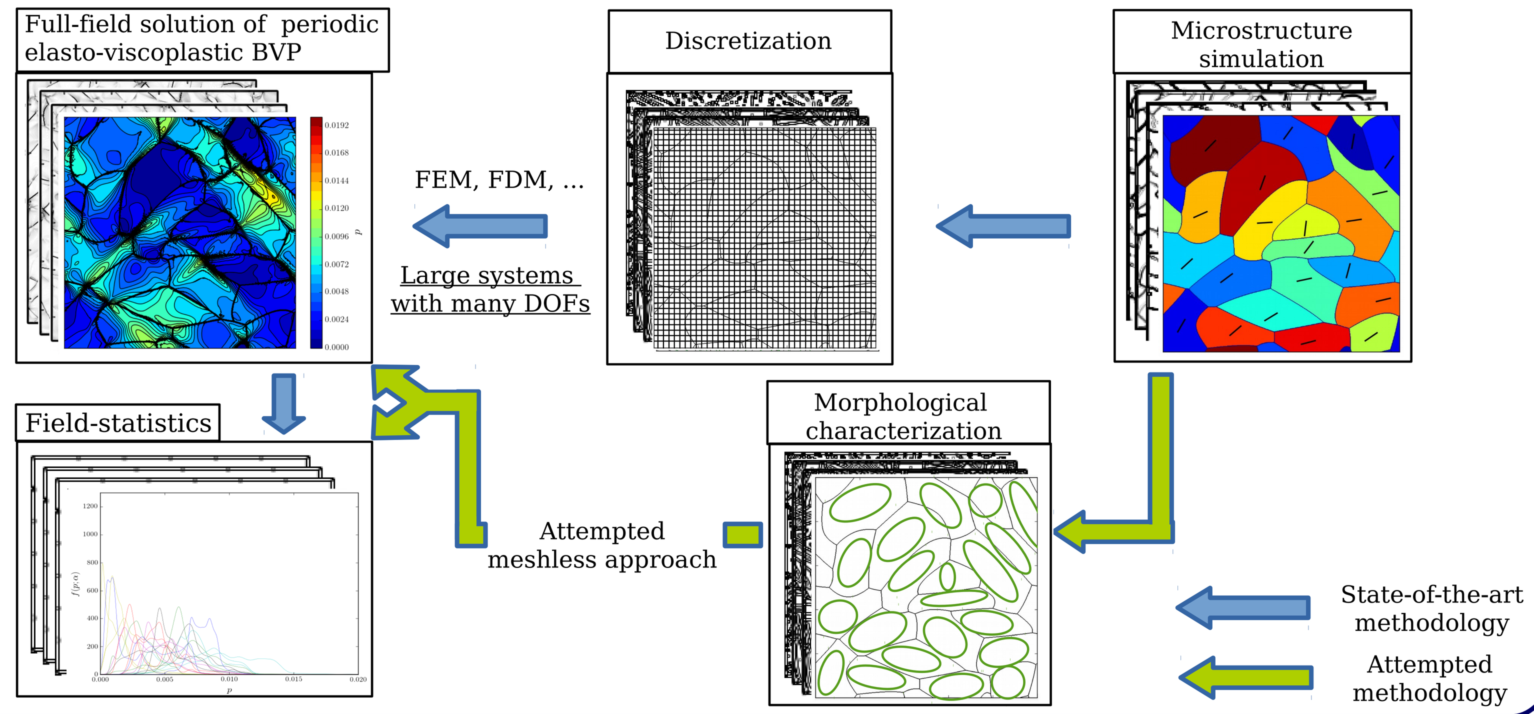
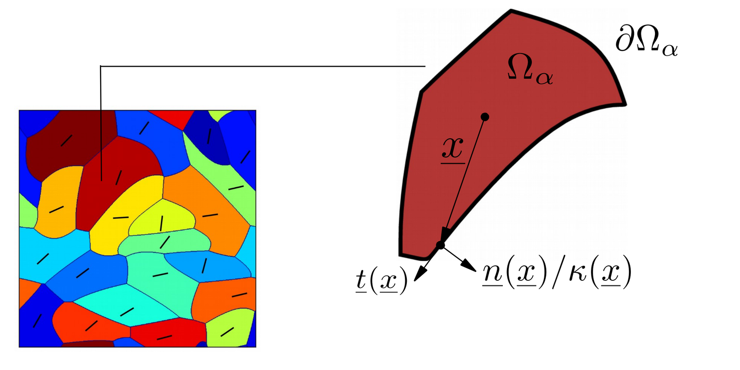
1. Objective

