Stochastic simulation of spherical growth tessellation models

Approach Using a Collective Rearrangement Algorithm

Nicolas Venkovic
nvenkov1@jhu.edu

Kirubel Teferra
kteferr1@jhu.edu

Lori Graham-Brady
lori@jhu.edu

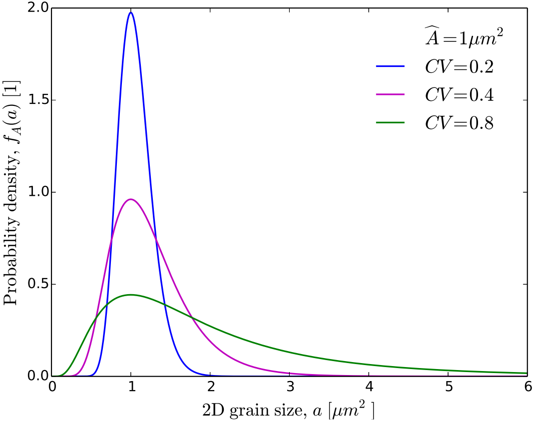
Johns Hopkins University

January 18, 2015

Some target 2D grain size distributions

Log-normal probability density functions (PDF) of 2D grain size A:

$$f_A(a|\mu,\sigma) = \frac{1}{a\sqrt{2\pi}} \exp\left[-\left(\frac{\log(a)-\mu}{\sqrt{2\sigma^2}}\right)^2\right],\ a \in]0,+\infty[$$



Mean:

$$\mathbb{E}[A] = \exp[\mu + \sigma^2/2]$$

Variance:

$$\mathbb{V}[A] = [\exp(\sigma^2) - 1]\exp[2\mu + \sigma^2]$$

Mode:

$$\widehat{A} = \exp[\mu - \sigma^2]$$

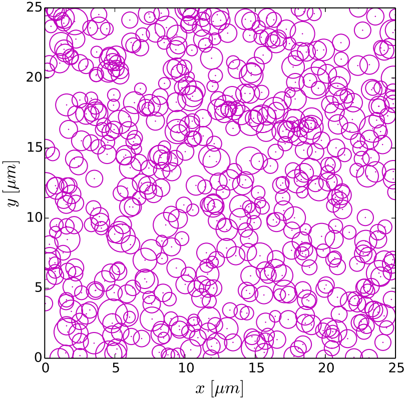
Coefficient of variation:

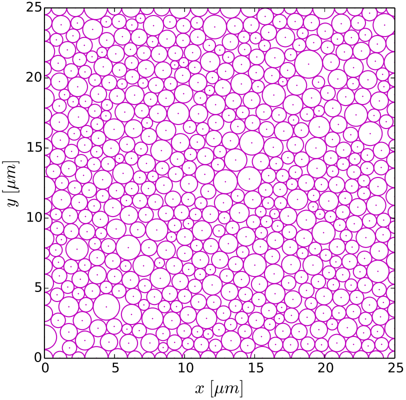
$$CV = \sqrt{\exp(\sigma^2) - 1}$$

MPP simulation by collective rearrangement

Force-bias algorithm, see Bezrukov et al. (2002):

1. Draw a realization of a Poisson point process with independent mark realizations drawn after $f_A(a)$.
2. Apply these two steps until convergence:
    1. uniformly scale all the marks to avoid any contact,
    2. move every point after the effect of some prescribed pair potentials.

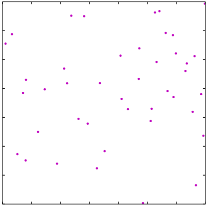


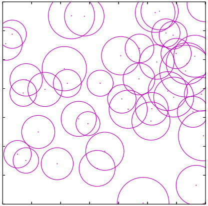


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} |\, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



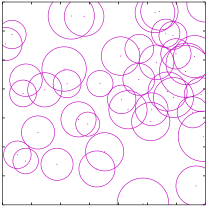


Simulation of the marks

Simulate the mark set $\{r_{i,0} |\, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

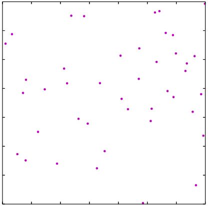
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

