Structural invariance of stochastic fibrous networks

C.T.J. Dodson
School of Mathematics

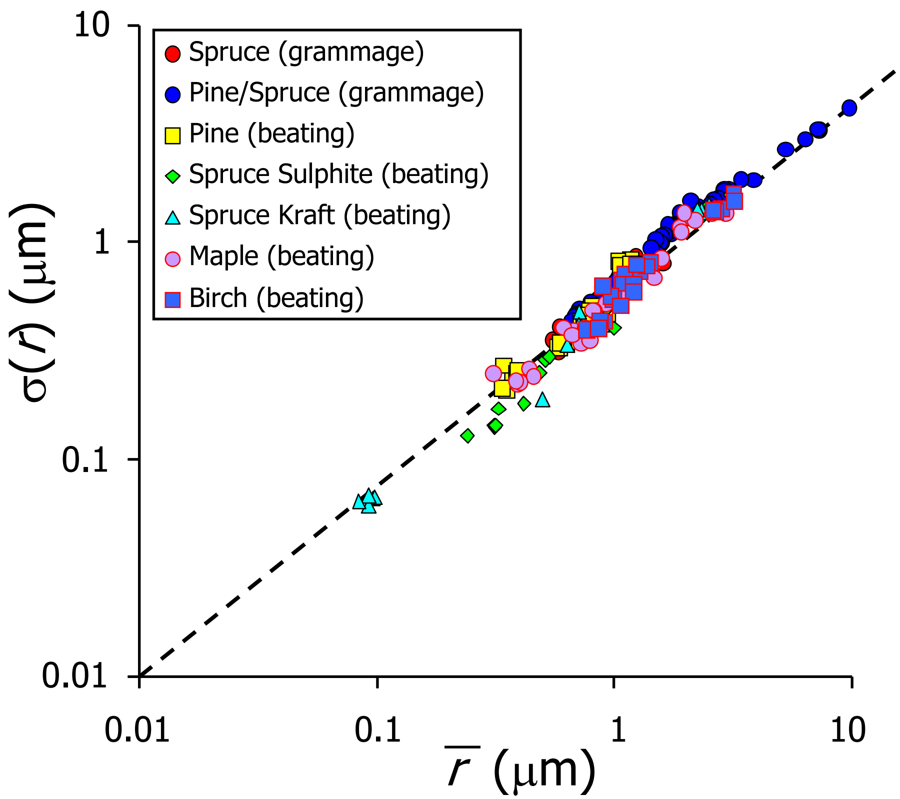
W.W. Sampson
School of Materials

University of Manchester

MANCHESTER 1824

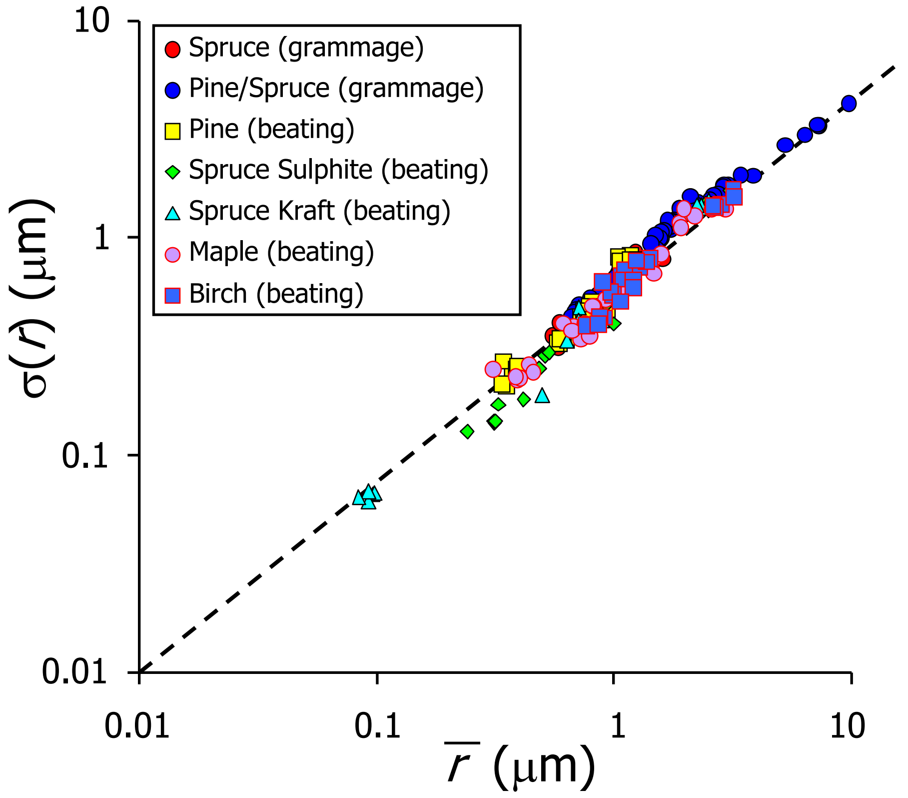
Structural invariance of voids: Pore size distribution

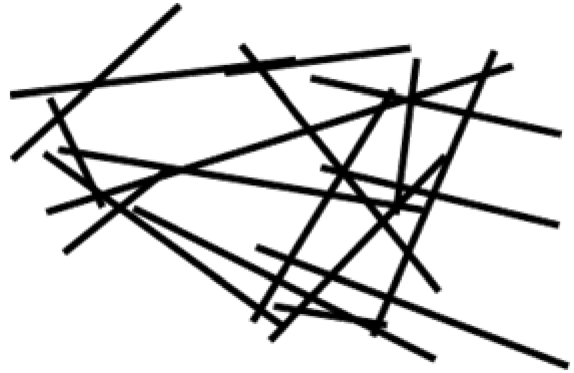
- Standard deviation of pore radii proportional to the mean:
  - Property of the gamma distribution
  - Measurements in real paper dominated by pore height distribution (exponential)
  - Insensitive to formation



Structural invariance of voids: Pore size distribution

- Standard deviation of pore radii proportional to the mean:
  - Property of the gamma distribution
  - Measurements in real paper dominated by pore height distribution (exponential)
  - Insensitive to formation
- Polygons tend to be 'roundish'
  - Conjecture, FRS13: correlated free-fibre-lengths



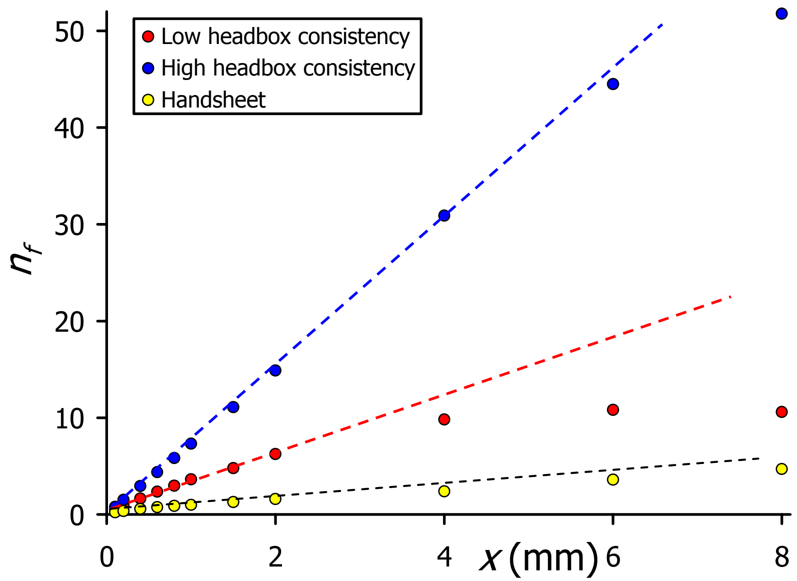


Structural invariance of mass: Formation number

- Variance of local grammage, $\sigma_x^2(\tilde{\beta})$, of random fibre networks known analytically
- Formation number (variance ratio):

$$n_f = \frac{\sigma_x^2(\tilde{\beta})^{\text{measured}}}{\sigma_x^2(\tilde{\beta})^{\text{random}}}$$