- Leverage high-order morphological characterization of microstructures to derive full-field approximation and statistics of mechanical behaviors in polycrystals.



2. Morphological characterization

- Single grains are characterized using Minkowski tensors:.



Measures of mass distribution:

$$\mathcal{W}_0^{r,0} = \int_{\Omega_\alpha} \underline{x}^{\otimes^r} \mathrm{d}V$$

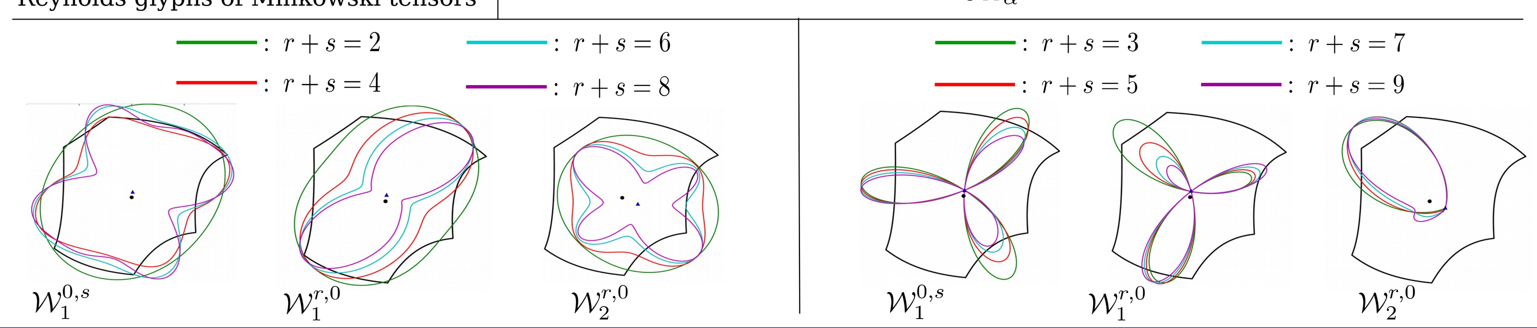
Measures of surface distribution:

$$\mathcal{W}_1^{r,s} = \int_{\partial\Omega_\alpha} \underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}S$$

Curvature-weighted measures of surface distribution:

$$\mathcal{W}_2^{r,s} = \int_{\partial\Omega_\alpha} \kappa(\underline{x})\underline{x}^{\otimes^r} \odot [\underline{n}(\underline{x})]^{\otimes^s} \mathrm{d}S$$

Reynolds glyphs of Minkowski tensors



3. Problem formulation

- Periodic boundary value problem (D): The underlying strain field of the problem

$$\text{(D)}: \text{Find } \Omega\text{-periodic } \underline{u} \text{ s.t. } \nabla\cdot[\mathbb{L}(\underline{x}):\boldsymbol{\varepsilon}(\underline{x})] = \underline{0}\,, \quad \boldsymbol{\varepsilon}(\underline{x}) = \{\nabla\underline{u}(\underline{x})\}_{sym}, \quad |\Omega|^{-1}\int_\Omega \boldsymbol{\varepsilon}(\underline{x})\mathrm{d}\underline{x} =: \overline{\boldsymbol{\varepsilon}} = \boldsymbol{\varepsilon}_0.$$

is equivalently expressed as the solution of the Lippmann-Schwinger (LS) equation:

$$\Delta\mathbb{L}(\underline{x})^{-1}:\boldsymbol{\tau}(\underline{x}) + \boldsymbol{\Gamma}*\boldsymbol{\tau}(\underline{x}) = \boldsymbol{\varepsilon}_0 \text{ for all } \underline{x}\,, \text{ where } \boldsymbol{\tau}(\underline{x}) := [\mathbb{L}(\underline{x})-\mathbb{L}^0]:\boldsymbol{\varepsilon}(\underline{x}) = \Delta\mathbb{L}(\underline{x}):\boldsymbol{\varepsilon}(\underline{x}).$$

