Anisotropic cylinder processes

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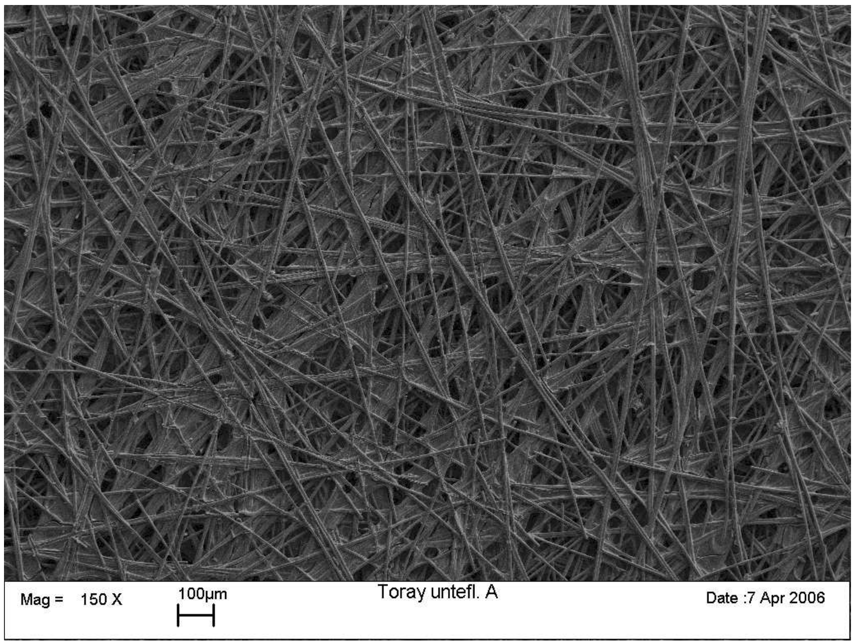
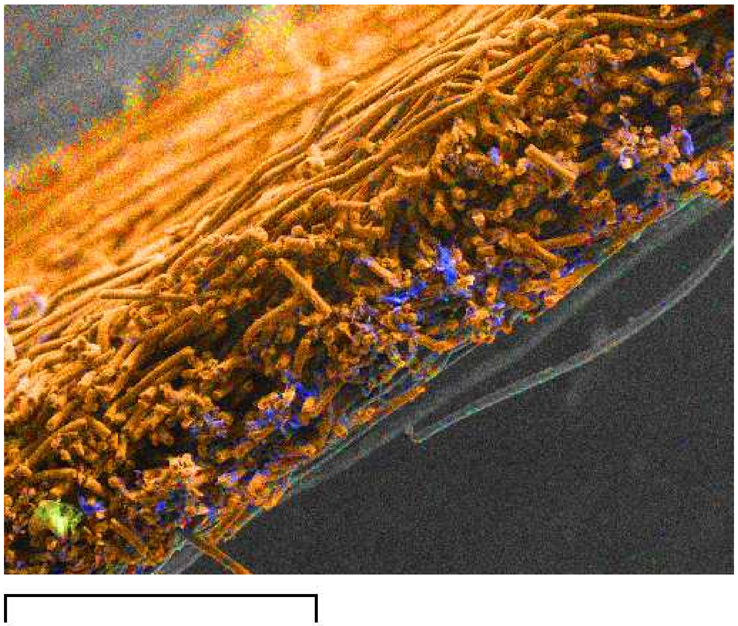
Modelling the structure of materials