- n_f *vs*. inspection zone size (x) `linear' for $x < 4$ mm



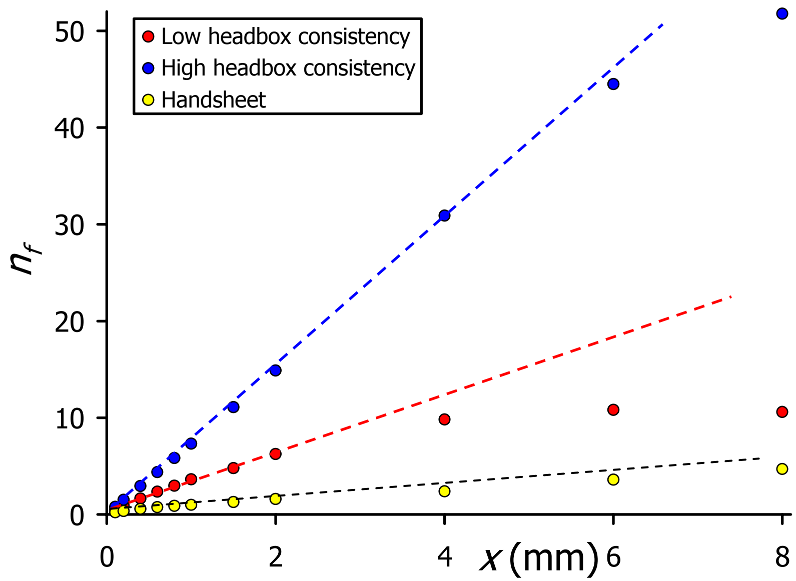
Structural invariance of mass: Formation number

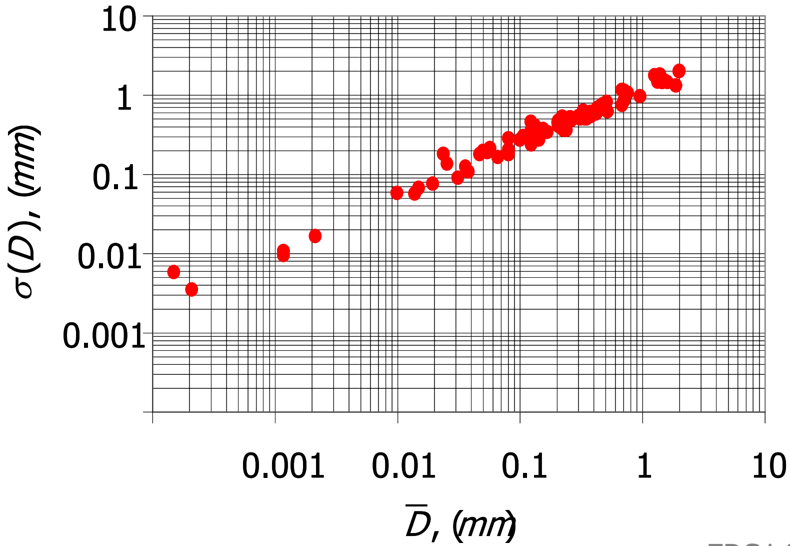
- Variance of local grammage, $\sigma_x^2(\tilde{\beta})$, of random fibre networks known analytically
- Formation number (variance ratio):

$$n_f = \frac{\sigma_x^2(\tilde{\beta})^{\text{measured}}}{\sigma_x^2(\tilde{\beta})^{\text{random}}}$$

- n_f *vs*. inspection zone size (x) `linear' for $x < 4$ mm
- Random disk model:

$$\sigma(D) \propto \bar{D}^{2/3}$$





MANCHESTER 1824

Objectives and Approach

Objective:

- **To explain the seemingly narrow class of structures realised in papermaking processes:**

  pore shape, pore size distribution and mass distribution

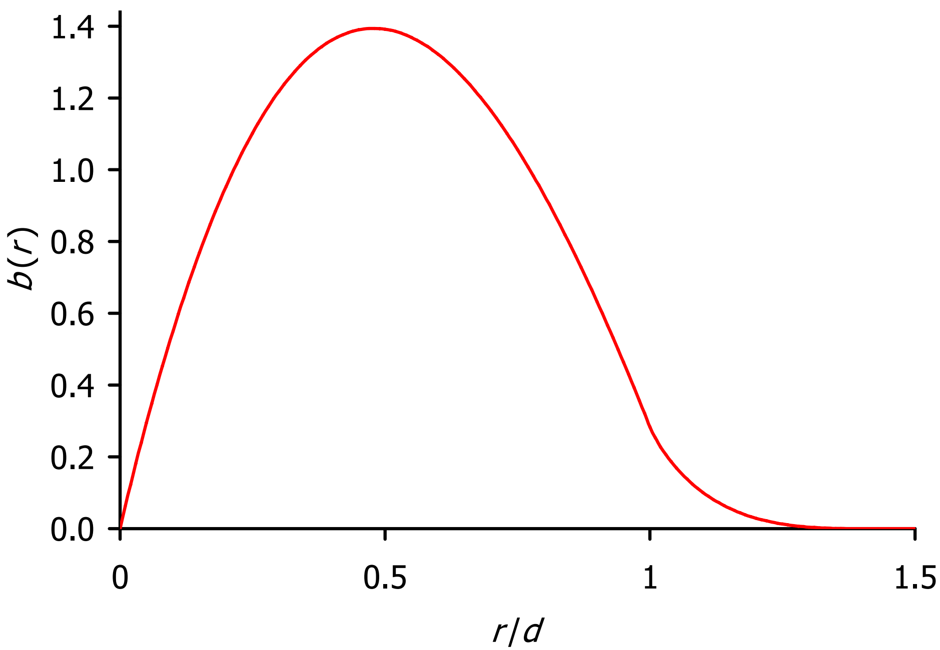
Approach:

- **Simulation** of random and clustered processes of:
  - **Points**, to represent fibre centres
  - **Infinite lines** to generate free-fibre-lengths
  - **Finite lines**, to represent fibres and generate mass maps.

Fibre centre statistics: Poisson points

Probability density of distance, *r*, between fibre centres occurring in a square of side, *d*, is known for the **random** (Poisson) case (Ghosh, 1951):

$$b(r,d)=\begin{cases}\dfrac{2r}{d^4}\left(\pi d^2-4dr+r^2\right) & \text{for } 0\le r\le d\\[2ex] \dfrac{2r}{d^4}\left(\begin{array}{l}4d\sqrt{r^2-d^2}-r^2\\ \qquad -d^2\left(2+\pi-4\sin^{-1}(d/r)\right)\end{array}\right) & \text{for } d<r\le\sqrt{2}\,d\end{cases}$$