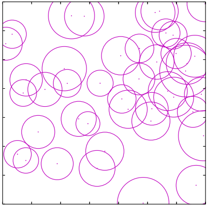


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



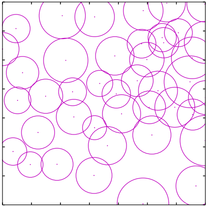


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

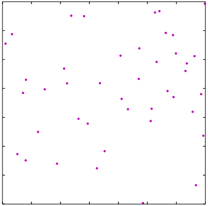
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

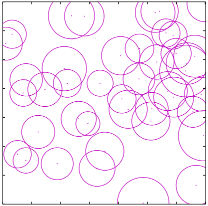


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



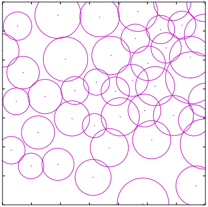


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

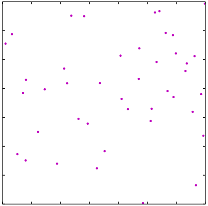
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

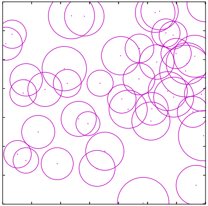


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



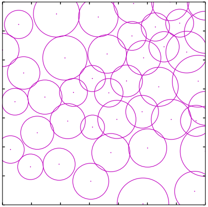


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

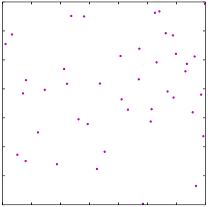
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

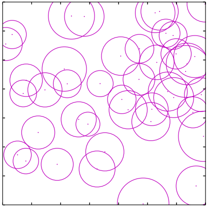


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



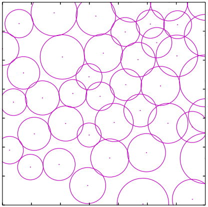


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

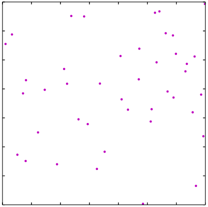
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

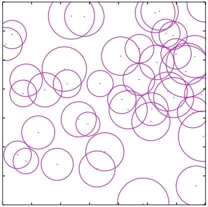


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



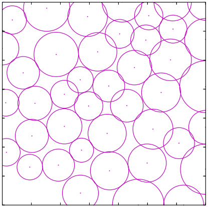


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

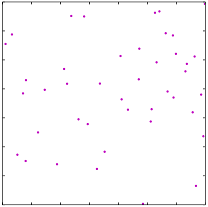
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

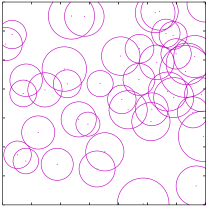


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



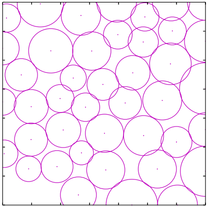


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

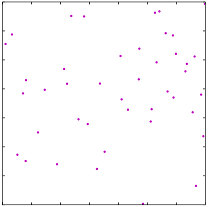
Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.

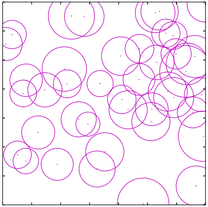


MPP simulation by collective rearrangement

Simulation of the point process

Simulate the point set $\{\vec{x}_{i,0} | \, i = 1, N\}$ in the container of size A_{cont} after a Poisson point process with rate $\lambda = 1/\mathbb{E}[A]$.



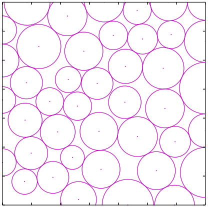


Simulation of the marks

Simulate the mark set $\{r_{i,0} | \, i = 1, N\}$ independently of the points after the prescribed grain distribution $f_A(a)$ and where $r = \sqrt{a/\pi}$.

Rearrangement of the marked point set

Assuming a pair potential p_{ij} between arbitrary marked points $(\vec{x}_i; r_i)$ and $(\vec{x}_j; r_j)$, modify the marked point set using the force-biased algorithm.