- Gas diffusion layer of polymer electrolyte fuel cells

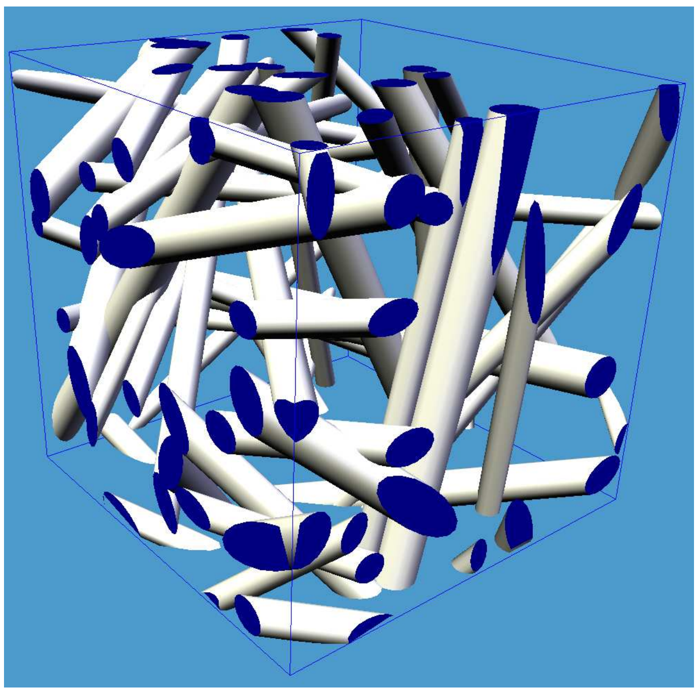




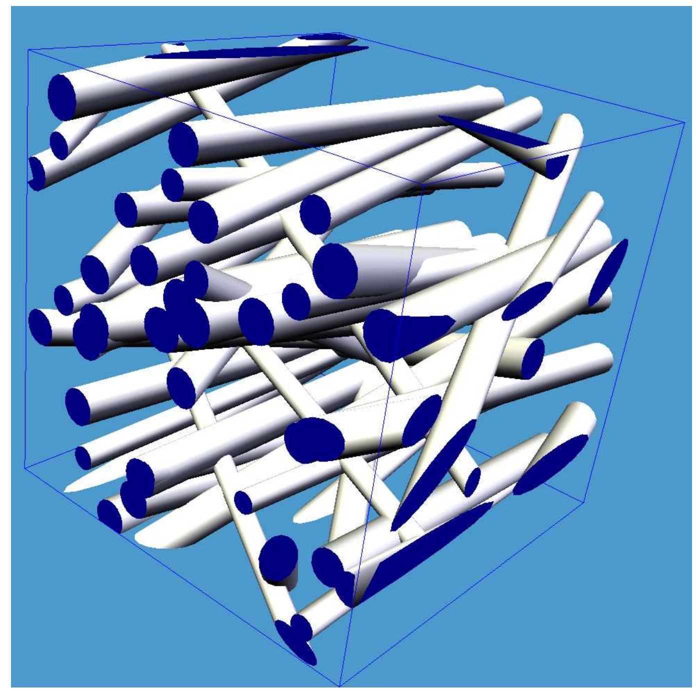
Courtesy of ZSW Ulm

Modelling approach

- (Poisson) processes of fibres or thick flats (cylinders, lamellae, membranes)



Before pressing: isotropy



After pressing: anisotropy

Overview

- Stationary anisotropic Poisson processes of cylinders
- Capacity functional and related characteristics
- Specific intrinsic volumes
- Isoperimetric problems
- Estimation of directional distribution via numerical inversion of generalized cosine transform
- Outlook

Point processes of cylinders

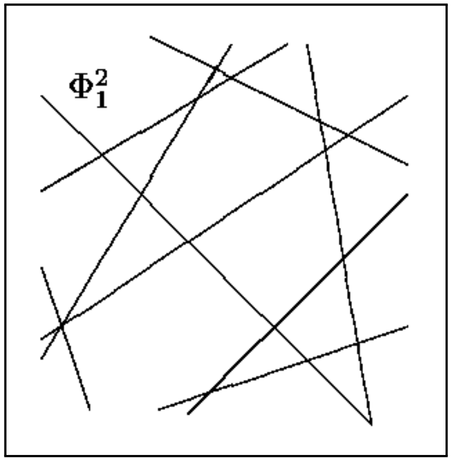
- Isotropic
  - Matheron (1975)
  - Davy (1978)
  - Schneider (1987)
  - Weil (1987)
  - Ohser, Mücklich (2000)
  - Michel, Paroux (2002)
- Anisotropic
  - Spiess, Spodarev (2009)
  - Hoffmann (2009)