Fibre centre statistics: Non-Poisson points

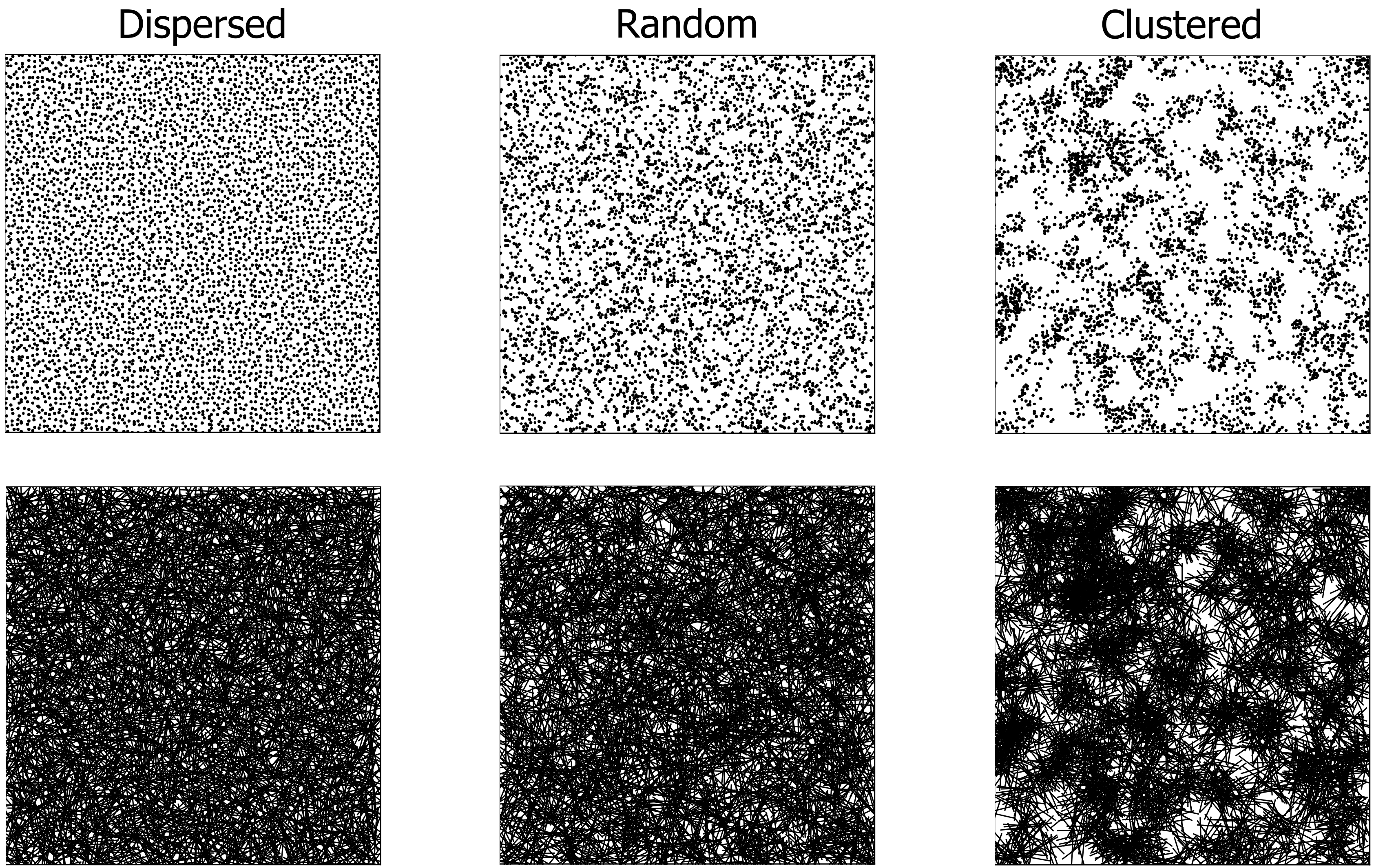
For flocculated and dispersed cases, we use simulation to deposit 50,000 fibre centres in a unit square.

Clustered: Compound Poisson process

- Cluster centres distributed as a 2D Poisson process
- Number of centres per cluster has a Poisson distribution
- Inputs:
  - mean number of centres per cluster
  - cluster diameter

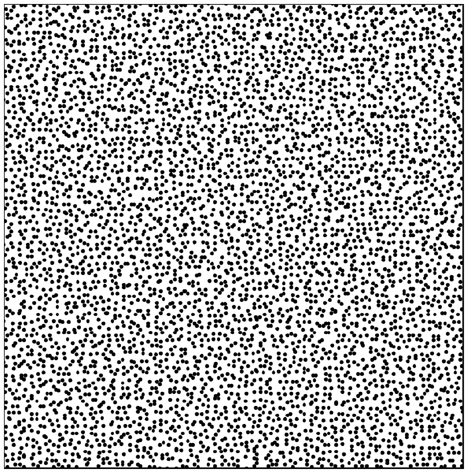
Dispersed: Small random perturbation from square lattice

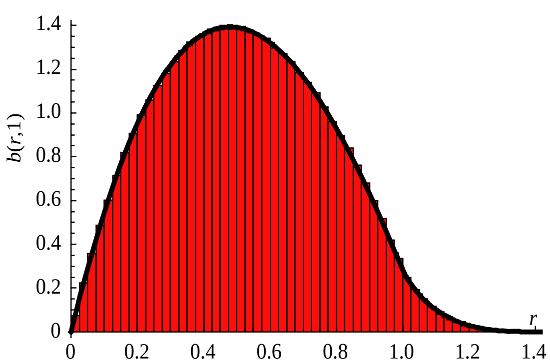
Fibre centres: Distributions of points and fibres



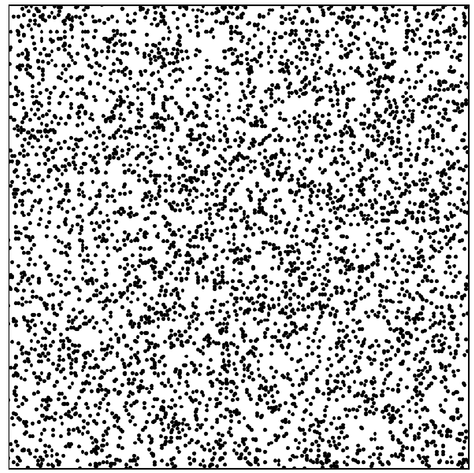
Fibre centres: Distributions of points and their separations

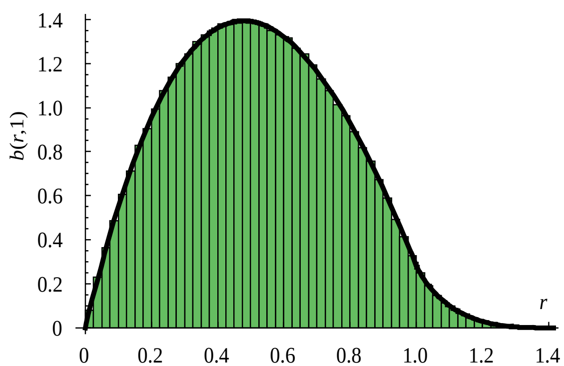
Dispersed



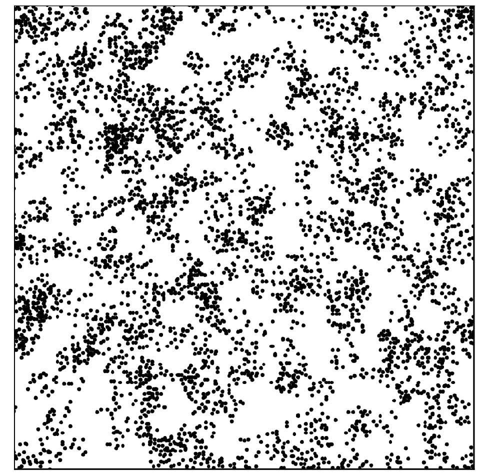


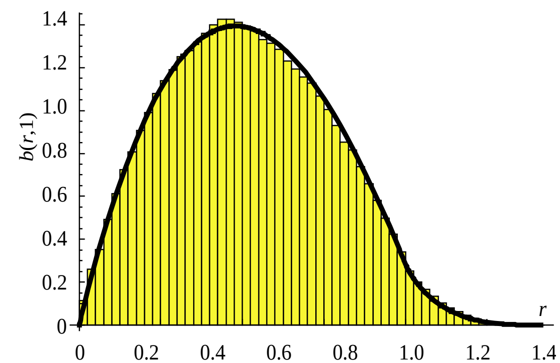
Random





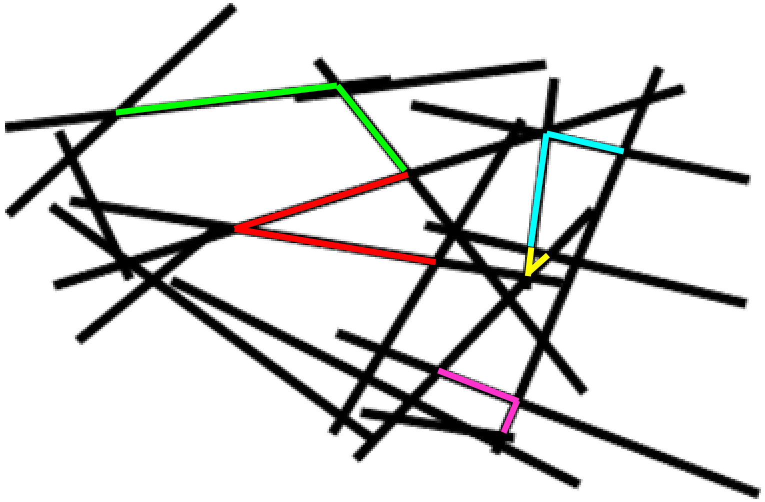
Clustered





Random networks: Correlation of adjacent free-fibre-lengths?