2D adaptation of the force-biased algorithm

for $i = 1, N$:
    $(\vec{x}_i; r_i) = (\vec{x}_{i,0}; r_{i,0})$
$\eta = \min_{i \neq j} \{\|\vec{x}_j - \vec{x}_i\| / (r_i + r_j)\}$
$\rho = 1$
while $\eta < 1$:
    for $i = 1, N$:
        for $j \neq i$:
            $\vec{n}_{ij} = (\vec{x}_j - \vec{x}_i) / \|\vec{x}_j - \vec{x}_i\|$
            $p_{ij} = r_i r_j \left[\frac{\|\vec{x}_j - \vec{x}_i\|^2}{(r_i + r_j)^2} - 1 \right]$
            $\vec{F}_{ij} = \varphi \mathbf{1}_{ij} p_{ij} \vec{n}_{ij}$
            $\vec{x}_i = \vec{x}_i + \frac{1}{r_i} \sum_{j \neq i} \vec{F}_{ij}$
    $A_{nom} = \sum_{i=1}^{N} \pi r_i^2 / A_{cont}$
    $\delta = -\log_{10} \left[(1 - \eta^2) A_{nom} \right]$
    $\rho = \rho - 2^{-\delta} / \tau$
    for $i = 1, N$:
        $r_i = \rho r_{i,0}$
    $\eta = \min_{i \neq j} \{\|\vec{x}_j - \vec{x}_i\| / (r_i + r_j)\}$

Size of the container:

$$A_{cont}$$

Indicator function:

$$\mathbf{1}_{ij} = \begin{cases} 1 \text{ if } b(\vec{x}_i, r_i) \cap b(\vec{x}_j, r_j) \neq \emptyset \\ 0 \text{ otherwise} \end{cases}$$

Contraction rate:

$$\tau \approx 3000 - 100000$$

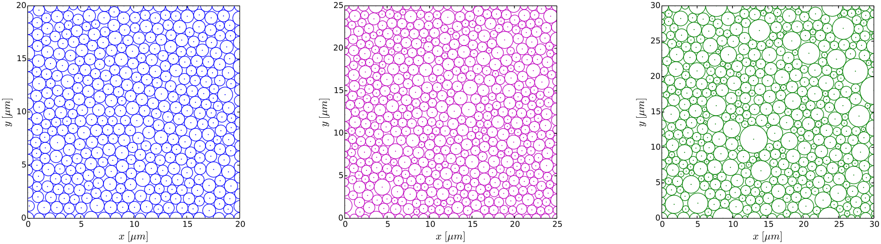
Force bias parameter:

$$\varphi \approx 0.3 - 0.6$$

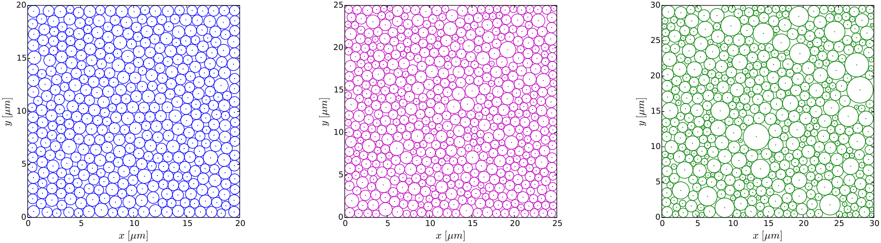
NB: Because $\vec{F}_{ij} \propto \mathbf{1}_{ij} p_{ij} \vec{n}_{ij}$, only repulsive potentials, *i.e.* $p_{ij} < 0$, affect the configuration of the system.