Preliminaries

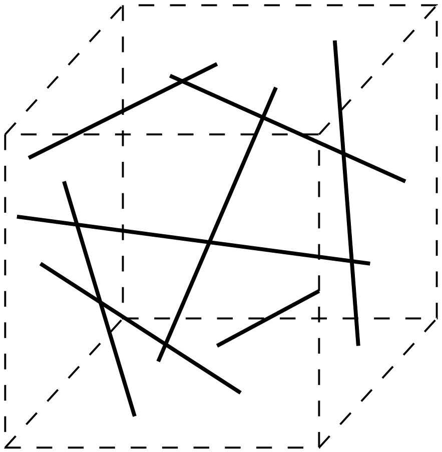
$\mathcal{K}$	family of all compact convex sets (bodies) in $\mathbb{R}^d$
$\mathcal{R}$	$= \{\bigcup_{i=1}^{n} K_i : K_i \in \mathcal{K},\ i = 1, \ldots, n,\ \forall n\}$ convex ring
$F(k, d)$	the set of affine k–flats in $\mathbb{R}^d$
$G(k, d)$	the set of linear k–subspaces in $\mathbb{R}^d$ (Grassmannian)
$\mathfrak{F},\ \mathfrak{G}$	Borel σ–algebras of $F(k, d)$, $G(k, d)$
$B_r(a)$	ball with center in a and radius r
$\mathbf{S}^{d-1}$	unit sphere in $\mathbb{R}^d$
$\omega_j(k_j)$	surface area (volume) of $B_1(o)$ in $\mathbb{R}^j$, $j = 0, \ldots, d$
$K_1 \oplus K_2$	$= \{x_1 + x_2 : x_1 \in K_1,\ x_2 \in K_2\}$ Minkowski addition

Processes of cylinders

A process Φ_k^d of cylinders with k–dim. direction space in $\mathbb{R}^d$ is a random element $(\Omega, \Gamma, P) \to (\mathcal{M}, \mathfrak{M})$, where $\mathcal{M}$ is the set of all at most countable "locally finite" systems of cylinders of the form $Z = K \oplus \xi$, $\xi \in G(k,d)$ and $K \subset \xi^{\perp}$, $K \in \mathcal{R}$.



Φ_1^2



Φ_1^3

Processes of cylinders

- Stationarity: $P\{\Phi_k^d \in \cdot\} = P\{x + \Phi_k^d \in \cdot\}$ for all $x \in \mathbb{R}^d$
- Intensity measure: $\Lambda(B) = E\,\Phi_k^d(B)$ for all $B \in \mathfrak{M}$.
  Define $i\colon (x, Z) \mapsto x + Z$ for $x \in \mathbb{R}^d$ and $Z \in \mathcal{Z}_k^o$ (the space of "centered" cylinders). If Φ_k^d is stationary, then a number $\lambda \geq 0$ and a probability measure θ on $\mathcal{Z}_k^o$ exist such that

$$\Lambda(i(A \times C)) = \lambda \int_C \nu_{d-k}^{L(Z)}(A) d\theta(Z)$$

  for all Borel sets $A \subset \mathbb{R}^d, C \subset \mathcal{Z}_k^o$, where $\nu_k^{\xi}(\cdot)$ is the Lebesgue measure in $\xi^{\perp} = \mathbb{R}^k$. Then λ is called the intensity and θ the shape distribution of Ξ.

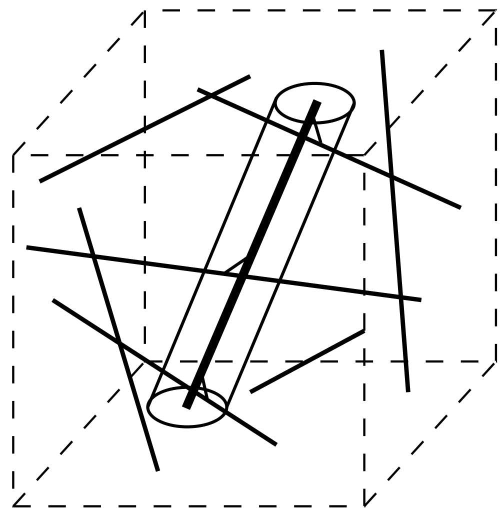
Processes of cylinders

- Directional distribution
  Define $j\colon (\varrho \times \xi) \mapsto \varrho \oplus \xi$ for $\varrho \in \mathcal{R}$ and $\xi \in G(k,d)$. Then there exist a probability measure α on $\mathfrak{G}$ (directional distribution of Φ_k^d) and a probability kernel $\beta\colon \mathfrak{R} \times G(k,d) \to [0,1]$ such that

$$\theta(j(R \times G)) = \int_G \beta(R,\xi)\alpha(d\xi), \quad R \in \mathfrak{R}, \quad G \in \mathfrak{G}.$$