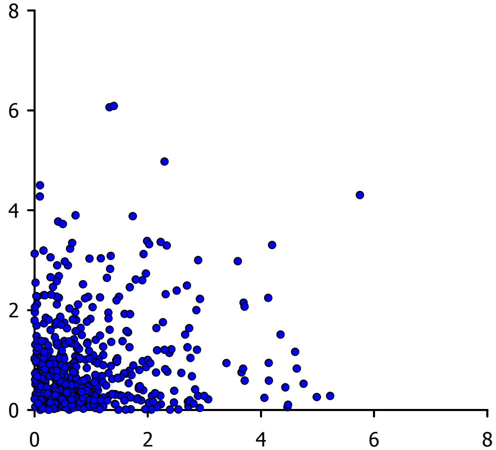
- Conjecture, FRS13: adjacent free-fibre-lengths are correlated, such that polygons tend to be 'roundish'.

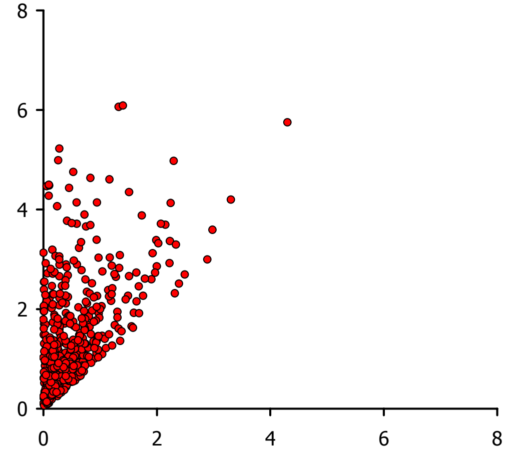


- Free-fibre-length distribution is exponential. For unit mean

$$f(x) = e^{-x} \text{ and } \sigma^2(x) = \bar{x} = 1$$

- To reveal correlation between pairs of free-fibre-lengths, $\{x_i\ y_i\}$, we must order the pairs such that $x_i \leq y_i$





Correlation of adjacent free-fibre-lengths: Independent pairs

- First we must obtain the correlation for <u>**independent**</u> sorted pairs
- Start with a pair of numbers, $\{x_i, y_i\}$, drawn from the exponential distribution
- Convert each pair into an ordered pair (x_i, y_i) such that $x_i \leq y_i$
- Two distributions arise, one for x and one for y:

$$g_{\leq}(x) = \frac{1}{2} e^{-2x} \qquad \text{with } \bar{x} = 1/2 \text{ and } \sigma^2(x) = 1/4$$

$$g_{\geq}(y) = 2e^{-2y}(1 - e^{-y}) \qquad \text{with } \bar{y} = 3/2 \text{ and } \sigma^2(y) = 5/4$$

Correlation of adjacent free-fibre-lengths: Independent pairs

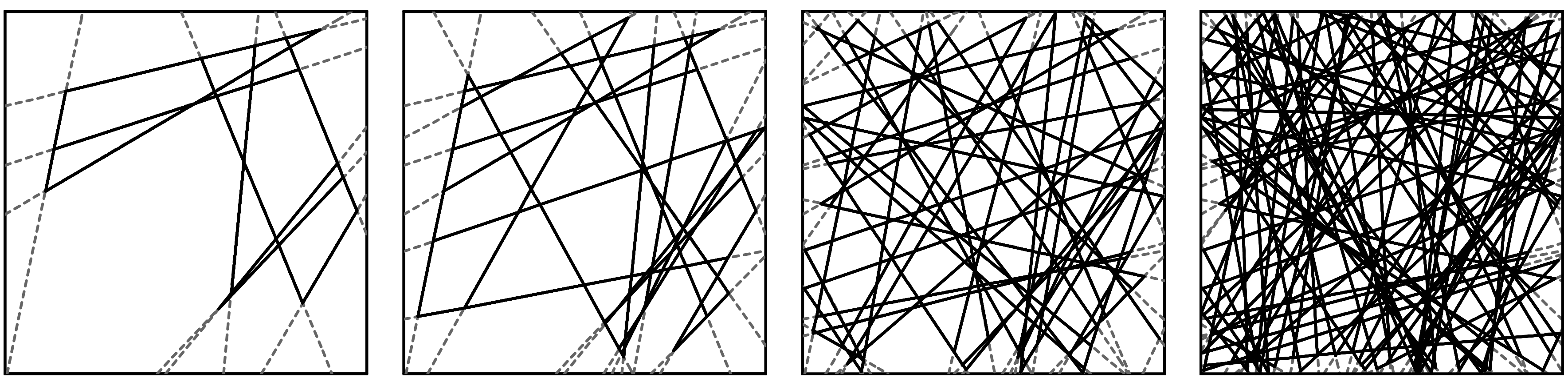
- The correlation ρ is given by

$$\rho = \frac{\overline{x\,y} - \bar{x}\,\bar{y}}{\sigma(x)\,\sigma(y)} = \frac{1}{\sqrt{5}}$$

- So for **independent** pairs $\rho \approx 0.447$. We use simulation to obtain ρ for stochastic line networks. If the simulation yields $\rho > 0.447$, then we have intrinsic correlation in our networks.

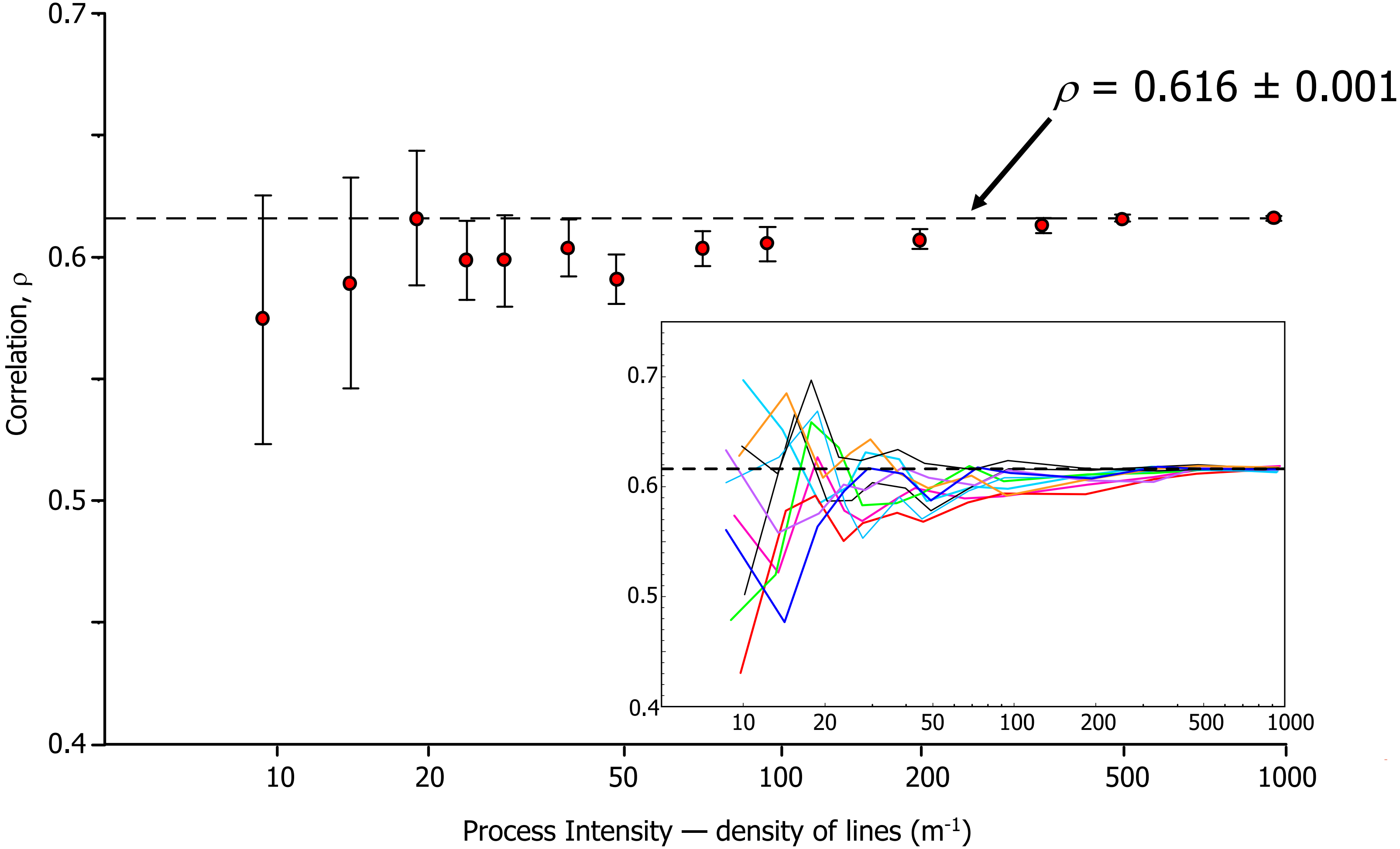
Correlation of adjacent free-fibre-lengths: Random networks