Different ways to handle boundaries

Enforce points to be within the domain:

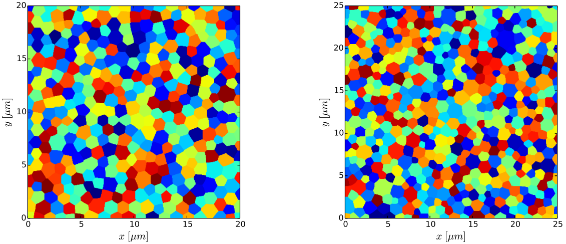


Enforce particles to be within the domain:

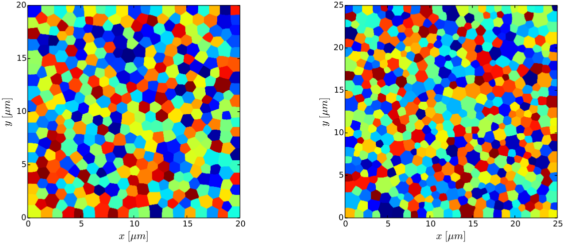


Different ways to handle boundaries – resulting tessellations

Enforce points to be within the domain:

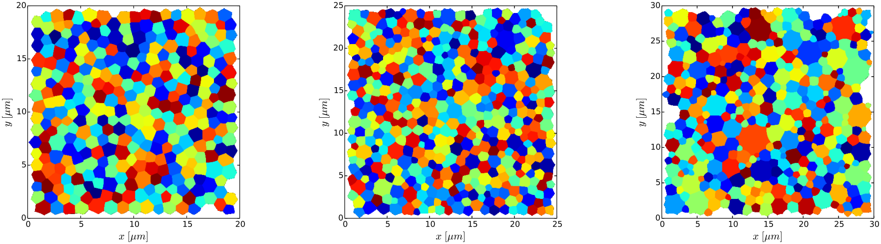


Enforce particles to be within the domain:

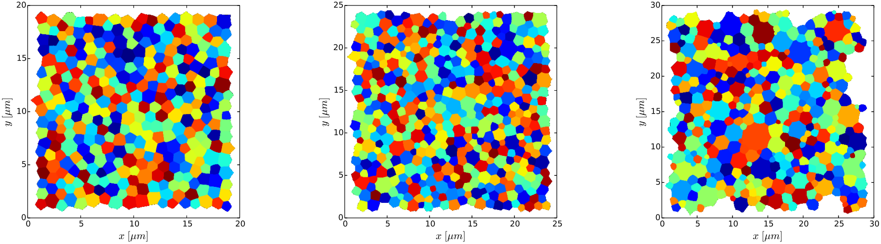


Different ways to handle boundaries – resulting tessellations

Enforce points to be within the domain:

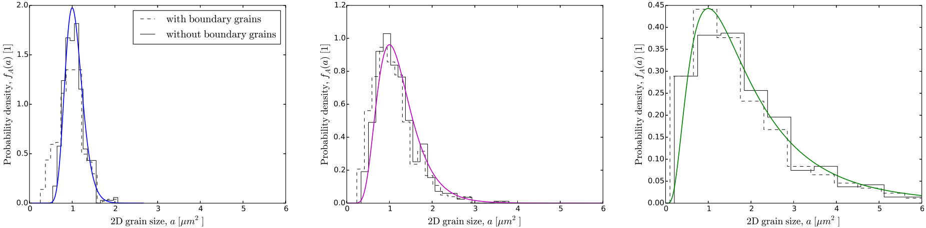


Enforce particles to be within the domain:

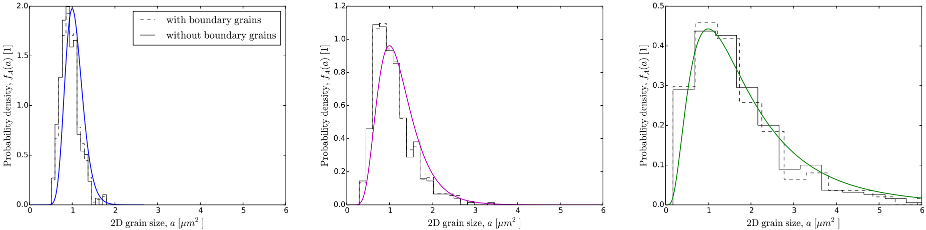


Effect of boundary grains on the recovered grain size PDF

Enforce points to be within the domain:

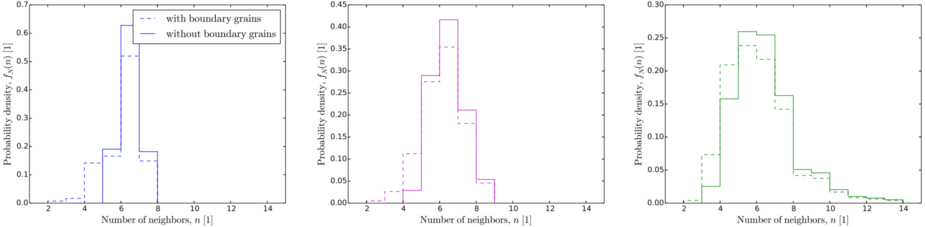


Enforce particles to be within the domain:

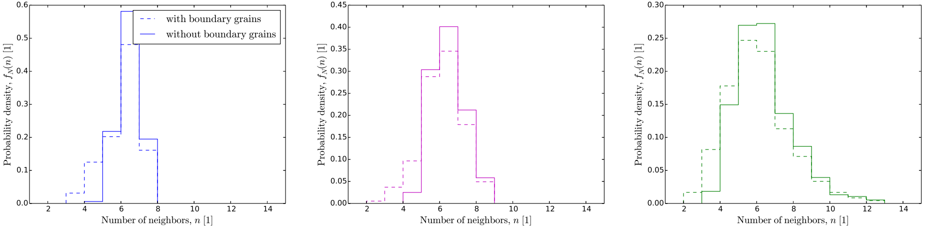


Effect of boundary grains on the number of neighbors

Enforce points to be within the domain:



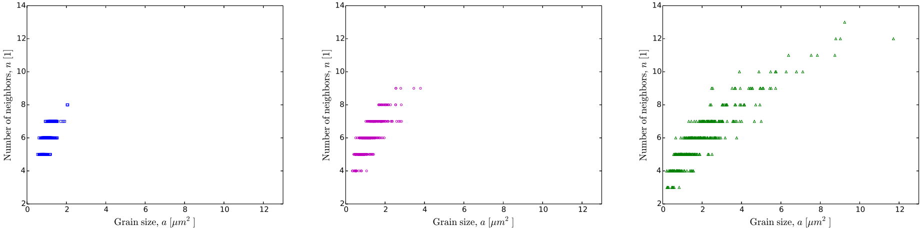
Enforce particles to be within the domain:



Correllation between number of neighbors and grain size

Yet to investigate:

- How would these scatters change if convergence of the FBA was stated for a prescribed value of $\eta < 1$?
- How do these scatters evolve as a function of φ and τ?
- Can we relate the random number of neighbors to the random grain size for a prescribed $f_A(a)$?



NB: The results presented are for the bulk grains in simulations where the points only are constrained to be within the domain.

Computation time

MPP simulation

- serial implementation
- convergence at $\eta = 1$
- $\varphi = 0.5$, $\tau = 40000$

SGT model resolution

- parallel implementation: 6 threads
- $\Delta x = 0.01\ \mu m$

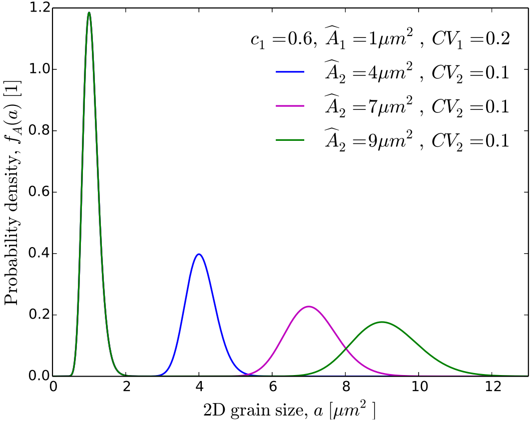
Target, $f_A(a \vert \widehat{A} = 1\ \mu m^2)$	**MPP**	**SGT**	**Total**
$CV = 0.1$, $A_{cont} = 20 \times 20\ \mu m^2$	67 s (5950 it.)	29 s	96 s
$CV = 0.4$, $A_{cont} = 25 \times 25\ \mu m^2$	132 s (6172 it.)	63 s	195 s
$CV = 0.8$, $A_{cont} = 30 \times 30\ \mu m^2$	85 s (5596 it.)	90 s	175 s

NB: The results presented are only for points constrained to be within the domain. MPP simulations enforcing particles to be within the domain are more time-consuming. The simulation times for SGT might be underestimated.