- Isotropy: $\alpha(d\xi) = d\xi$, the unique probability measure on $G(k,d)$ that is invariant with respect to rotations (Haar measure).
- Poisson processes: The stationary process Φ_k^d is Poisson if $\Phi_k^d(\mathcal{B}) \sim$ Poisson $(\Lambda(\mathcal{B}))$ for all $\mathcal{B} \in \mathfrak{M}$ with $\Lambda(\mathcal{B}) < \infty$.

Random closed sets of cylinders



Introduce the stationary RACS $\Xi = \bigcup_{i=1}^{\infty} Z_i$, where

$\Phi_k^d = \{Z_1, Z_2, Z_3, \ldots\}$ is a stationary Poisson process of cylinders with intensity λ and shape distribution θ.

Capacity functional

- Cross section of a cylinder: For a cylinder $Z = K \oplus \xi$ we define the functions $L(Z) = \xi$ and $K(Z) = K$.
- Capacity functional: $T_\Xi(C) = P(\Xi \cap C \neq \emptyset)$ for any compact set C. It holds

$$T_\Xi(C) = 1 - \exp\left\{ -\lambda \int_{\mathcal{Z}_k^o} \nu_{d-k}^{L(Z)}(-K(Z) \oplus \mathrm{Pr}_{L(Z)}(C))\, \theta(dZ) \right\}.$$

where Pr_ξ is the orthogonal projection onto $\xi^\perp$.

Covariance function

$$C_\Xi(h) = P(o, h \in \Xi) = 2T_\Xi(\{o\}) - T_\Xi(\{o, h\}).$$

Let γ_A denote the covariogram of a set $A \subset L(Z)^\perp$ defined by

$$\gamma_A(x) = \nu_{d-k}^{L(Z)}(A \cap (A - x))$$

for $x \in L(Z)^\perp$. For $A(Z) = \nu_{d-k}^{L(Z)}(K(Z))$ and $h \in \mathbb{R}^d$ it holds

$$C_\Xi(h) = 1 - 2\exp\left\{-\lambda \int_{\mathcal{Z}_k^o} A(Z)\,\theta(dZ)\right\} + \exp\left\{-2\lambda \int_{\mathcal{Z}_k^o} A(Z)\,\theta(dZ) + \lambda \int_{\mathcal{Z}_k^o} \gamma_{K(Z)}(\mathrm{Pr}_{L(Z)}(h))\,\theta(dZ)\right\}.$$

Contact distribution function

For any compact set $B \subset \mathbb{R}^d$, $o \in B$, $r > 0$, introduce

$$H_B(r) = P(\Xi \cap rB \neq \emptyset | o \notin \Xi) = \frac{T_\Xi(rB) - T_\Xi(\{o\})}{1 - T_\Xi(\{o\})}$$

In our case:

$$H_B(r) = 1 - \exp\left\{ -\lambda \int_{\mathcal{Z}_k^o} \left[\nu_{d-k}^{L(Z)}(-K(Z) \oplus \mathrm{Pr}_{L(Z)}(rB)) - A(Z) \right] \theta(dZ) \right\}.$$

Specific intrinsic volumes

$\overline{V}_j(\Xi)$, $j = 0, \ldots, d$ are defined as intensities of the corresponding curvature measures.

- Specific intrinsic volumes: Hoffmann; Spiess, Spodarev (2009).
- Volume fraction: $p_\Xi = \overline{V}_d(\Xi) = P(o \in \Xi)$.
  Here:

$$p_\Xi = 1 - \exp\left\{ -\lambda \int_{\mathcal{Z}_k^o} A(Z)\, \theta(dZ) \right\}.$$

- Specific surface area: $S_\Xi = 2\overline{V}_{d-1}(\Xi)$.