- Simulation solves equations of random lines drawn in a unit square to compute coordinates of crossings and polygon sides (free-fibre-lengths)
- Adjacent polygon sides are paired
- Polygon sides crossing boundaries of unit square are discarded
- Correlation of sorted and paired polygon side lengths computed
- Correlation tracked as number of lines increased



10 lines | 20 lines | 50 lines | 100 lines

Correlation of adjacent free-fibre-lengths: Random networks

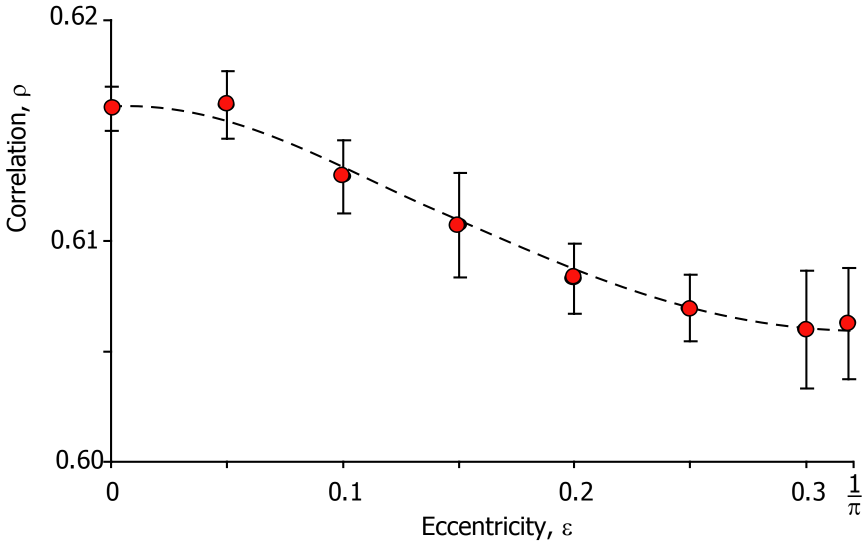


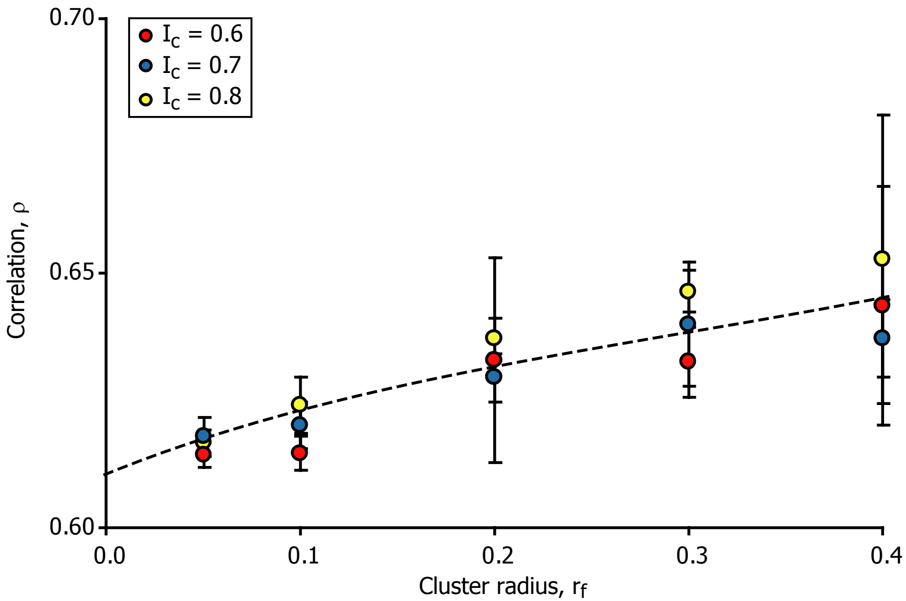
Correlation of adjacent free-fibre-lengths: Oriented & clustered

- Very small influence of fibre orientation using 1-parameter cosine distribution

- Very small influence of clustering. Lines pass through clusters of points with varying cluster radius, r_{fl} and cluster intensity, I_c

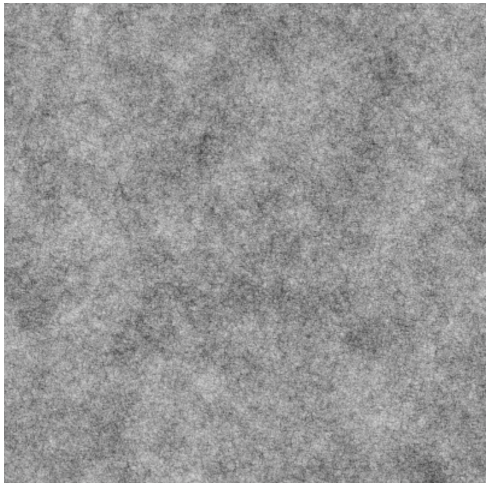
$$f(\theta) = \frac{1}{\pi} - \varepsilon \cos(2\theta) \qquad 0 \leq \theta \leq 1/\pi$$



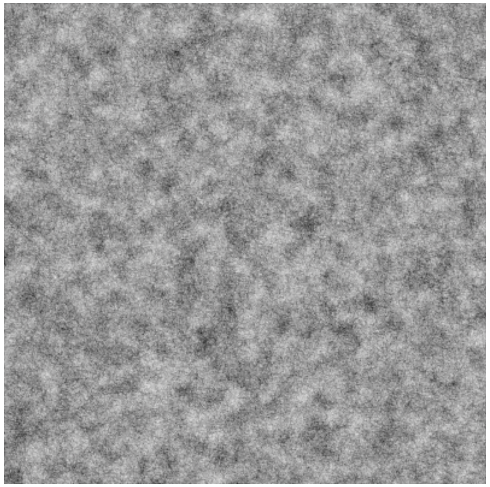


Formation simulator

Cloudy



Grainy



- Formation easily visually classified as 'cloudy' (large flocs, low floc grammage) or 'grainy' (small flocs, high floc grammage)
- Experimentally difficult to vary scale and intensity of flocculation independently
- Simulator generates 4 cm × 4 cm grammage maps where scale and intensity of clusters (flocs) can be varied independently

MANCHESTER 1824

Formation simulator

Inputs:

- Grammage, $\overline{\beta}$
- Fibre properties:
  - Length, λ
  - Coarseness, δ
  - Width, ω
- Mean floc radius, r_f
- Floc intensity, $0 \leq I \leq 1$
- Expected number of fibres per cluster, $\overline{n_c}$

Formation simulator for flocculated networks

Inputs:

- Grammage, $\bar{\beta}$
- Fibre properties:
  - Length, λ
  - Coarseness, δ
  - Width, ω
- Mean floc radius, r_f
- Floc intensity, $0 \leq I \leq 1$
- Expected number of fibres per cluster, $\bar{n}_c$

Simulation:

- Number of fibres per cluster, n_c, is a Poisson variable with mean, $\bar{n}_c$
- Mean grammage, G, of each cluster is assumed constant (*cf.* Farnood *et al.* 1995)

