Physics-compatible numerical approximations to the Fokker-Planck model of fiber orientation

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Fiber orientation modeling

- Evolution of the probability distribution function $\psi(\mathbf{p},t) \geq 0$ of fiber orientation is governed by the Fokker-Planck equation

$$\frac{\partial \psi}{\partial t} + \nabla_{\mathbf{p}} \cdot (\dot{\mathbf{p}}\psi) = \Delta_{\mathbf{p}}(D_r\psi), \qquad \dot{\mathbf{p}} = \mathbf{W}\cdot\mathbf{p} + \lambda[\mathbf{D}\cdot\mathbf{p} - \mathbf{D} : (\mathbf{p}\otimes\mathbf{p})\mathbf{p}].$$

- Important quantities are the orientation tensors $\mathbb{A}_2 \in \mathbb{R}^{n\times n}$ and $\mathbb{A}_4 \in \mathbb{R}^{n\times n\times n\times n}$

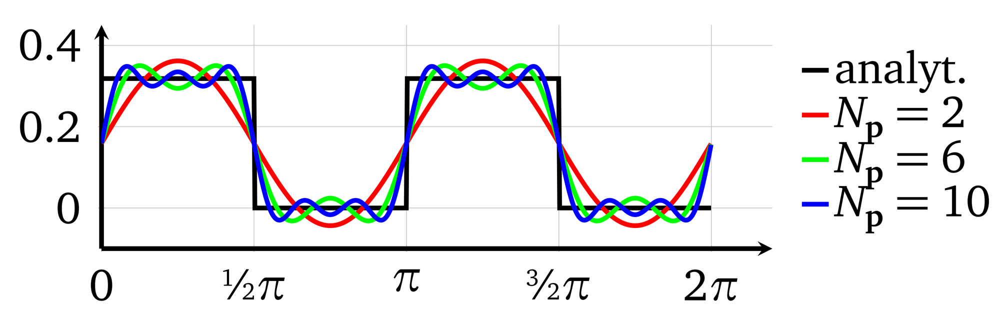
$$\mathbb{A}_{2m} = (\mathbb{A}_{i_1\dots i_{2m}}), \qquad \mathbb{A}_{i_1\dots i_{2m}} = \langle \mathbf{p}_{i_1}\cdots\mathbf{p}_{i_{2m}}\rangle = \int_{\mathbb{S}} \mathbf{p}_{i_1}\cdots\mathbf{p}_{i_{2m}}\psi(\mathbf{p})\,\mathrm{d}\mathbf{p}. \qquad (1)$$

- In two dimensions ψ is approximated by the truncated Fourier series ψ^{N_p} of order N_p

$$\psi^{N_\mathrm{p}}(\phi) = a_0\tfrac{1}{\sqrt{2\pi}} + \sum_{j=1}^{N_\mathrm{p}/2}\left(a_{2j}\tfrac{1}{\sqrt{\pi}}\cos(2j\phi) + b_{2j}\tfrac{1}{\sqrt{\pi}}\sin(2j\phi)\right).$$

Fourier analysis

Figure 1: Gibbs phenomenon



Truncated Fourier expansions should correspond to valid "nonnegative" approximations. However, the condition $\psi^{N_\mathrm{p}}(\mathbf{p}) \geq 0$ for all $\mathbf{p} \in \mathbb{S}$ is too restrictive.

Definition: nonnegative Fourier approximation

A Fourier approximation ψ^{N_p} is called "nonnegative" if and only if there exists $\bar{\psi} \geq 0$ s.t. $\mathcal{P}_{N_\mathrm{p}}\bar{\psi} = \psi^{N_\mathrm{p}}$, where $\mathcal{P}_{N_\mathrm{p}}\cdot$ denotes the truncated Fourier expansion of order N_p.