Some bimodal target 2D grain size distributions

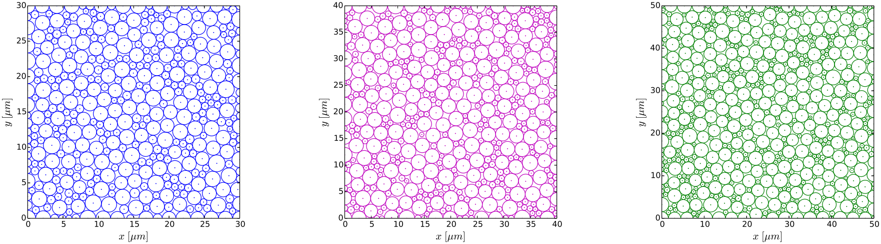
Bimodal log-normal PDF of 2D grain size A:

$$f_A(a|\mu_1,\sigma_1,\mu_2,\sigma_2,c_1) = c_1 f_A(a|\mu_1,\sigma_1) + (1-c_1) f_A(a|\mu_2,\sigma_2),\ a \in]0,+\infty[$$

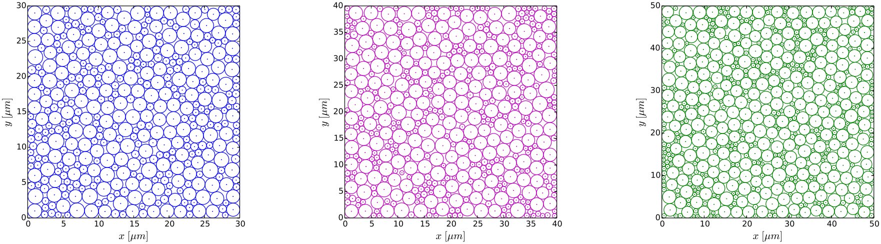


Different ways to handle boundaries

Enforce points to be within the domain:

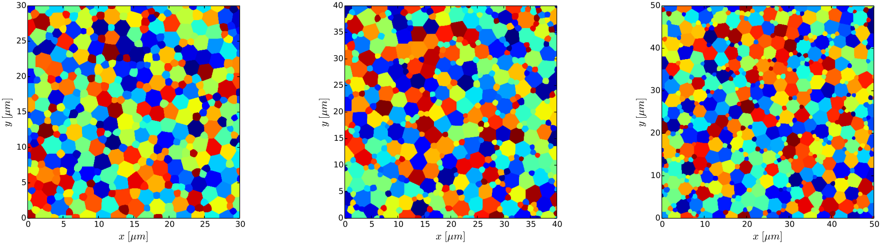


Enforce particles to be within the domain:

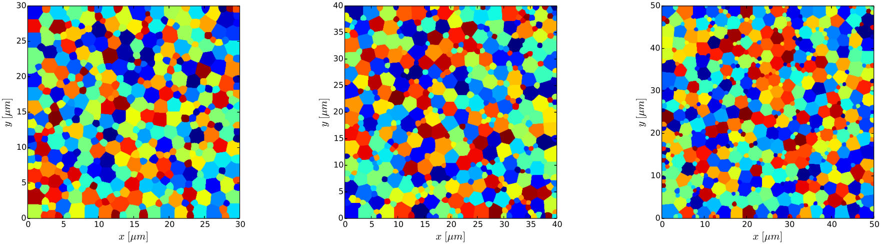


Different ways to handle boundaries – resulting tessellations

Enforce points to be within the domain:

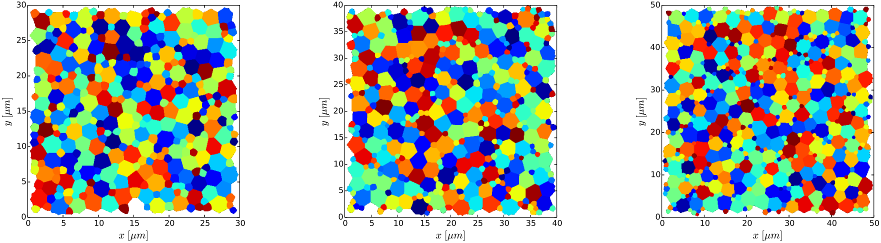


Enforce particles to be within the domain:

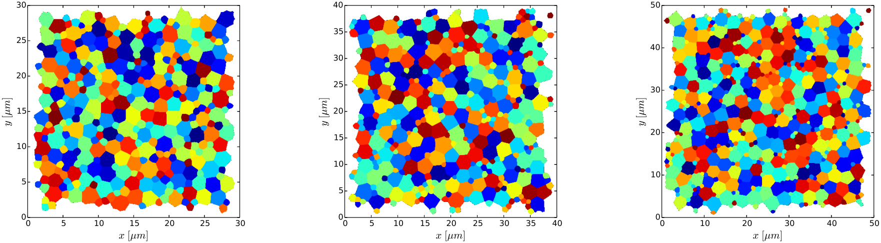


Different ways to handle boundaries – resulting tessellations

Enforce points to be within the domain:

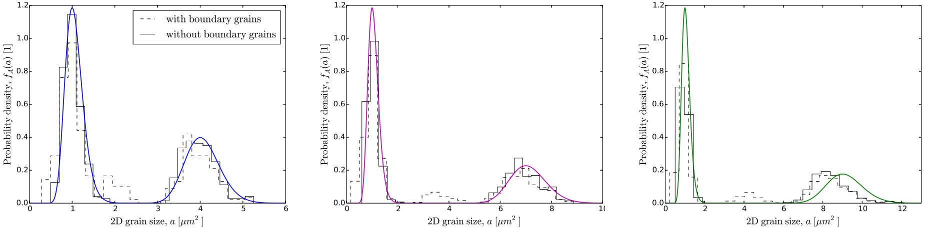


Enforce particles to be within the domain:

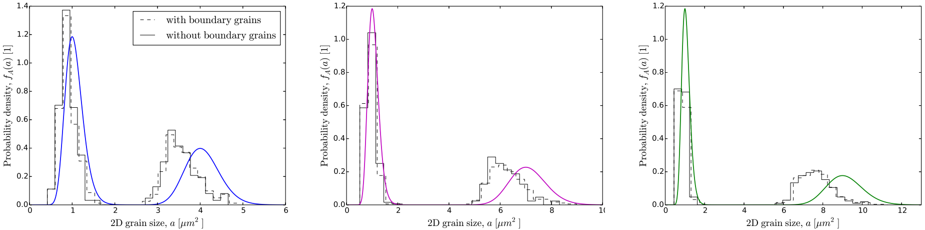


Effect of boundary grains on the recovered grain size PDF

Enforce points to be within the domain:

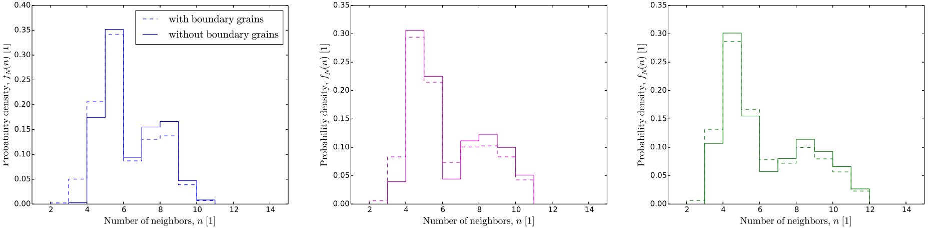


Enforce particles to be within the domain:

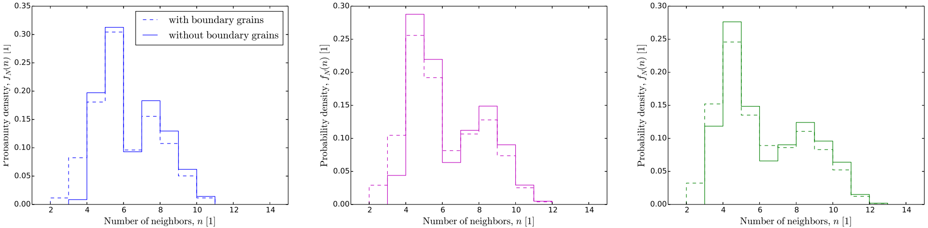


Effect of boundary grains on the number of neighbors

Enforce points to be within the domain:



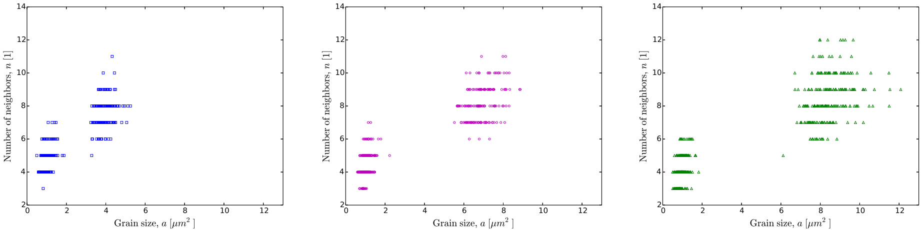
Enforce particles to be within the domain:



Correllation between number of neighbors and grain size

Yet to investigate:

- How would these scatters change if convergence of the FBA was stated for a prescribed value of $\eta < 1$?
- How do these scatters evolve as a function of φ and τ?
- Can we relate the random number of neighbors to the random grain size for a prescribed $f_A(a)$?



NB: The results presented are for the bulk grains in simulations where the points only are constrained to be within the domain.

Computation time

MPP simulation

- serial implementation
- convergence at $\eta = 1$
- $\varphi = 0.5$, $\tau = 40000$

SGT model resolution

- parallel implementation: 6 threads
- $\Delta x = 0.02\ \mu m$

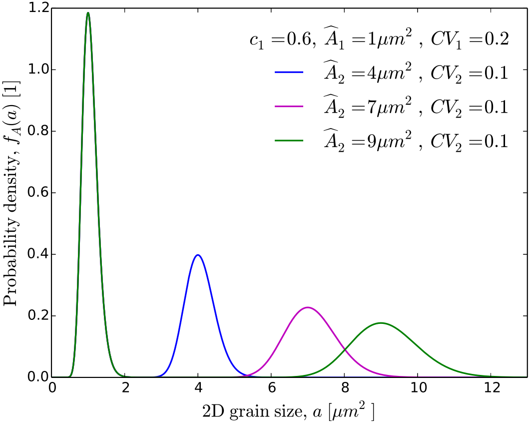
Target, $f_A(a \mid \widehat{A} = 1\ \mu m^2)$	**MPP**	**SGT**	**Total**
$\widehat{A}_2 = 4\ \mu m^2$, $A_{cont} = 30 \times 30\ \mu m^2$	66 s (5265 it.)	25 s	91 s
$\widehat{A}_2 = 7\ \mu m^2$, $A_{cont} = 40 \times 40\ \mu m^2$	85 s (4826 it.)	57 s	142 s
$\widehat{A}_2 = 9\ \mu m^2$, $A_{cont} = 50 \times 50\ \mu m^2$	157 s (5596 it.)	109 s	266 s

NB: The results presented are only for points constrained to be within the domain. MPP simulations enforcing particles to be within the domain are more time-consuming. The simulation times for SGT might be underestimated.

A target 2D grain size PDF of nanoengineered material

Bimodal log-normal PDF of 2D grain size A:

$$f_A(a|\mu_1,\sigma_1,\mu_2,\sigma_2,c_1) = c_1 f_A(a|\mu_1,\sigma_1) + (1-c_1) f_A(a|\mu_2,\sigma_2),\ a \in]0,+\infty[$$



Volume fractions:

$$\phi_1 = \frac{c_1 \widehat{A}_1}{c_1 \widehat{A}_1 + (1-c_1)\widehat{A}_2 \exp(CV_2^2 - CV_1^2)}$$

$$\phi_2 = 1 - \phi_1$$

Ratio of modes:

Points and questions to address

1. Can we fit a inhomogeneous rate of Poisson process onto such results? If so, what about the marks?
2. Improve the efficiency of the current force-biased algorithm implementation

References I

Bezrukov, A., Bargiel, M., and Stoyan, D. (2002). Statistical analysis of simulated random packings of spheres. *Particle and Particle Systems Characterization*, 19(2):111–118.

Teferra, K. and Graham-Brady, L. (Under review). Grain growth tessellation models for polycrystalline microstructures. *Computational Materials Science*.