Specific intrinsic volumes

- Specific surface area: Let Ξ have cylinders with regular closed cross-section $K(Z) \in \mathcal{R}$ for θ-almost all $Z \in \mathcal{Z}_k$. Then

$$S_\Xi = -\lambda \frac{\kappa_d d}{\kappa_{d-1}} \int_{\mathcal{Z}_k^o} \int_{G(1,d)} \gamma'_{K(Z)}(o, \mathrm{Pr}_{L(Z)}(r_\xi)) \, [\xi, L(Z)] \, d\xi \, \theta(dZ) \times$$

$$\times \exp\left\{ -\lambda \int_{\mathcal{Z}_k^o} A(Z) \, \theta(dZ) \right\}.$$

where $\gamma'_{K(Z)}(o, \mathrm{Pr}_{L(Z)}(r_\xi))$ is the derivative of the above set covariogram at zero in direction $Pr_{L(Z)}(r_\xi)$ and $[\xi, \eta]$ is the volume of the parallelepiped spanned by the orthonormal bases in ξ and η.

Isoperimetric problem

For a fixed intensity λ of the Poisson cylinder process Φ_1^3, find a shape distribution of cylinders θ which maximizes the volume fraction p_Ξ provided that the variance of the typical pore radius H is small:

$$\begin{cases} p_\Xi \longrightarrow \max_\theta, \\ \text{Var} H < \varepsilon, \end{cases}$$

where H is a random variable with distribution function $H_{B_1(o)}(r)$ (typical pore radius).

Isoperimetric problem

- Sufficient condition for Var$H < \varepsilon$:

$$c_s = \int_{\mathcal{Z}_1^o} S(K(Z))\theta(dZ) \leq 2\pi\sqrt{\varepsilon - \frac{1}{\pi\lambda}} = b,$$

where $S(K(Z))$ is the perimeter of cross section $K(Z)$.

- New optimization problem: for isotropic convex cross sections $K(Z)$

$$\begin{cases} E\,A(K(Z)) \to \max_\theta, \\ E\,S(K(Z)) \leqslant b \end{cases} \Longrightarrow$$ classical isoperimetric problem!

Isoperimetric problem

- Solution: $K(Z)$ is a circle with the random radius $a_0(K)$ which is the zero Fourier coefficient in the expansion of the support function of $K(Z)$ (Groemer (1996)).
- Summary: The volume fraction of $70\% - 80\%$ in the optimized gas diffusion layer of a fuel cell can be achieved best by taking fibers with circular cross sections, relatively small mean radius and high variance of this radius.

Rose of intersections of stat. fibre processes

Let Φ_k^d be a stationary thick fibre or cylinder process with intensity λ and directional distribution α.

- Rose of intersections: $f(\eta)$ is the intensity of $\Phi_k^d \cap \eta$, $\eta \in G(r,d)$
- Generalized cosine transform:

$$T_{kr}\alpha(\eta) = \int_{G(k,d)} [\eta^\perp, \xi^\perp]\, \alpha(d\xi), \quad \eta \in G(r,d)$$

- It holds: $f(\eta) = \lambda T_{kr}\alpha(\eta)$, $\eta \in G(r,d)$

Stereology for stat. fibre processes

- Inverse problem: given $T_{kr}\alpha(\eta)$, $\eta \in G(r,d)$, $r = d-k+j$, find α
- One-to-one correspondence?
  - $j = 0$:
    - $k = d-1$ or $k = 1$: Possible (Matheron (1975)),
    - $2 \leq k \leq d-2$: Impossible (Goodey, Howard (1990)),
  - $1 \leq j < k \leq d-1$ (Goodey, Howard (1990)):
    - $k < d-1$: Impossible,
    - $k = d-1$: Possible.

Stereology for stat. fibre processes

- Inversion formulae:
  - $d = 2$: Mecke (1981). For a measurable direction distribution density γ and a π-periodic function $g \in C^2([0, \pi])$

    $$\langle g, \gamma \rangle = \frac{1}{2} \langle T_{11} \gamma, g + g'' \rangle,$$

    where $\langle \cdot, \cdot \rangle$ is the scalar product in $L^2(0, \pi)$.
  - $d = 3$: Mecke and Nagel (1980).
  - $d \geqslant 3$: Spodarev (2001). Formulae for $k = d - 1, r = 1$ and $k = d - 1, 1 < r \leq d - 1$ if α is absolutely continuous with respect to the Haar measure ω_d on the unit sphere S^{d-1}.