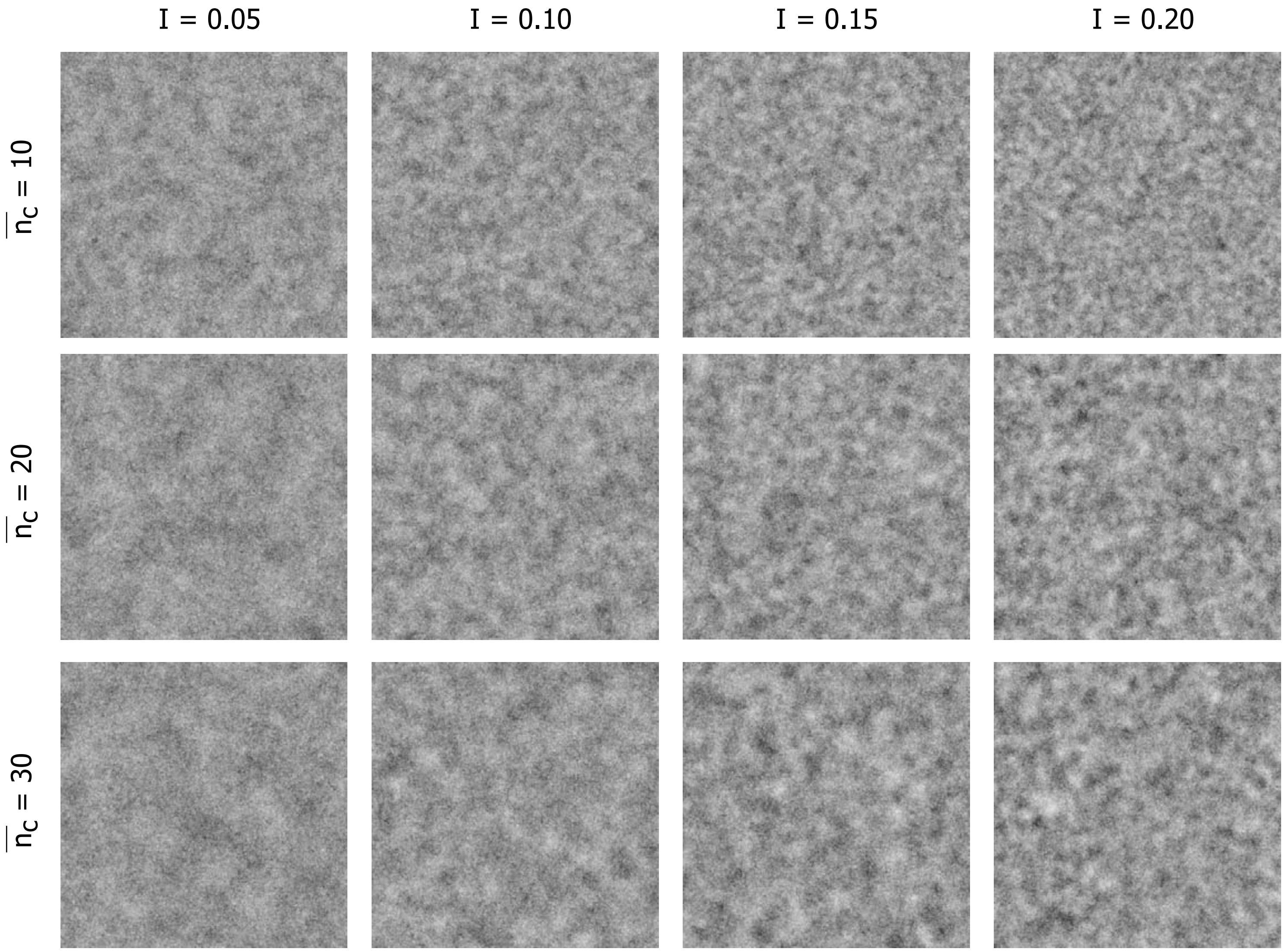
$$G = I\,\beta_{\text{fib}} = \frac{I\,\delta}{\omega}$$

- Radius of each cluster is

$$r = \sqrt{\frac{n_c\,\lambda\,\omega}{\pi\,I}}$$

- n_c fibre centres deposited within circles of radius r.
- For each fibre, contribution to mass of each pixel calculated.

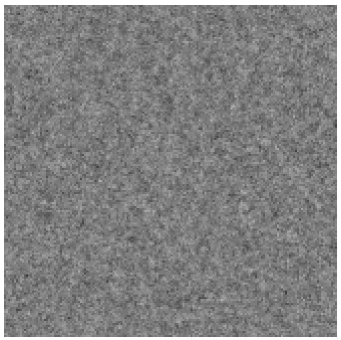
Formation simulator: Example outputs



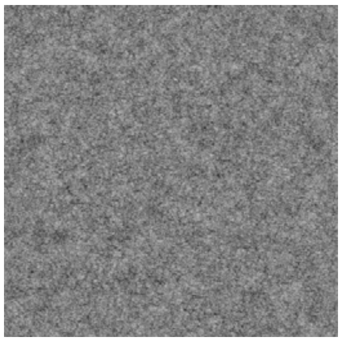
Formation simulator: Random case, fibre length effect

- Simulator generated Poisson random networks ($n_c = 1$) for different fibre lengths and computed n_f