- Variational problem (V) formulation: The weak form of the LS equation is

$$\text{(V)}: \quad \text{Find } \boldsymbol{\tau}\in\mathbb{V} \text{ such that } a(\boldsymbol{\tau},\boldsymbol{\omega}) = \ell(\boldsymbol{\omega})\ \forall\boldsymbol{\omega}\in\mathbb{V}, \text{ where}$$

$$\begin{aligned} a: \mathbb{V}\times\mathbb{V} &\to \mathbb{R} \\ (\boldsymbol{\omega},\boldsymbol{\tau}) &\mapsto \overline{\boldsymbol{\omega}:\Delta\mathbb{L}^{-1}:\boldsymbol{\tau}} + \overline{\boldsymbol{\omega}:(\boldsymbol{\Gamma}*\boldsymbol{\tau})} \end{aligned} \quad \text{and} \quad \begin{aligned} \ell: \mathbb{V} &\to \mathbb{R} \\ \boldsymbol{\omega} &\mapsto \overline{\boldsymbol{\omega}}:\boldsymbol{\varepsilon}_0 \end{aligned}\,.$$

- Optimization problem (O) formulation:

$\Delta\mathbb{L}(\underline{x}) \prec 0$ (resp. $\Delta\mathbb{L}(\underline{x}) \succ 0$) for all $\underline{x}$ implies that the Hashin-Shtrikman (HS) functional $\mathcal{H}:\boldsymbol{\tau}\mapsto a(\boldsymbol{\tau},\boldsymbol{\tau})/2 - \ell(\boldsymbol{\tau})$ is strictly convex (resp. concave). (V) is then equivalent to

$$\text{(O)}: \quad \text{Find } \boldsymbol{\tau}\in\mathbb{V} \text{ such that } \partial_\epsilon[\mathcal{H}(\boldsymbol{\tau}+\epsilon\delta\boldsymbol{\tau})]|_{\epsilon=0} = 0\,.$$

4. Piecewise polynomial Galerkin method

- We consider piecewise polynomial trial fields $\boldsymbol{\tau}^p \in \mathbb{V}_p \subset \mathbb{V}$ of the form

$$\boldsymbol{\tau}^p(\underline{x}) := \sum_\alpha \left(\chi_\alpha(\underline{x})\boldsymbol{\tau}^\alpha + \chi_\alpha(\underline{x})\sum_{k=1}^p \left\langle \boldsymbol{\tau}^\alpha\boldsymbol{\partial}^k, (\underline{x}-\underline{x}^\alpha)^{\otimes^k}\right\rangle_k\right)$$

and intend to solve (V_p) : Find $\boldsymbol{\tau}^p\in\mathbb{V}_p$ such that $a(\boldsymbol{\tau}^p,\boldsymbol{\omega}^p) = \ell(\boldsymbol{\omega}^p)\ \forall\boldsymbol{\omega}^p\in\mathbb{V}_p$.

- The functionals then take the following forms

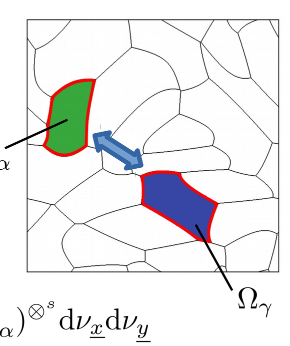
$$\ell(\boldsymbol{\omega}^p) = \sum_\alpha \left(c_\alpha\boldsymbol{\omega}^\alpha:\boldsymbol{\varepsilon}_0 + \sum_{r=1}^p \left\langle \boldsymbol{\omega}^\alpha\boldsymbol{\partial}^r, \mathcal{W}_0^{r,0}(\Omega'_\alpha)\right\rangle_r : \boldsymbol{\varepsilon}_0\right)$$