Definition: Positive semi-definite tensor

A tensor $\mathbb{B} \in \mathbb{R}^{n\times\dots\times n}$, $n \in \mathbb{N}$, of order $2m \in 2\mathbb{N}$ (i.e., $n\times\dots\times n$ $2m$ times) is positive semi-definite if and only if

$$\mathbf{S}_{i_1\dots i_m}\mathbb{B}_{i_1\dots i_m j_1\dots j_m}\mathbf{S}_{j_1\dots j_m} = \mathbf{S} : (\mathbb{B} : \mathbf{S}) \geq 0$$

for all tensors $\mathbf{S} \in \mathbb{R}^{n\times\dots\times n}\setminus\{\mathbf{0}\}$ of order m.

Theorem: Positive semi-definiteness of an orientation tensor

Let $\psi \geq 0$ be a nonnegative function. Then each orientation tensor $\mathbb{A}_{2m}$ of order $2m \in 2\mathbb{N}$ (see eq. (1)) is positive semi-definite.

Lemma: Nonnegativity criterion for polynomial roots

Let $p(x) = p_n x^n + p_{n-1}x^{n-1} + \ldots + p_0$, $p_k \in \mathbb{R}$, be a polynomial of order $n \in \mathbb{N}$ with exclusively real-valued roots. These are nonnegative if and only if

$$(-1)^k p_k \geq 0 \quad \text{for all } 0 \leq k \leq n \qquad \text{or} \qquad (-1)^k p_k \leq 0 \quad \text{for all } 0 \leq k \leq n.$$

Derivation of nonnegativity conditions

The orientation tensor $\mathbb{A}_4 \in \mathbb{R}^{2\times2\times2\times2}$ of order 4 can be written as

$$\mathbb{A}_4 = \frac{\sqrt{\pi}}{8}\begin{pmatrix} 3\sqrt{2}a_0+4a_2+a_4 & 2b_2+b_4 & 2b_2+b_4 & \sqrt{2}a_0-a_4 \\ 2b_2+b_4 & \sqrt{2}a_0-a_4 & \sqrt{2}a_0-a_4 & 2b_2-b_4 \\ 2b_2+b_4 & \sqrt{2}a_0-a_4 & \sqrt{2}a_0-a_4 & 2b_2-b_4 \\ \sqrt{2}a_0-a_4 & 2b_2-b_4 & 2b_2-b_4 & 3\sqrt{2}a_0-4a_2+a_4 \end{pmatrix}.$$

Then the characteristic polynomial of this tensor is given by

$$\chi_{\mathbb{A}_4}(\lambda) = \lambda^4 - \sqrt{\pi}\sqrt{2}a_0\lambda^3 + \tfrac{\pi}{16}(10a_0^2 - 4c_2^2 - c_4^2)\lambda^2 - \tfrac{\sqrt{\pi^3}}{32}(2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2)\lambda.$$

The lemma above yields the following inequality constraints

$$\begin{cases} 0 \leq a_0, \\ 0 \leq 10a_0^2 - 4c_2^2 - c_4^2, \\ 0 \leq 2\sqrt{2}a_0^3 - 2\sqrt{2}a_0c_2^2 - \sqrt{2}a_0c_4^2 + 2a_2^2a_4 + 4a_2b_2b_4 - 2a_4b_2^2. \end{cases}$$

Correction techniques

Constrained least-squares minimization

$$\begin{cases} \inf & F(\psi^{n+1}) = \left\|\mathcal{P}^{-1}(\mathcal{A}\psi^{n+1} - \mathbf{b})\right\|_2^2, \\ \text{s.t.} & \text{inequalities hold and mass is preserved } (a_0^{n+1} = a_0^n). \end{cases}$$

Artificial Diffusion

reduces especially high frequency oscillations

$$\frac{\partial\psi(\mathbf{p},t)}{\partial t} + \mathrm{div}_{\mathbf{p}}(\dot{\mathbf{p}}\psi(\mathbf{p},t)) - \Delta_{\mathbf{p}}(D_r\psi(\mathbf{p},t)) - \tilde{\mu}\Delta_{\mathbf{p}}(\psi(\mathbf{p},t)) = 0.$$