Stereology for stat. fibre processes

- Inversion formula for $k = 1, r = d-1$: If α has density γ then

$$\gamma(\xi) = \frac{c_R^2}{\lambda}\left(\frac{d}{d(\mu^2)}\right)^{d-2}\left[\int_{\langle\xi,\eta\rangle^2>\mu^2}\frac{\Box T_{1,d-1}\gamma(\eta)\,|\langle\xi,\eta\rangle|}{(\langle\xi,\eta\rangle^2-\mu^2)^{2-d/2}}\omega_d(d\eta)\right]\Bigg|_{\mu=0},$$

  where $c_R^2 = \frac{(-1)^{d-2}\,2^{d-3}}{(d-3)!\,\omega_{d-1}}$, $\Box = \frac{1}{2\omega_{d-1}}(\triangle_0 + d - 1)$, and $\triangle_0$ is the Beltrami-Laplace operator on S^{d-1}.

- Numerical inversion?
  - Discrete α: Kiderlen and Pfrang (2005), Hoffmann (2008)
  - Absolutely continuous α: Louis, Riplinger, Spiess, Spodarev (2009)

Numerical inversion of T_{kr}

- Method of approximative inverse: Schuster (2007)
  Let $e_\delta(x, \cdot)$ be an approximation of the Dirac delta function:

$$e_\delta(x, \cdot) \longrightarrow \delta_x(\cdot) \quad \text{as } \delta \to 0$$

for any $x \in G(k, d)$. If the function $\psi_\delta(x, \cdot)$ (mollifier) with

$$(T_{kr}\psi_\delta(x, \cdot))(y) = e_\delta(x, y), \quad x \in G(k, d), \quad y \in G(r, d)$$

is found and $\langle \cdot, \cdot \rangle$ is the scalar product in $L^2(G(r, d))$ then

$$\gamma(x) = \lim_{\delta \to 0} \langle \psi_\delta(x, \cdot), T_{kr}\gamma(\cdot) \rangle, \quad x \in G(k, d).$$

Numerical inversion of T_{11}

- Sine transform ($d = 2$): If α has a density γ then

$$T_{11}\gamma(x) = \int_0^\pi |\sin(x-y)|\gamma(y)\,dy/\pi, \quad x \in [0,\pi)$$

  is the rose of intersections of a stationary process of fibres Φ_1^2 in $\mathbb{R}^2$ (intensity $\lambda = 1$) with the line at angle $x \in [0,\pi)$.

- Numerical inversion: for a π-periodic C^2–smooth $e_\delta(x,y)$ it holds

$$\psi_\delta(x,y) = \frac{1}{2}e_\delta(x,y) + \frac{1}{2}\frac{\partial^2}{\partial y^2}e_\delta(x,y).$$

Numerical inversion of T_{11}

- Example of mollifiers: for $\nu \in \mathbb{N}$ consider

$$e_\delta(x,y) = \delta^{-1} k_\nu \left(1 - \frac{(x-y)^2}{\delta^2}\right)^\nu \mathbf{1}\{|x-y| \le \delta\}$$

with $k_\nu = \Gamma(\nu + \frac{3}{2})/(\Gamma(\nu+1)\sqrt{\pi})$. If $\nu = 3$ then $k_3 = 35/32$ and for $|x-y| < \delta$ we get

$$\psi_\delta(x,y) = \frac{k_3}{2\delta}\left(1 - \frac{(x-y)^2}{\delta^2}\right)^3 + \frac{3k_3}{\delta^3}\left(4\left(1 - \frac{(x-y)^2}{\delta^2}\right)\frac{(x-y)^2}{\delta^2} - \left(1 - \frac{(x-y)^2}{\delta^2}\right)^2\right).$$

Outlook

- Approximative inversion formulas for the generalized cosine transform and spherical Radon transform in dimension $d \geqslant 3$
- Statistics for this inversion for noisy incomplete data
- Metrics for comparison of two different fibre processes?

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