$$a(\boldsymbol{\tau}^p,\boldsymbol{\omega}^p) = \sum_\alpha \Delta\mathbb{M}^\alpha :: \left(c_\alpha\boldsymbol{\omega}^\alpha\otimes\boldsymbol{\tau}^\alpha + \sum_{r=1}^p\sum_{s=1}^p \left\langle \boldsymbol{\omega}^\alpha\boldsymbol{\partial}^r, \left\langle \mathcal{W}_0^{r+s,0}(\Omega'_\alpha), \boldsymbol{\partial}^s\boldsymbol{\tau}^\alpha\right\rangle_s\right\rangle_r\right)$$

$$+\sum_\alpha\sum_\gamma \left(\boldsymbol{\omega}^\alpha : \mathbb{T}_{0,0}^{\alpha\gamma} : \boldsymbol{\tau}^\gamma + \sum_{r=1}^p\sum_{s=1}^p \left\langle \boldsymbol{\partial}^r\boldsymbol{\omega}^\alpha, \left\langle \mathbb{T}_{r,s}^{\alpha\gamma}, \boldsymbol{\tau}^\gamma\boldsymbol{\partial}^s\right\rangle_{s+2}\right\rangle_{r+2}\right)$$

Minkowski tensors (see Frame 2)

Influence tensors (see Frame 5)



with influence tensors capturing the effect of pairwise grain interactions

$$\mathbb{T}_{r,s}^{\alpha\gamma} = \int_{\Omega_\alpha}\int_{\Omega_\gamma} (\underline{x}-\underline{x}_\alpha)^{\otimes^r}\otimes\boldsymbol{\Gamma}(\underline{x}-\underline{y})\otimes(\underline{x}-\underline{x}_\alpha)^{\otimes^s}\mathrm{d}\nu_{\underline{x}}\mathrm{d}\nu_{\underline{y}}$$

5. Non-consistent approximation

- Computing $\mathbb{T}_{r,s}^{\alpha\gamma}$ is the main source of difficulty of this work. We approach this problem by expressing the Green operator as a Taylor expansion around $\underline{x}_{\gamma\alpha} := \underline{x}_\alpha - \underline{x}_\gamma$ for each pair (α,γ) of grains respectively centered at $(\underline{x}_\alpha,\underline{x}_\gamma)$:

$${}^n\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha}) := {}^n\boldsymbol{\Gamma}(\underline{x}_{\gamma\alpha}) + \sum_{k=1}^n\sum_{i=0}^k \frac{(-1)^i}{(k-i)!i!}\left\langle \boldsymbol{\Gamma}^{(k)}(\underline{x}_{\gamma\alpha}), \underline{x}^{\otimes^{k-i}}\otimes\underline{y}^{\otimes^i}\right\rangle_k \text{ for all } (\underline{x},\underline{y})\in\mathring{\Omega}'_\alpha\times\mathring{\Omega}'_\gamma$$

- We denote the order of the expansion by *n* and construct the following estimates:

for any $\gamma\neq\alpha$

$$({}^nT_{r,s}^{\alpha\gamma})_{r_1\dots r_r ijkl s_1\dots s_s} = \frac{1}{|\Omega|}[W_0^{r,0}(\Omega'_\alpha)]_{r_1\dots r_r}\Gamma_{ijkl}(\underline{x}_{\gamma\alpha})[W_0^{s,0}(\Omega'_\gamma)]_{s_1\dots s_s}$$
$$+\frac{1}{|\Omega|}\sum_{k=1}^n\sum_{i=0}^k\frac{(-1)^i}{(k-i)!i!}\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})[W_0^{r+k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}r_1..r_r}[W_0^{i+s,0}(\Omega'_\gamma)]_{k_{k-i+1}..k_k s_1..s_s}$$