Nonnegative reconstruction

- Boltzmann-Shannon entropy maximization

$$\begin{cases} \inf\limits_{\psi} & \int_0^{2\pi} \psi(\phi)\log(\psi(\phi)) - \psi(\phi)\,\mathrm{d}\phi, \\ \text{s.t.} & \int_0^{2\pi} \psi(\phi)\tfrac{1}{\sqrt{\pi}}\cos(2j\phi)\,\mathrm{d}\phi = a_{2j} \quad \text{for all } 1 \leq j \leq N_\mathrm{p}/2, \\ & \int_0^{2\pi} \psi(\phi)\tfrac{1}{\sqrt{\pi}}\sin(2j\phi)\,\mathrm{d}\phi = b_{2j} \quad \text{for all } 1 \leq j \leq N_\mathrm{p}/2, \\ & \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \psi(\phi)\,\mathrm{d}\phi = a_0, \quad 0 \leq \psi(\phi). \end{cases}$$

- Under certain assumptions the solution has the form

$$\bar{\psi}^{N_\mathrm{p}}(\phi) = \exp\left(\hat{\psi}^{N_\mathrm{p}}(\phi)\right) = \exp\left[\hat{a}_0\tfrac{1}{\sqrt{2\pi}} + \sum_{j=1}^{N_\mathrm{p}/2}\left(\hat{a}_{2j}\tfrac{1}{\sqrt{\pi}}\cos(2j\phi) + \hat{b}_{2j}\tfrac{1}{\sqrt{\pi}}\sin(2j\phi)\right)\right].$$

- The coefficients of $\hat{\psi}^{N_\mathrm{p}}(\phi)$ are determined by solving

$$\begin{cases} \inf\limits_{\hat{a}_{2j},\hat{b}_{2j}} & \sum_{j=1}^{N_\mathrm{p}/2}\left(\int_0^{2\pi}\bar{\psi}^{N_\mathrm{p}}(\phi)\tfrac{1}{\sqrt{\pi}}\cos(2j\phi)\,\mathrm{d}\phi - \tilde{a}_{2j}\right)^2 + \left(\int_0^{2\pi}\bar{\psi}^{N_\mathrm{p}}(\phi)\tfrac{1}{\sqrt{\pi}}\sin(2j\phi)\,\mathrm{d}\phi - \tilde{b}_{2j}\right)^2 \\ \text{s.t.} & \frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\bar{\psi}^{N_\mathrm{p}}(\phi)\,\mathrm{d}\phi = \tilde{a}_0. \end{cases}$$

The truncated Fourier series of $\bar{\psi}^{N_\mathrm{p}}$ satisfies the nonnegativity condition for Fourier approximations

Numerical example

Figure 2: Euclidean error of calculated coefficients

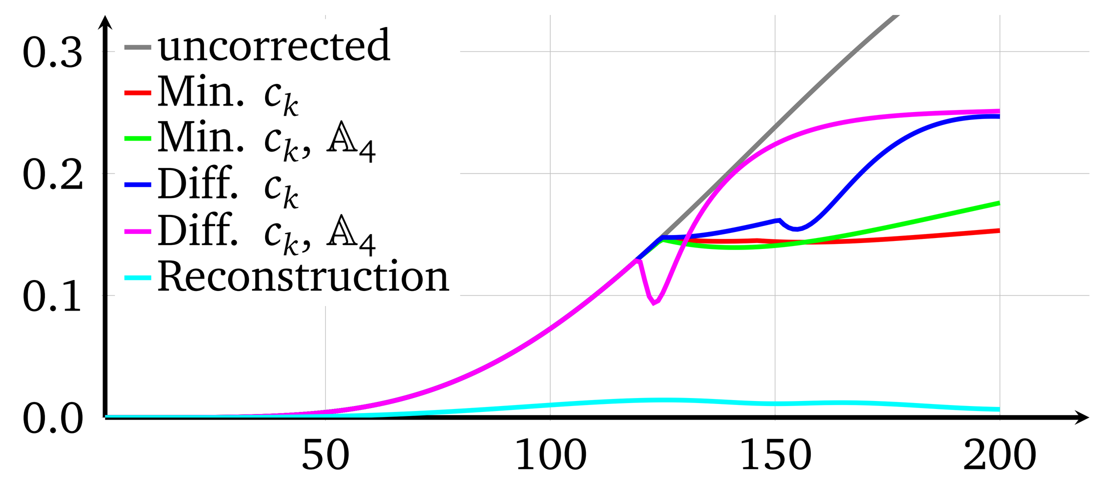


Figure 3: Minimal eigenvalue of second order orientation tensor $\mathbb{A}_2$

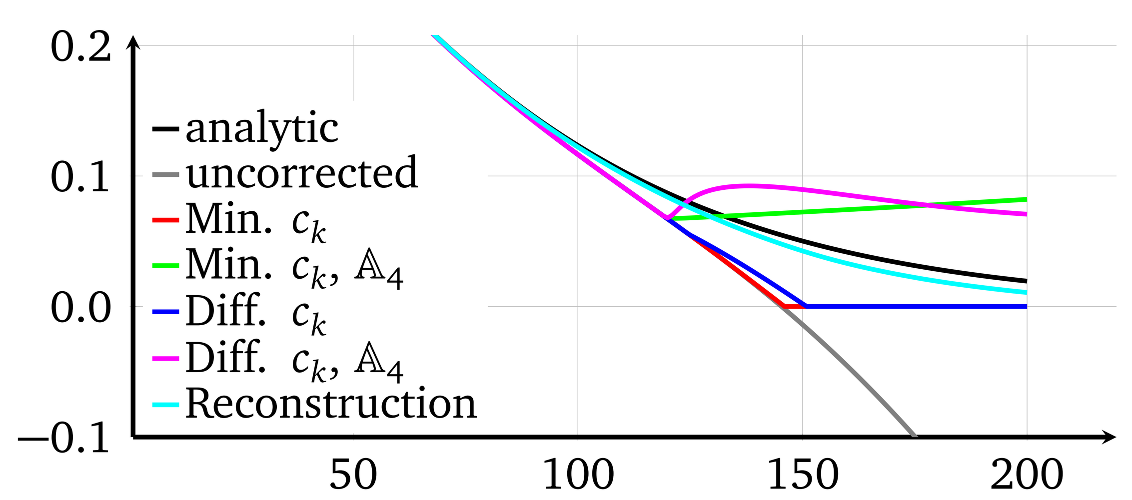
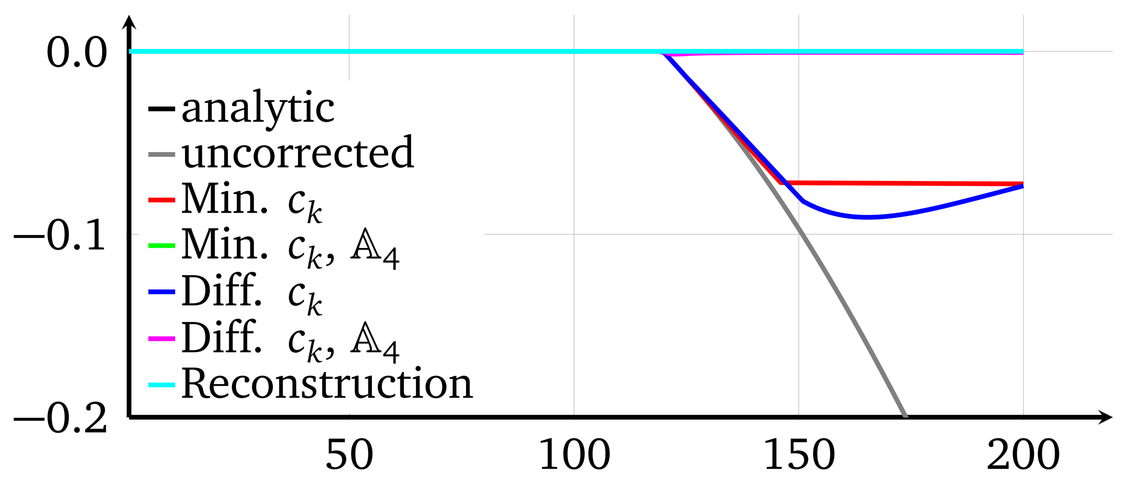


Figure 4: Minimal eigenvalue of fourth order orientation tensor $\mathbb{A}_4$



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