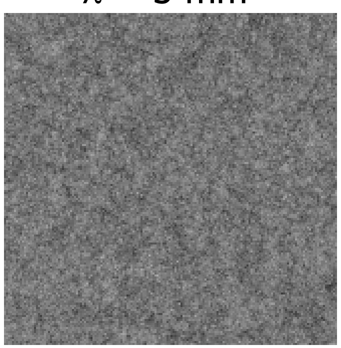
λ = 1 mm



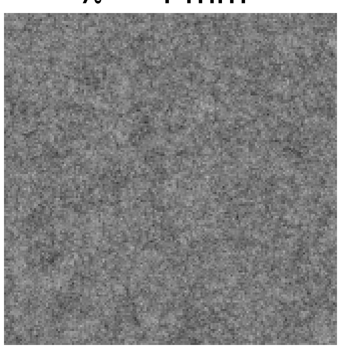
λ = 2 mm



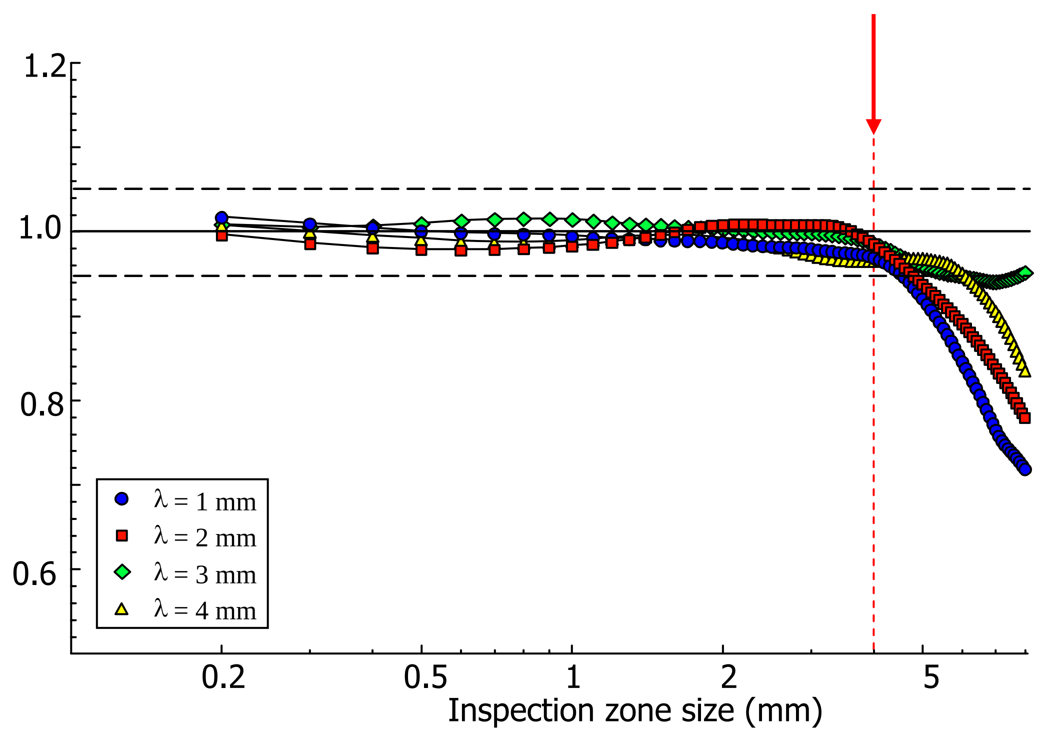
λ = 3 mm



λ = 4 mm



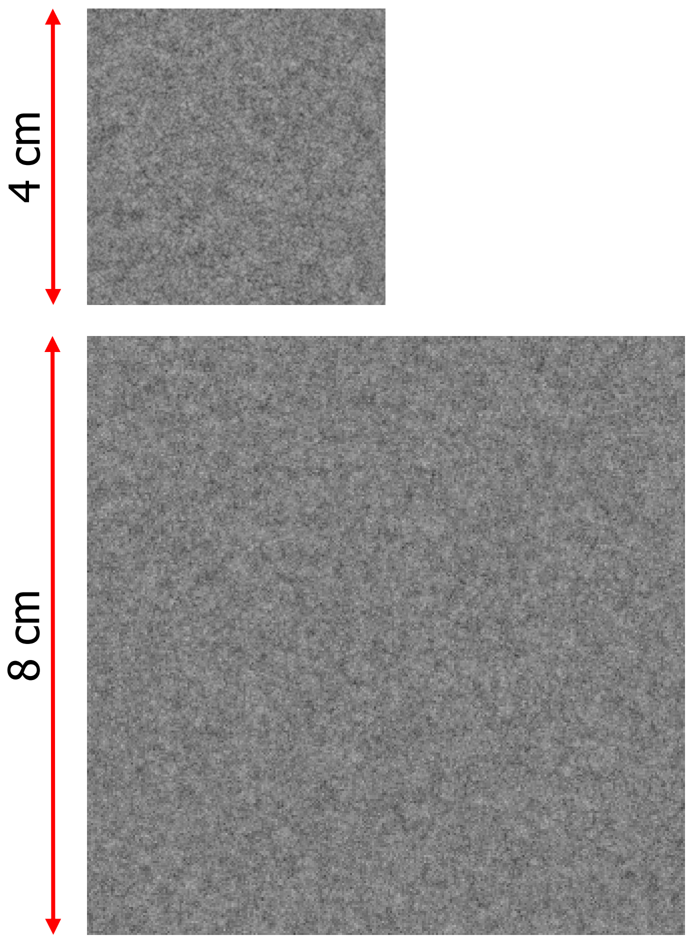
4 cm

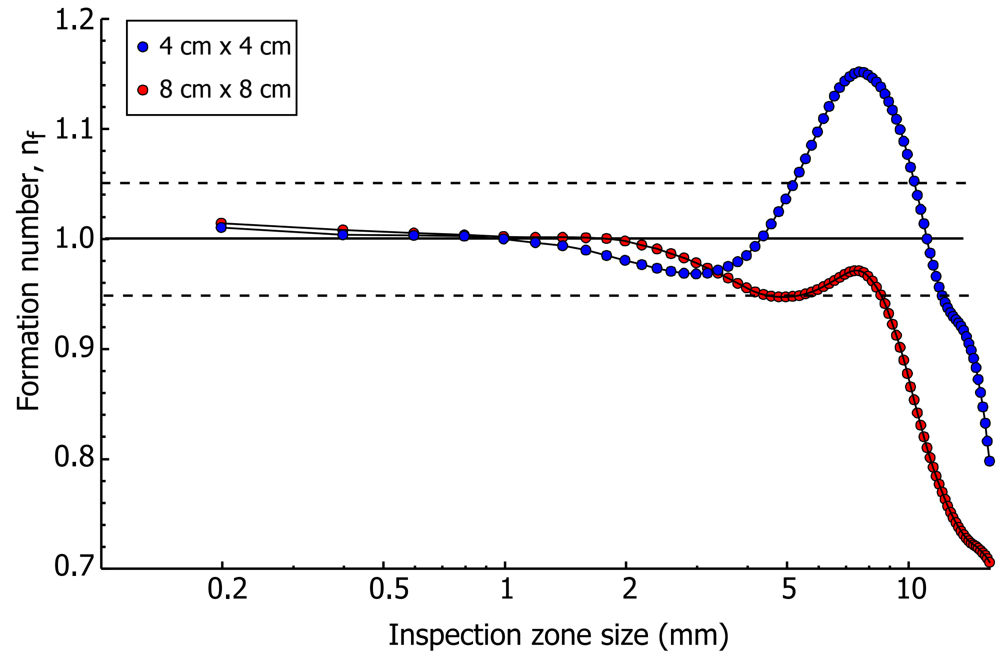


MANCHESTER 1824

Formation simulator: Random case, scale sensitivity

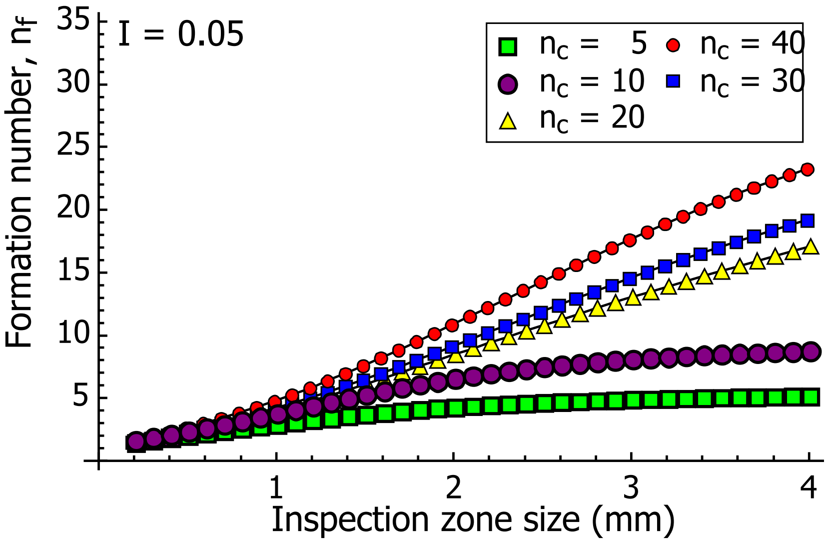
- Different areas

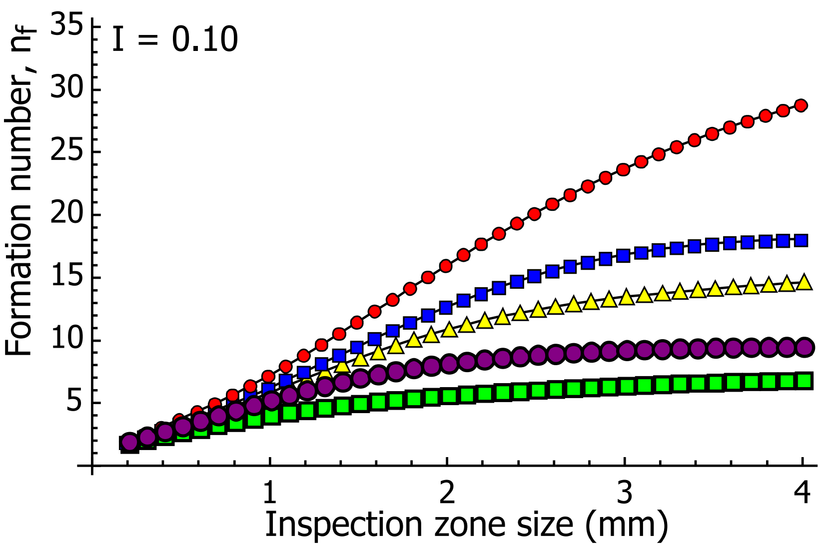




- Sufficient data reliably to compute variance only for scales up to about 10% of imaging area

Formation simulator: Scale dependence of n_f

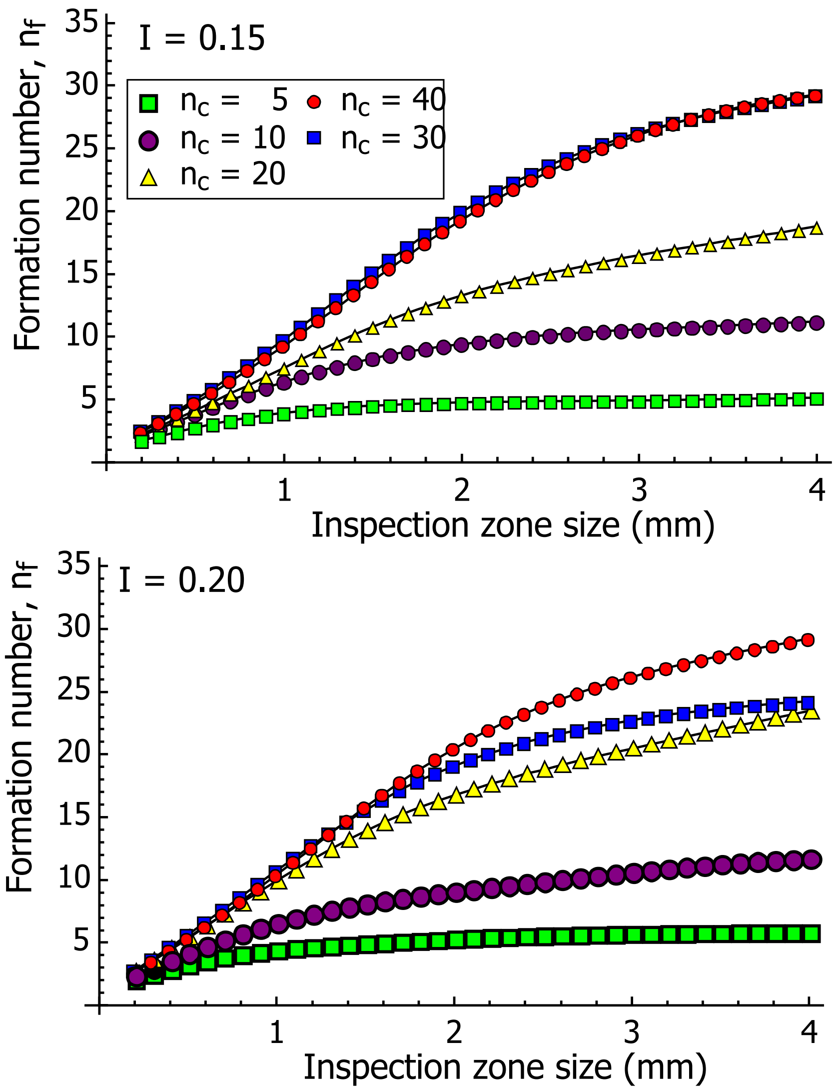




- n_f increases with
  - inspection zone size
  - flocculation intensity, I
  - number of fibres per cluster, n_c
- Dependence on zone size nonlinear
  - literature data sparse
  - linear regression gives $r^2>0.9$ on these data

λ = 1 mm; ω= 20 μm; $\delta = 2 \times 10^{-7}$ kg m^{-1}; β = 60 g m^{-2}

Formation simulator: Scale dependence of n_f



- n_f increases with
  - inspection zone size
  - flocculation intensity, I
  - number of fibres per cluster, n_c
- Dependence on zone size nonlinear
  - literature data sparse
  - linear regression gives $r^2>0.9$ on these data
- No simple scaling law found, but
  - when n_c and I are both large, n_f exhibits similar dependence on zone size at small scales

λ = 1 mm; ω= 20 μm; δ = 2 × 10^{-7} kg m^{-1}; β = 60 g m^{-2}

Analytic approximation of formation number n_f

For a Poisson structure of sparse disks with grammage, *G*, and uniform diameter, *D*, the variance of local grammage for square zones of side *x* is

$$\sigma^2{}_{\text{disks},x}(\tilde{\beta}) = \bar{\beta}\, G \int_0^{\sqrt{2}\,x} \alpha_{\text{disks}}(D,r)\, b(r,x)\, dr$$

where

$$\alpha_{\text{disks}}(D,r) = \frac{2}{\pi D}\left(D \cos^{-1}(r/D) - r\sqrt{1-(r/D)^2}\right)$$

Also

$$n_f(x) = \frac{\sigma^2_{\text{disks},x}(\tilde{\beta})}{\sigma^2_{\text{fibres},x}(\tilde{\beta})}$$

Where $\sigma^2_{\text{fibres},x}(\tilde{\beta})$ is the variance of local grammage of a random fibre network and is known analytically:

$$\sigma^2{}_{\text{fibres},x}(\tilde{\beta}) = \bar{\beta}\, \beta_{\text{fib}} \int_0^{\sqrt{2}\,x} \alpha(r,\omega,\lambda)\, b(r,x)\, dr$$

Analytic approximation of formation number n_f

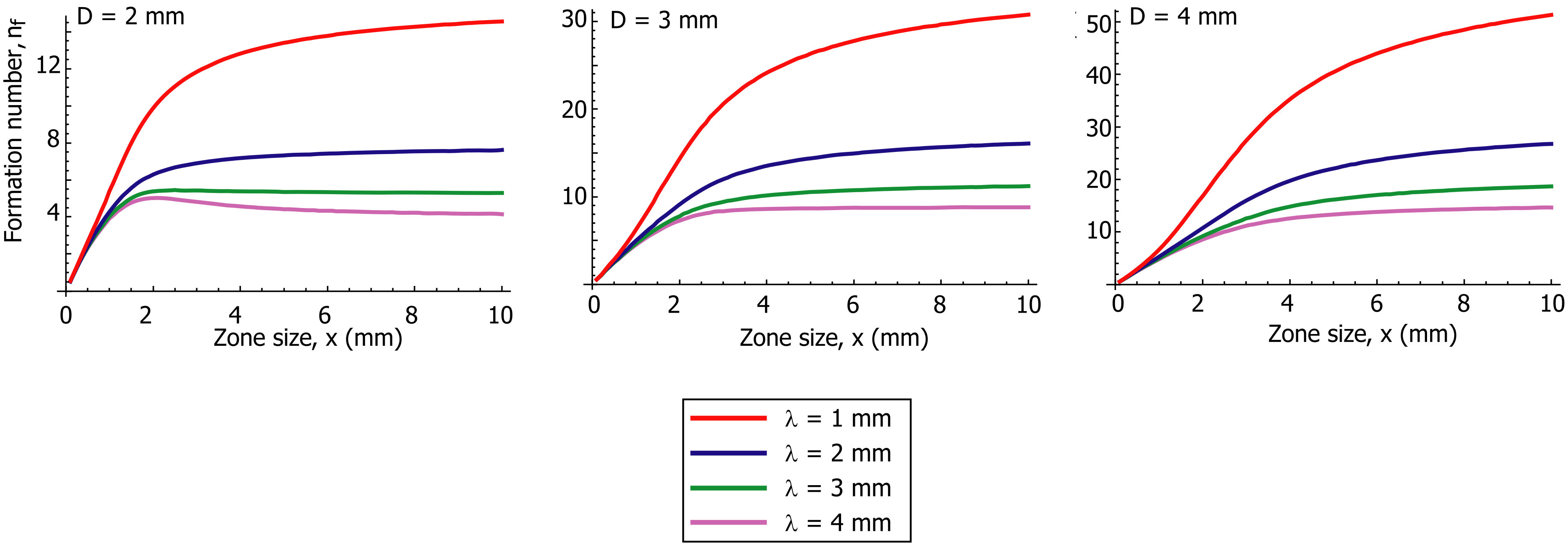
$$n_f(x) = \frac{\sigma^2_{\text{disks},x}(\tilde{\beta})}{\sigma^2_{\text{fibres},x}(\tilde{\beta})}$$

$$= I \, \frac{\int_0^{\sqrt{2x}} \alpha_{\text{disks}}(D,r)\, b(r,x)\, dr}{\int_0^{\sqrt{2x}} \alpha(r,\omega,\lambda)\, b(r,x)\, dr}$$

Analytic approximation of formation number n_f

$$n_f(x) = \frac{\sigma^2_{\text{disks},x}(\tilde{\beta})}{\sigma^2_{\text{fibres},x}(\tilde{\beta})}$$

$$= I \frac{\int_0^{\sqrt{2x}} \alpha_{\text{disks}}(D,r)\, b(r,x)\, dr}{\int_0^{\sqrt{2x}} \alpha(r,\omega,\lambda)\, b(r,x)\, dr}$$



Analytic approximation of formation number asymptotics

For large inspection zones

$$\lim_{x \to \infty} n_f(x) = n_c$$

At small inspection zones, the initial slope is

$$\lim_{x \to 0} \frac{dn_f}{dx} = I \left. \frac{\alpha_{\text{disks}}(D,r)\, b(r,x)}{\alpha(r,\omega,\lambda)\, b(r,x)} \right| r \to x \to 0$$

$$= I$$

So the initial slope of a plot of formation number against inspection zone size depends on the intensity of flocculation and the asymptotic value depends on the expected number of fibres per floc.

Conclusions

- **Pores ARE roundish:** Natural stochastic clusters, which generate local free-fibre-length correlations, overwhelm any effects on pore shape of fibre orientation or flocculation.

- **Trapped polygon void sizes:** Local free-fibre-length correlations force coefficient of variation for in-plane pore sizes to be insensitive to flocculation and orientation.

- **Trapped formation:** Variance ratio to random (n_f) asymptotic to number of fibres per cluster (n_c) and convergence rate is intensity of flocculation (I).