$$({}^nT_{r,s}^{\alpha\alpha})_{r_1\dots r_r ijkl s_1\dots s_s} = \frac{1}{|\Omega|}[W_0^{r,0}(\Omega'_\alpha)]_{r_1\dots r_r}\Gamma_{ijkl}(\underline{x}_{\gamma\alpha})[W_0^{s,0}(\Omega'_\alpha)]_{s_1\dots s_s}$$
$$+\frac{1}{|\Omega|}\sum_{k=1}^n\sum_{i=0}^k\frac{(-1)^i}{(k-i)!i!}\Gamma^{(k)}_{ijklk_1..k_k}(\underline{x}_{\gamma\alpha})[W_0^{r+k-i,0}(\Omega'_\alpha)]_{k_1..k_{k-i}r_1..r_r}[{}^\gamma\widetilde{\mathcal{W}}_0^{i|s,0}(\Omega'_\alpha)]_{k_{k-i+1}\dots k_k s_1\dots s_s}$$

$${}^\gamma\widetilde{\mathcal{W}}_0^{i|s,0}(\Omega'_\alpha) := \sum_{t=0}^i\binom{i}{t}(\underline{x}_{\gamma\alpha})^{\otimes^{i-t}} \overset{i-t,t}{\odot} \mathcal{W}_0^{t+s,0}(\Omega'_\alpha)$$

- We refer to a in which $\mathbb{T}_{r,s}^{\alpha\gamma}$ is replaced by ${}^n\mathbb{T}_{r,s}^{\alpha\gamma}$ as ${}^na$ and now focus on the non-consistent HS functional ${}^n\mathcal{H}:\boldsymbol{\tau}^p\mapsto{}^na(\boldsymbol{\tau}^p,\boldsymbol{\tau}^p)/2-\ell(\boldsymbol{\tau}^p)$.

6. Discretized system

- Eventually, we solve (${}^n\mathrm{O}_p$) : Find $\boldsymbol{\tau}^p\in\mathbb{V}_p$ such that $\partial_\epsilon[{}^n\mathcal{H}(\boldsymbol{\tau}^p+\epsilon\delta\boldsymbol{\tau}^p)]|_{\epsilon=0} = 0$.
- In 2D, this is equivalent to solving the system

$$\begin{Bmatrix}\{\overline{\boldsymbol{\varepsilon}}^0\}\\\{\overline{\boldsymbol{\varepsilon}}^1\}\\\{\overline{\boldsymbol{\varepsilon}}^2\}\\\vdots\\\{\overline{\boldsymbol{\varepsilon}}^p\}\end{Bmatrix} = \begin{bmatrix}[\mathbb{D}^{0,0}] & [\mathbb{D}^{0,1}] & [\mathbb{D}^{0,2}] & \dots & [\mathbb{D}^{0,p}]\\ [\mathbb{D}^{1,0}] & [\mathbb{D}^{1,1}] & [\mathbb{D}^{1,2}] & \dots & [\mathbb{D}^{1,p}]\\ [\mathbb{D}^{2,0}] & [\mathbb{D}^{2,1}] & [\mathbb{D}^{2,2}] & \dots & [\mathbb{D}^{2,p}]\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ [\mathbb{D}^{p,0}] & [\mathbb{D}^{p,1}] & [\mathbb{D}^{p,2}] & \dots & [\mathbb{D}^{p,p}]\end{bmatrix}\begin{Bmatrix}\{\boldsymbol{\partial}^0\boldsymbol{\tau}\}\\\{\boldsymbol{\partial}^1\boldsymbol{\tau}\}\\\{\boldsymbol{\partial}^2\boldsymbol{\tau}\}\\\vdots\\\{\boldsymbol{\partial}^p\boldsymbol{\tau}\}\end{Bmatrix}$$

$3n_\alpha\binom{p+2}{2}\times 1 \qquad 3n_\alpha\binom{p+2}{2}\times 3n_\alpha\binom{p+2}{2} \qquad 3n_\alpha\binom{p+2}{2}\times 1$

where $[\mathbb{D}^{r,s}] = [\mathbb{M}^{r,s}] + [{}^n\boldsymbol{\Gamma}^{r,s}]$

- $[\mathbb{M}^{r,s}] = \mathrm{diag}\left([\mathbb{M}^{r,s,1}], \underbrace{[\mathbb{M}^{r,s,2}]}_{3(r+1)\times 3(s+1)}, \dots, [\mathbb{M}^{r,s,n_\alpha}]\right)$ in which $[\mathbb{M}^{r,s,\alpha}]$ contains properly weighted components of $\mathcal{W}^{r+s}(\Omega'_\alpha)\otimes(\Delta\mathbb{L}_\alpha)^{-1}$.

- $$[{}^n\boldsymbol{\Gamma}^{r,s}] = \begin{bmatrix}[{}^n\boldsymbol{\Gamma}^{r,s,1,1}] & [{}^n\boldsymbol{\Gamma}^{r,s,1,2}] & \dots & [{}^n\boldsymbol{\Gamma}^{r,s,1,n_\alpha}]\\ [{}^n\boldsymbol{\Gamma}^{r,s,2,1}] & [{}^n\boldsymbol{\Gamma}^{r,s,2,2}] & \dots & [{}^n\boldsymbol{\Gamma}^{r,s,2,n_\alpha}]\\ \vdots & \vdots & \ddots & \vdots\\ [{}^n\boldsymbol{\Gamma}^{r,s,n_\alpha,1}] & [{}^n\boldsymbol{\Gamma}^{r,s,n_\alpha,2}] & \dots & \underbrace{[{}^n\boldsymbol{\Gamma}^{r,s,n_\alpha,n_\alpha}]}_{3(r+1)\times 3(s+1)}\end{bmatrix}$$ in which $[{}^n\boldsymbol{\Gamma}^{r,s,\alpha,\gamma}]$ contains properly weighted components of ${}^n\mathbb{T}_{r,s}^{\alpha\gamma}$.

7. Table of derivatives of the Green operator

- In order to compute the components of ${}^n\mathbb{T}_{r,s}^{\alpha\gamma}$, we need to evaluate $\Gamma_{ijkl,k_1}(\underline{x}_{\gamma\alpha})$ and the derivatives $\Gamma^{(1)}_{ijkl,k_1}(\underline{x}_{\gamma\alpha}),\ \Gamma^{(2)}_{ijkl,k_1k_2}(\underline{x}_{\gamma\alpha}),\ \dots,\Gamma^{(n)}_{ijkl,k_1\dots k_n}(\underline{x}_{\gamma\alpha})$.
- To do so, we use the Barnett-Lothe integral solution for anisotropic Green functions $G_{ij}(r,\theta)$, i.e.

$$4\Gamma_{ijkl}(\underline{x}) = G^{(2)}_{ik,jl}(\underline{x}) + G^{(2)}_{il,jk}(\underline{x}) + G^{(2)}_{jk,il}(\underline{x}) + G^{(2)}_{jl,ik}(\underline{x}) \ .$$

- We derive the following recurrence relations to compute the derivatives of anisotropic Green functions:

$$2\pi G^{(n)}_{ij,k_1\dots k_n}(r,\theta) = (-r)^{-n}h^n_{ijk_1\dots k_n}(\theta)$$

$$h^n_{ijk_1\dots k_n}(\theta) = (n-1)h^{n-1}_{ijk_1\dots k_{n-1}}(\theta)n_{k_n}(\theta) - \partial_\theta[h^{n-1}_{ijk_1\dots k_{n-1}}(\theta)]m_{k_n}(\theta) \ \text{ for } n\geq 2$$

$$\partial^k_\theta[h^n_{ijk_1\dots k_n}(\theta)] = \sum_{s=0}^k\binom{k}{s}\left\{(n-1)\partial_\theta^{k-s}[h^{n-1}_{ijk_1\dots k_{n-1}}(\theta)]\partial^s_\theta[n_{k_n}(\theta)] - \partial_\theta^{k-s+1}[h^{n-1}_{ijk_1\dots k_{n-1}}(\theta)]\partial_\theta^{s+1}[n_{k_n}(\theta)]\right\}$$

$$h^1_{ijk_1}(\theta) = H_{ij}n_{k_1}(\theta) + [N^1_{is}(\theta)H_{sj} + N^2_{is}(\theta)S_{js}]m_{k_1}(\theta)$$

$$\partial^k_\theta[h^1_{ijk_1}(\theta)] = H_{ij}\partial^k_\theta[n_{k_1}(\theta)] + \sum_{s=0}^k\binom{k}{s}\left\{H_{lj}\partial_\theta^{k-s}[N^1_{il}(\theta)] + S_{jl}\partial_\theta^{k-s}[N^2_{il}(\theta)]\right\}\partial^s_\theta[m_{k_1}(\theta)]$$

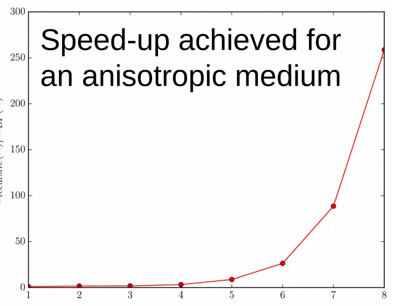
Barnett-Lothe integrands, see Ting (1996).

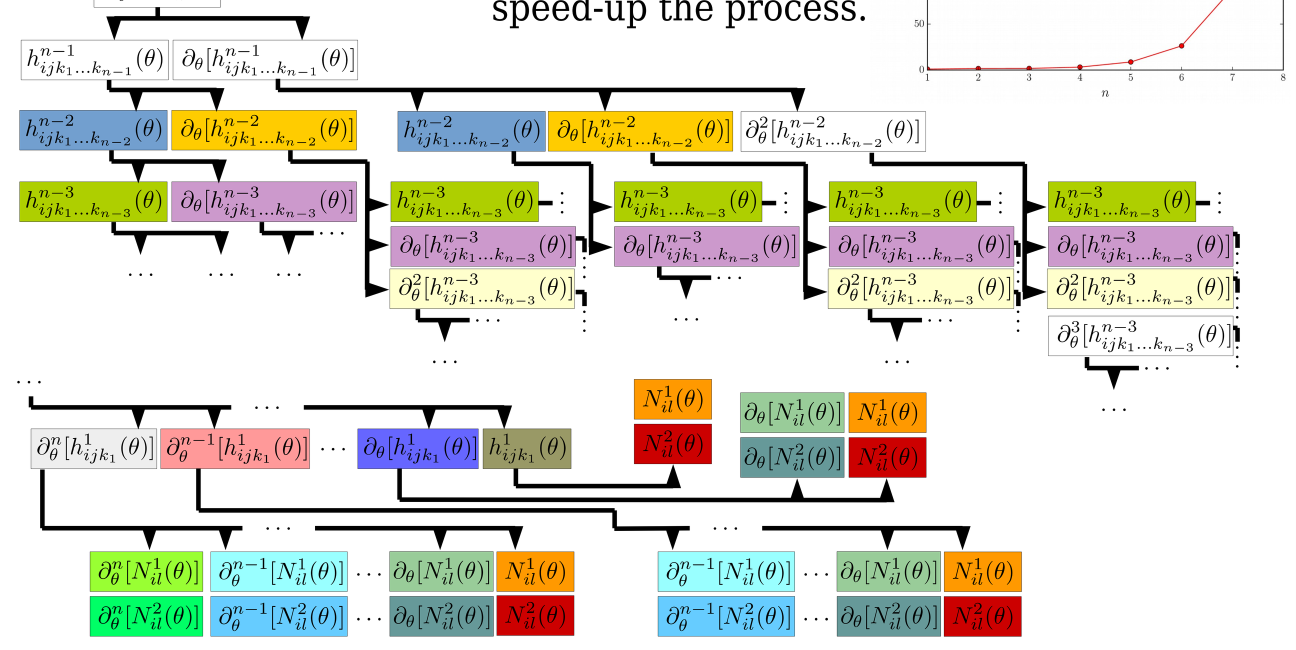
- Number of components of derivatives of the Green operator to build the system: $6\binom{n_\alpha}{2}\binom{n+2}{2}$.

Those components are "memoized" to avoid repeating computations.

8. Bottom-up dynamic evaluation

- Evaluation of the Barnett-Lothe (BL) integrands and their derivatives is costly. A naive implementation of the recursive scheme is not efficient. Instead, we derive a bottom-up dynamic algorithm to speed-up the process.

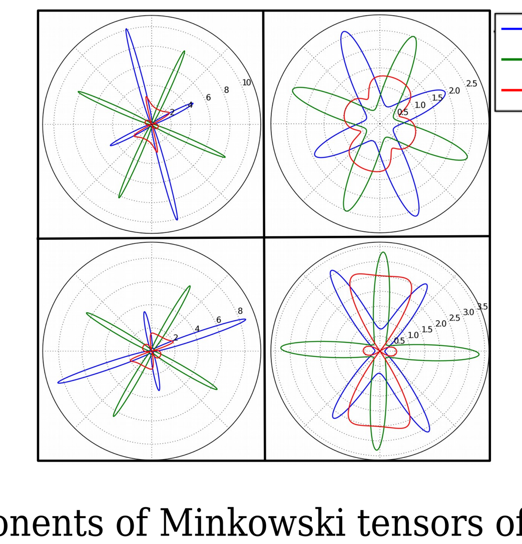




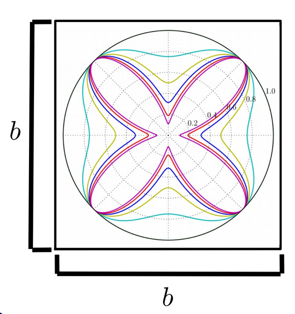
- [colored boxes] , , , , ..., : repeated evaluation of BL integrands by divide-and-conquer approach.

9. Preliminary results

- We consider a periodic array of 4 anisotropic squares with those generalized elastic moduli:



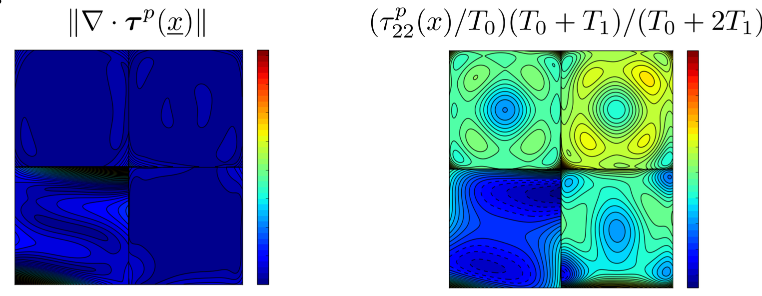
- Components of Minkowski tensors of each phase:



$$[\mathcal{W}_0^{r,0}](n_1) := [\mathcal{W}_0^{r,0}]_{\underbrace{11\dots1}_{(n_1\text{ times})}\underbrace{22\dots2}_{(r-n_1\text{ times})}}$$

$$[\mathcal{W}_0^{r,0}](n_1) = \frac{(b/2)^{n_1+n_2+2} - (-b/2)^{n_1+1}(b/2)^{n_2+1}}{(n_1+1)(n_2+1)} + \frac{(-b/2)^{n_1+1}(-b/2)^{n_2+1} - (b/2)^{n_1+1}(-b/2)^{n_2+1}}{(n_1+1)(n_2+1)}$$

- The array is subjected to $\overline{\boldsymbol{\varepsilon}} = \underline{e}_2\otimes\underline{e}_2$.
- $\mathbb{L}_0$ is picked such that $\Delta\mathbb{L}(\underline{x})\prec 0$.
- Let p=5 and n=5.
- Results:



- Those results do not qualitatively match the solution.
- Source of error: ${}^n\boldsymbol{\Gamma}$ is a poor estimate of $\boldsymbol{\Gamma}(\underline{x}-\underline{y}+\underline{x}_{\gamma\alpha})$ if $\underline{x}$ and $\underline{y}$ are near the grain boundary $\Omega_\alpha\cap\Omega_\gamma$: