Homogénéisation : les microstructures ont-elles leur mot à dire ?

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Colloque MECAMAT "Homogénéisation du comportement mécanique des matériaux hétérogènes", Aussois, 27-31 janvier 2025

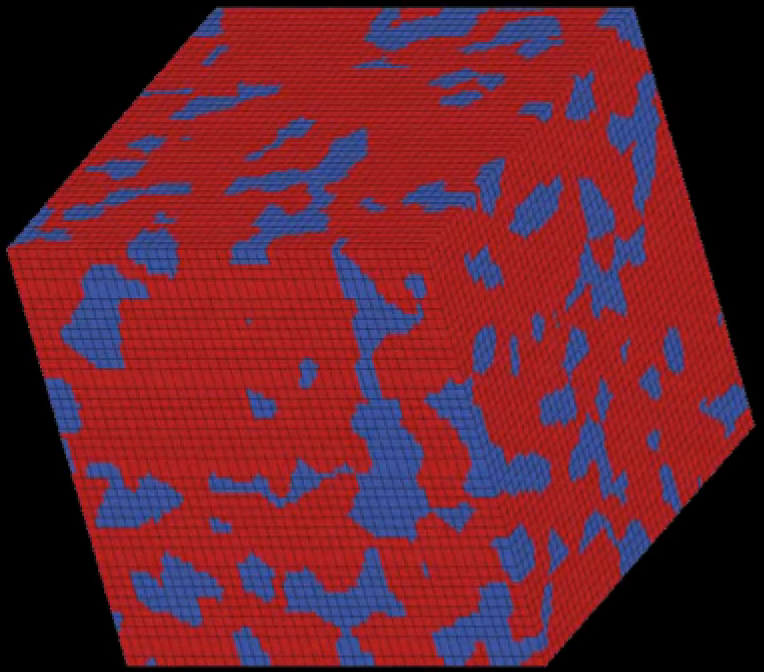
LGF cnrs MINES Saint-Étienne

Neper (https://neper.info)

FEPX (https://fepx.info)

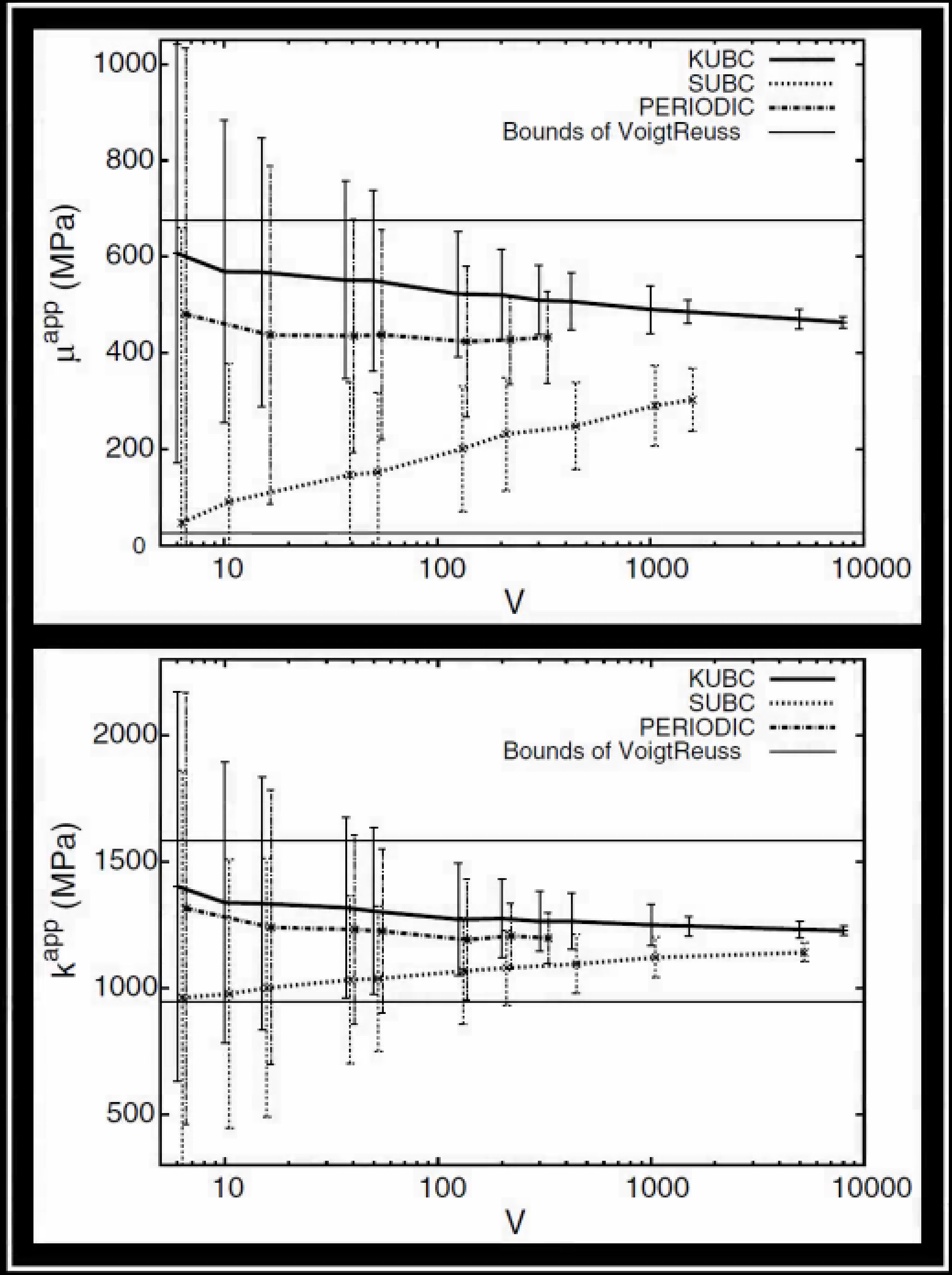
Numerical Homogenization

(Kanit et al, 2003)



2-phase microstructure

(AI-generated)



Periodic BCs are the best.

Relative error (95% confidence):

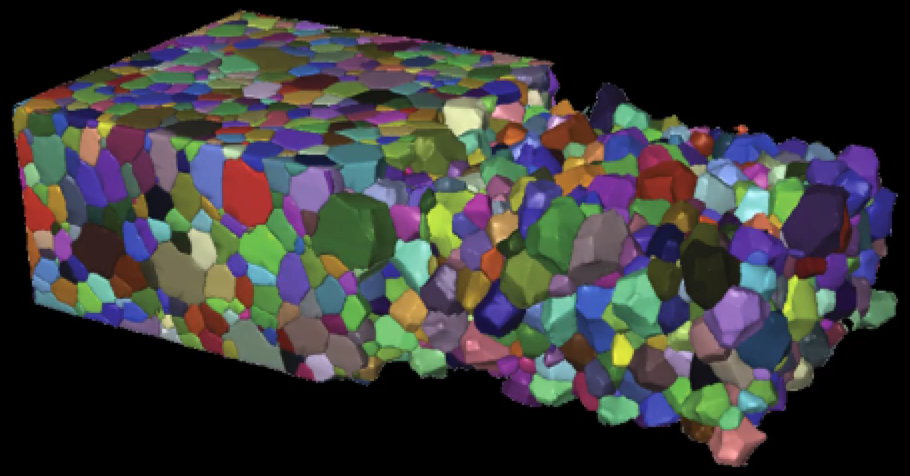
$$e(V) = \frac{2\,\sigma_\mu(V)}{\bar{\mu}(V)}$$

Knowing $e(V)$ and for a desired e, V can be obtained.

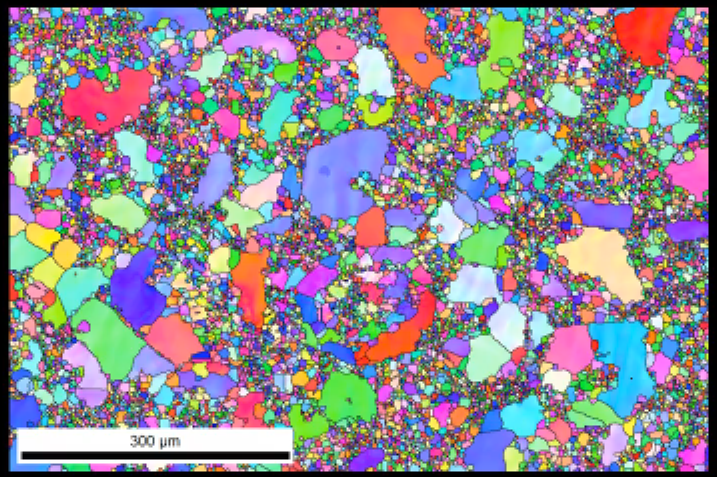
RVE = Domain for which a mean value can be estimated within a desired error (for a given property)

$e(V)$ can be related to microstructural properties (integral range).

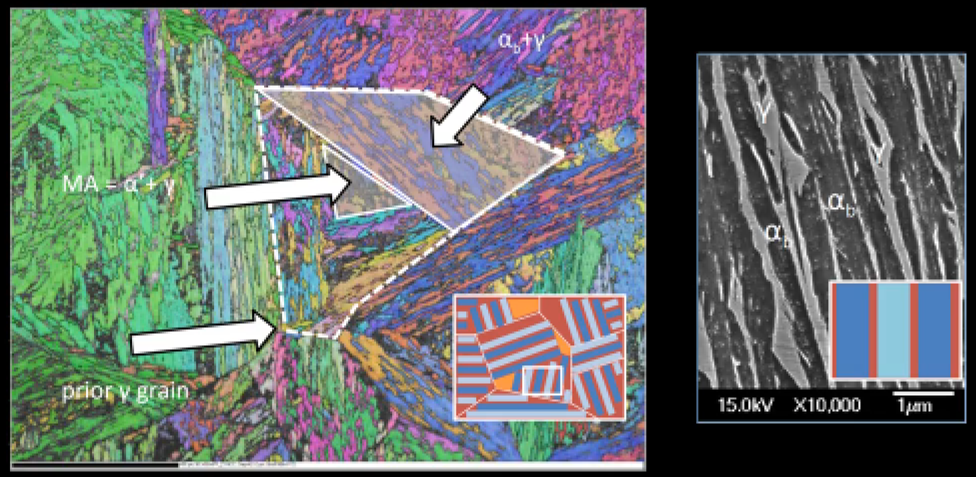
Polycrystalline Microstructures



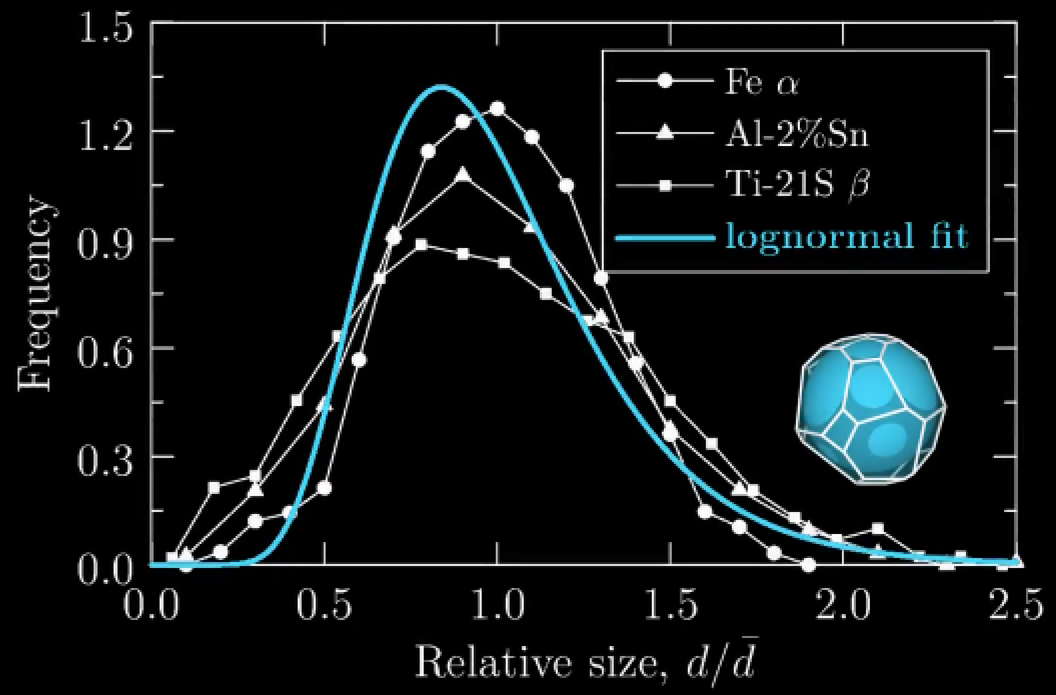
Ti-21S β (Rowenhorst et al, 2007)

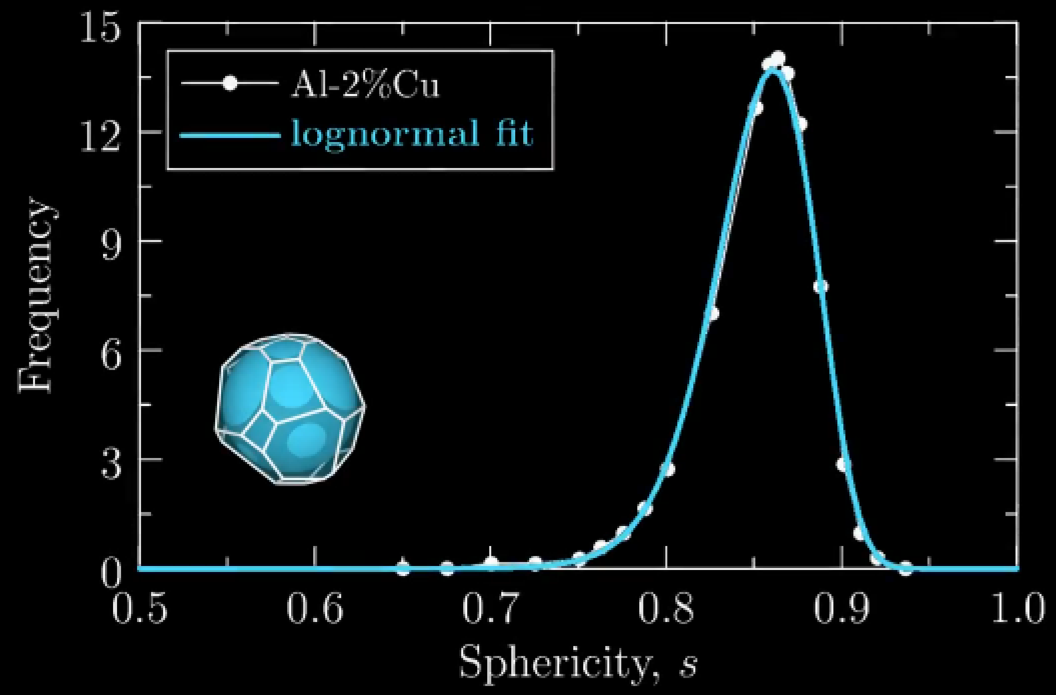


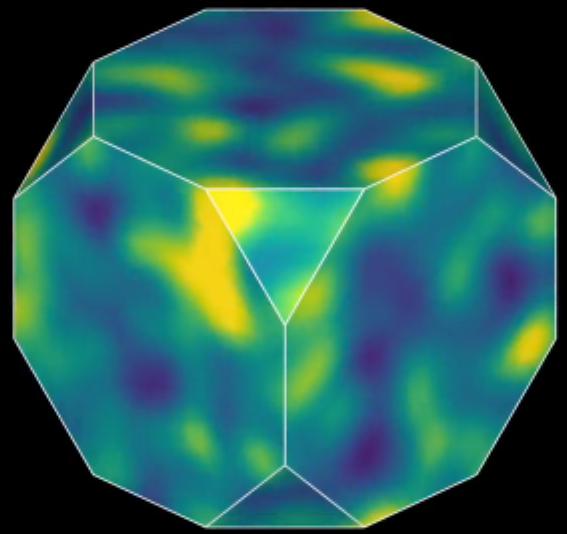
Bimodal 316L (Flipon, 2020)



Martensite (Hell, 2011)



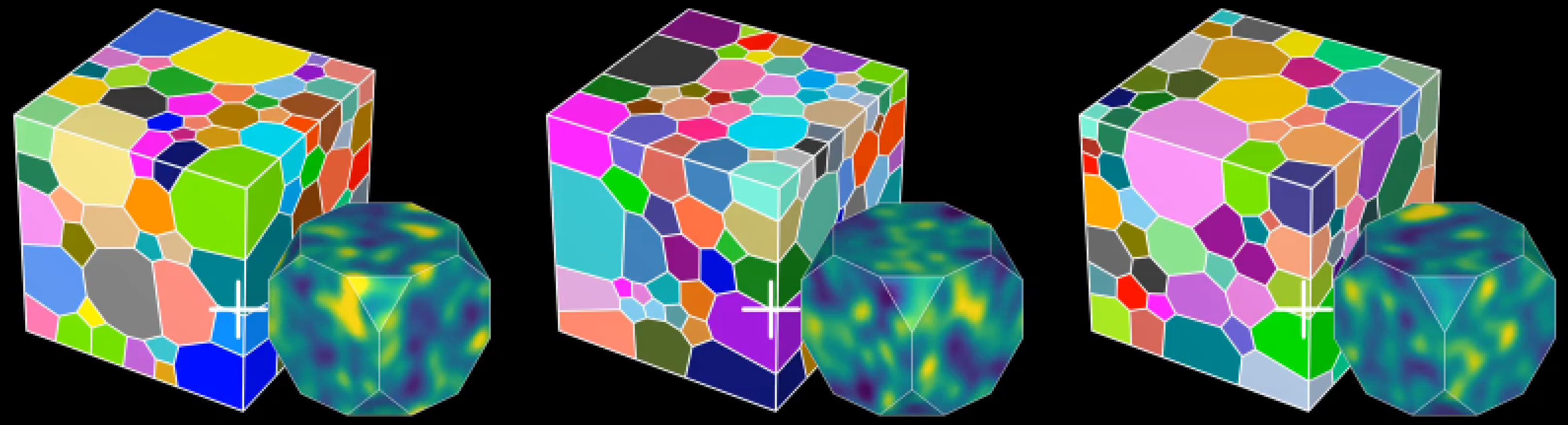




(Random) Orientations

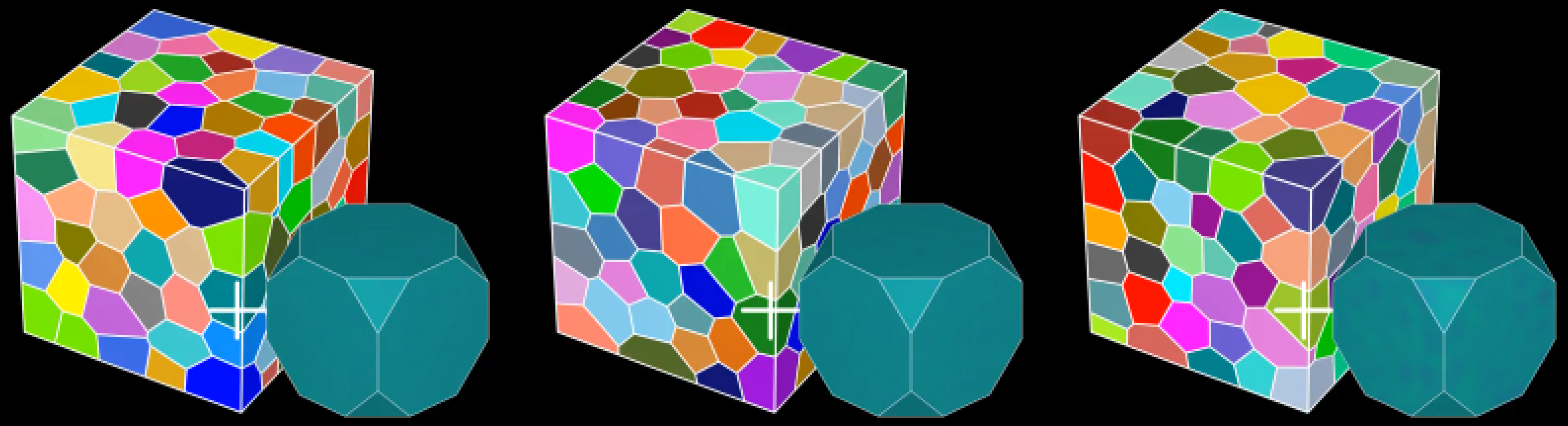
"Grain-growth statistics": Variabilities σ_d, σ_s and σ_f (standard deviation / average)

Motivation



$\cdots \longrightarrow \{\mu_1^{exp}, \mu_2^{exp}, \mu_3^{exp}, \ldots\} \longrightarrow \bar{\mu}^{exp}, e_\mu^{exp}(N)$

“Experimental”: Random orientation distribution (σ_f) + grain size distribution (σ_d)



$\cdots \longrightarrow \{\mu_1^{uni}, \mu_2^{uni}, \mu_3^{uni}, \ldots\} \longrightarrow \bar{\mu}^{uni}, e_\mu^{uni}(N)$

“Uniformized”: Uniform orientation distribution ($\sigma_f \simeq 0$) + no grain size distribution ($\sigma_d \simeq 0$)

- Can we go from “experimental” to “uniformized”? ($\bar{\mu}^{uni} = \bar{\mu}^{exp}$?)
- Is there an interest? ($e^{uni} < e^{exp}$ and so $N^{uni} < N^{exp}$?)
- How does e_μ relate to σ_d and σ_f?

Contents

Laguerre Tessellations

(aka "Weighted Voronoi" or "Radical" Tessellations)

Domain of space, D

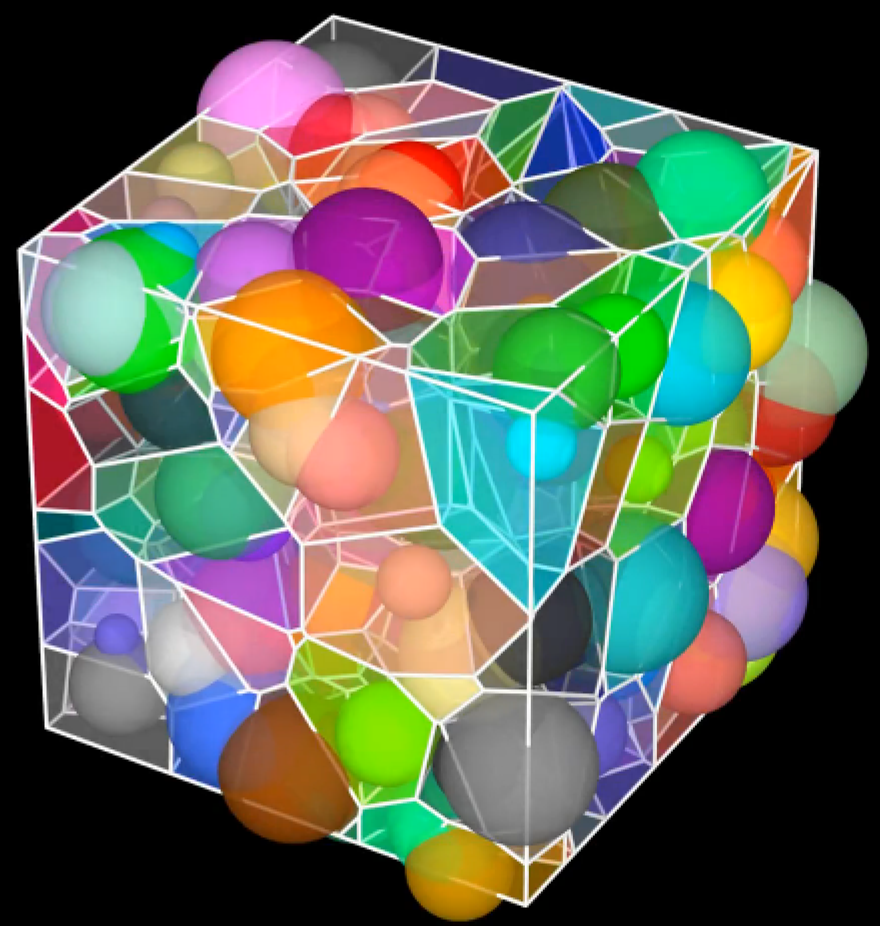
Seeds, S_i ($i \in [1, N]$), of positions $\mathbf{x}_i$ and weights w_i

$\longrightarrow$ Cells, $C_i = \{P(\mathbf{x}) \in D \mid \|P, S_i\|^2 - w_i < \|P, S_j\|^2 - w_j \;\; \forall j \neq i\}$

In general, the larger the weight (w_i), the bigger the cell (C_i).

No direct relation between $S_i(\mathbf{x_i}, w_i)$ and C_i

Grains are convex $\rightarrow$ conventional meshing



Laguerre tessellations = general parameterization of normal tessellations (assuming independent parameters) (Lautensack, 2007).

Optimization of Laguerre Tessellations

(Quey and Renversade, 2018)

Variables = Seed weights and coordinates
Objective Function = "actual vs target properties"
(grain statistics or individual grain properties)

→ non-linear, unknown gradient, large-scale, local optimization problem

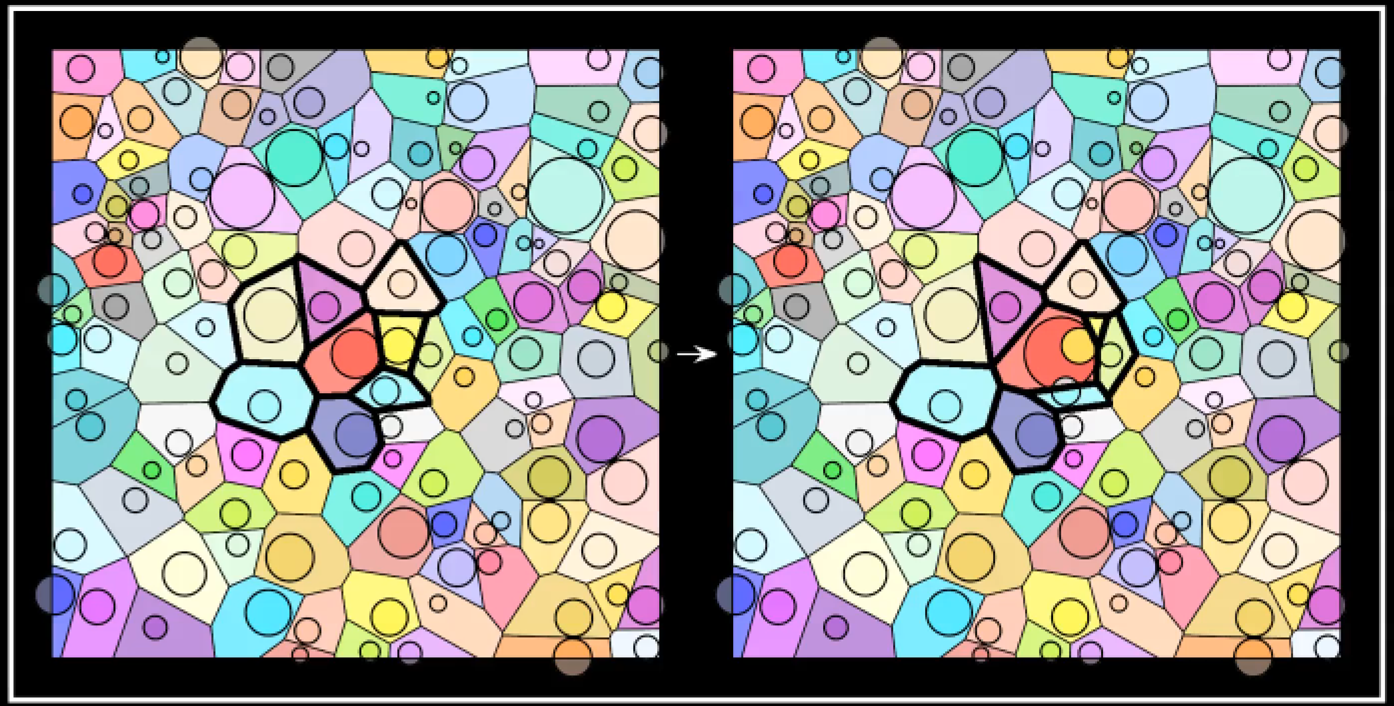
Resolution using

NLopt's *Subplex* algorithm

(one variable changed at each iteration)

+

a tessellation update algorithm

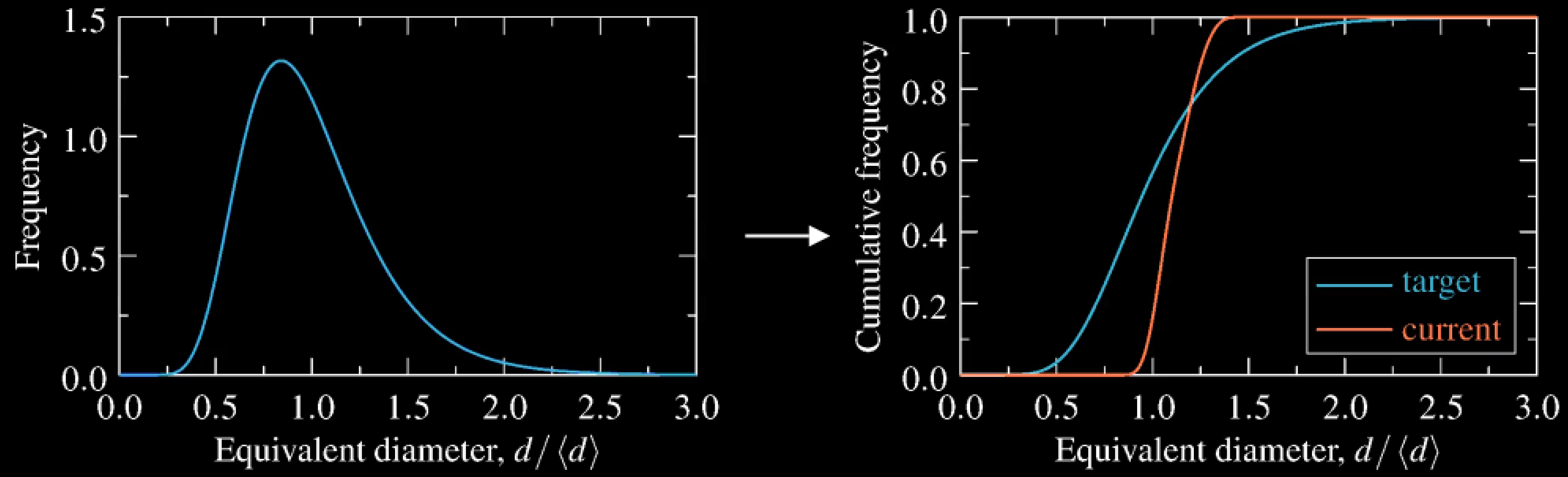


Tessellation update (red seed modified).

Any (convex-grain) polycrystal can be generated given a proper definition of the objective function.

Optimization of Laguerre Tessellations

(Quey and Renversade, 2018)



Modified Anderson-Darling test (1952):

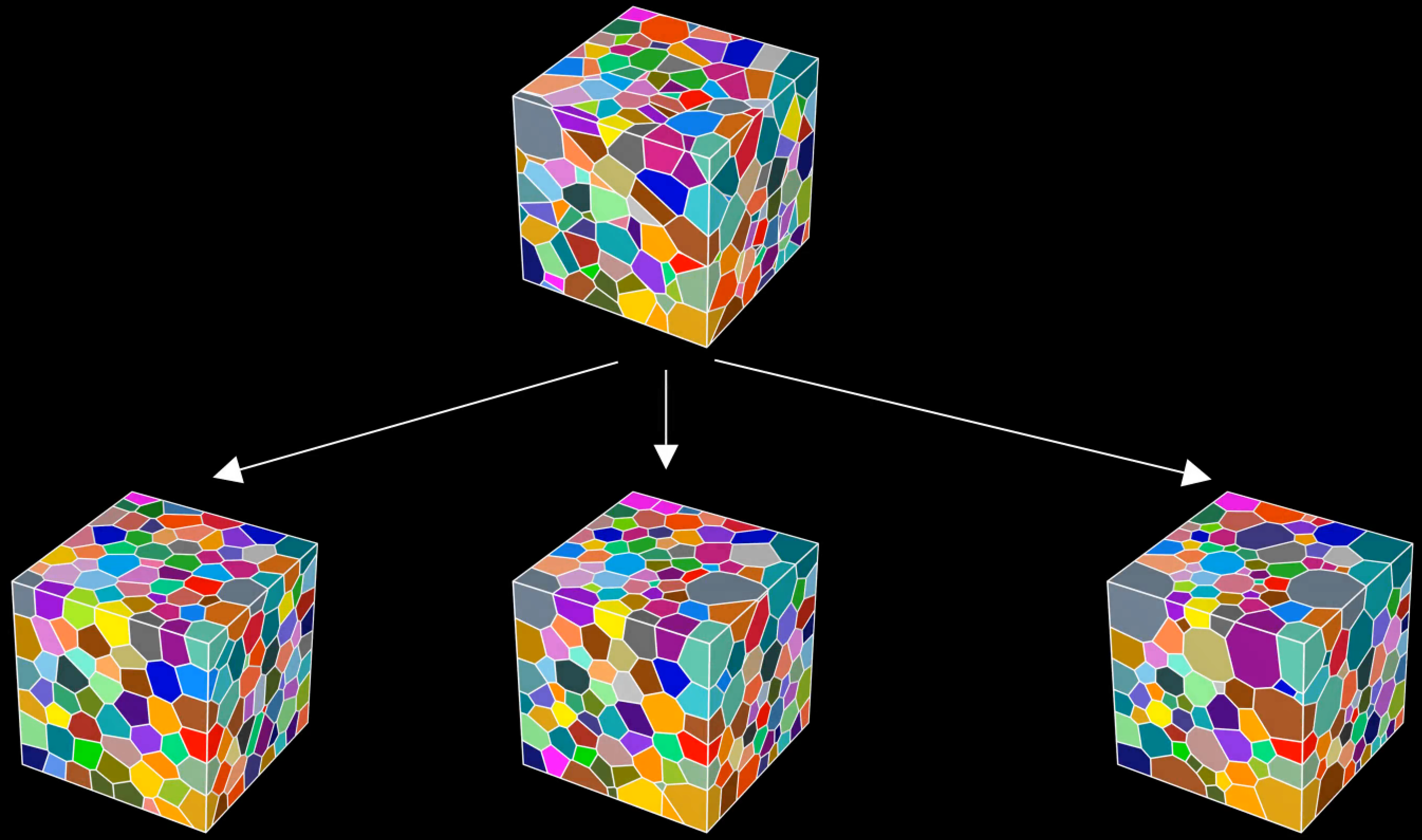
$$O_d = \int_{-\infty}^{+\infty} \frac{\left(F^* \circ s(x) - F \circ s(x)\right)^2}{F \circ s(x)\ \left(1 - F \circ s(x)\right)}\,\mathrm{d}x$$

Same for other distributions (sphericity)...

$$O = \sqrt{{O_d}^2 + {O_s}^2}$$

(Aggregated optimization)

Example Microstructures

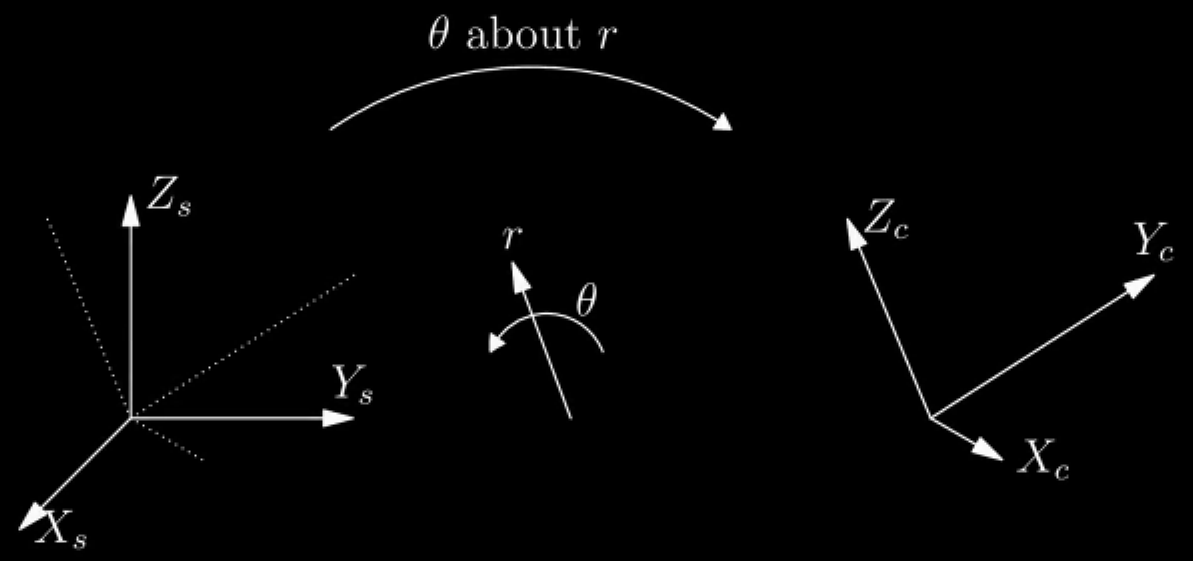


“Dirac” ($\sigma_d = 0$) “Voronoi” ($\sigma_d = 0.145$) “Grain-growth” ($\sigma_d = 0.35$)

Contents

Orientations Represented by Unit Quaternions (Hamilton, 1843)

Any orientation can be described by a rotation of angle $\theta \in [0, \pi]$ *around a unique axis,* $\mathbf{r}$ (Euler, 1775).



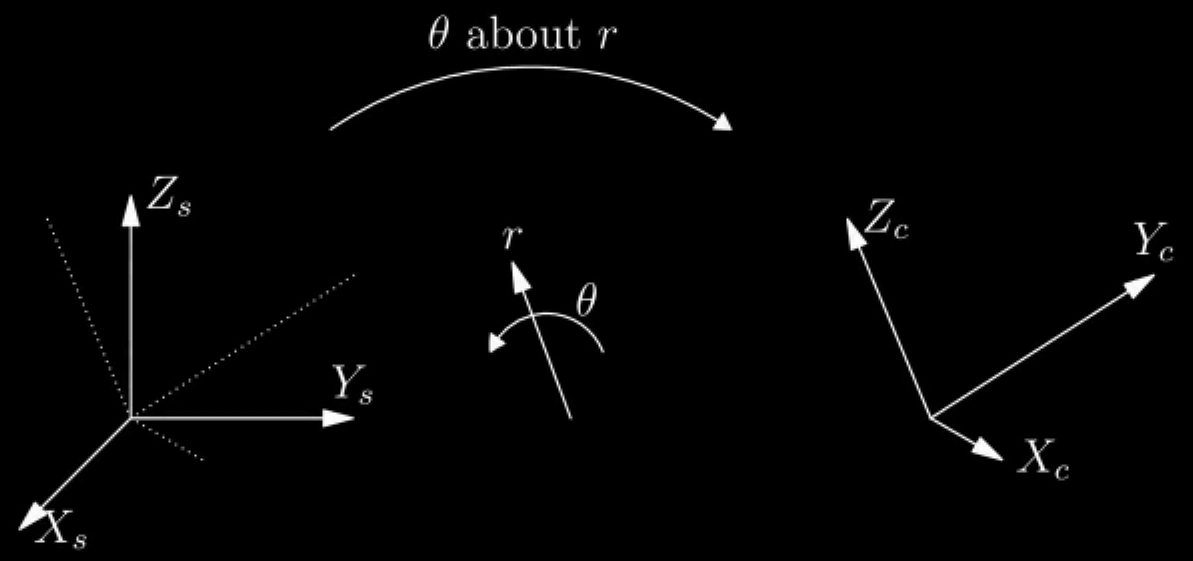
$$\boxed{\mathbf{q} = \cos\left(\frac{\theta}{2}\right) + \mathbf{r}\,\sin\left(\frac{\theta}{2}\right)} \longrightarrow \begin{cases} \text{4D vectors, } \|\mathbf{q}\| = 1,\ \mathbf{q} \in \mathbb{S}^3 \\ \text{1 orientation} = \text{2 quaternions } (\mathbf{q} \text{ and } -\mathbf{q}) \end{cases}$$

Easy computation: $\mathbf{q_3} = \mathbf{q_1}\,\mathbf{q_2},\ \mathbf{q_m} = \mathbf{q_2}\,\mathbf{q_1}^{-1},\ \mathbf{q^k} = \mathbf{q}\,\mathbf{u^k}, \ldots$

Misorientation angle = 2 × distance between quaternions (no distorsion)

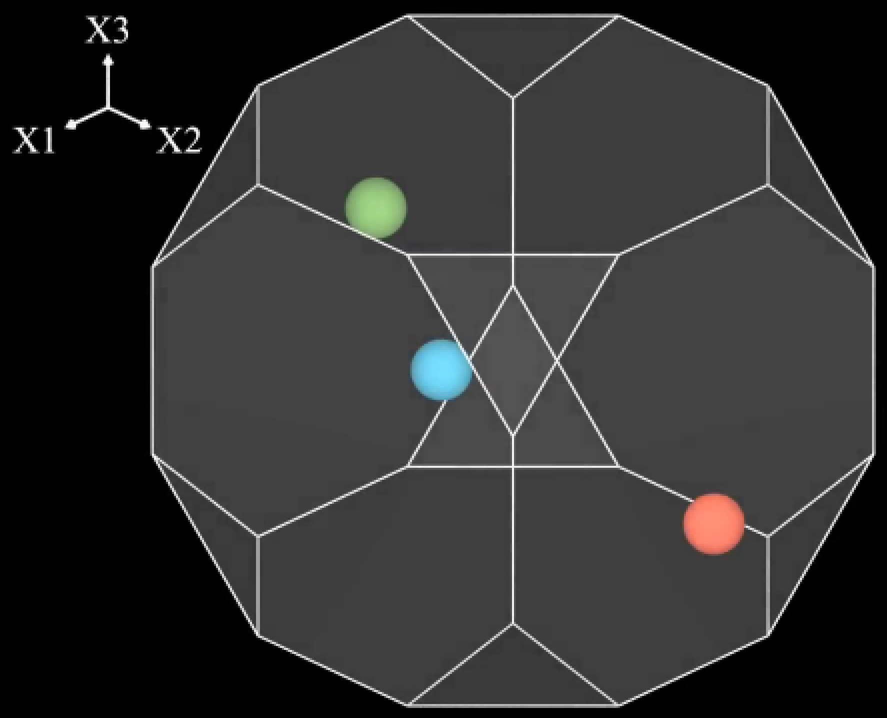
Visualization of Orientations using Rodrigues Vectors (Rodrigues, 1840)

Any orientation can be described by a rotation of angle $\theta \in [0, \pi]$ around a unique axis, $\mathbf{r}$ (Euler, 1775).



$$\boxed{\mathbf{v} = \mathbf{r}\,\tan\left(\frac{\theta}{2}\right)} \longrightarrow \begin{cases} \text{3D vectors, } v \in \mathbb{R}^3 \text{ (infinite space)} \\ \text{1 orientation} = \text{1 Rodrigues vector} \end{cases}$$

Cubic symmetry $\Rightarrow$ "fundamental region" = truncated cube

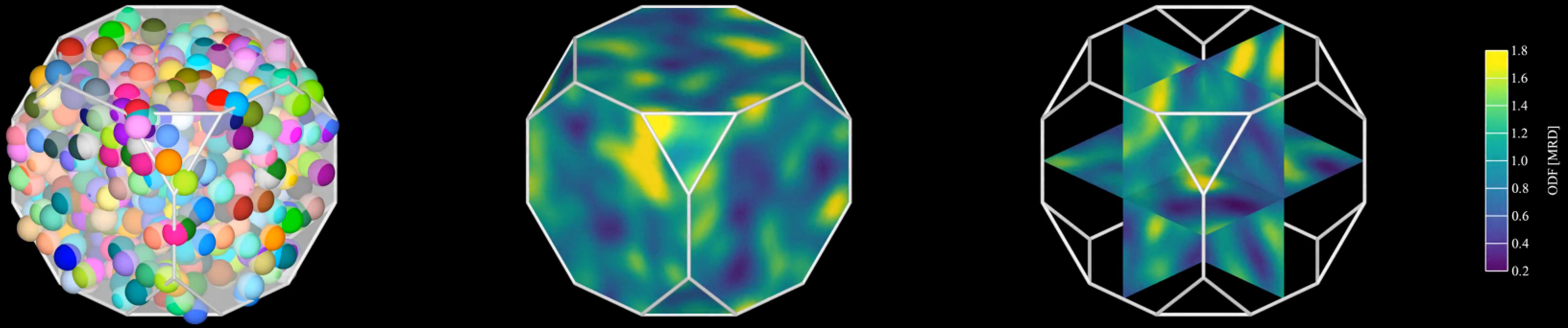


Random Distributions of Orientations

Rejection Sampling Algorithm:

1. Draw random numbers, n_1, n_2, n_3 and n_4, in $[-1, 1]$
2. If ${n_1}^2 + {n_2}^2 + {n_3}^2 + {n_4}^2 \leq 1$, accept orientation:

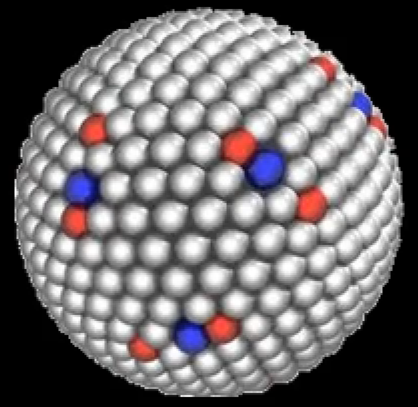
$$\mathbf{q} = \frac{(n_1, n_2, n_3, n_4)}{\sqrt{{n_1}^2 + {n_2}^2 + {n_3}^2 + {n_4}^2}}$$



1000 orientations, cubic symmetry

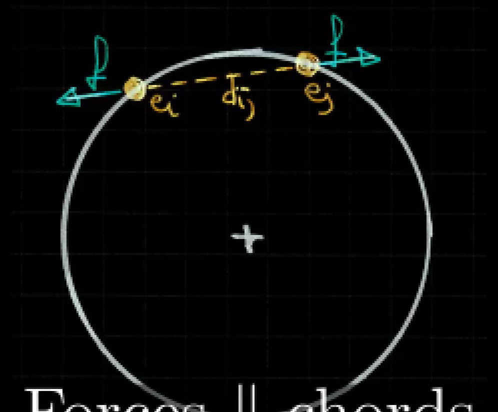
$\sigma_f \simeq 0.3 \,\forall\, N$

Nearly-Uniform Distributions of Orientations (Quey et al, 2018)



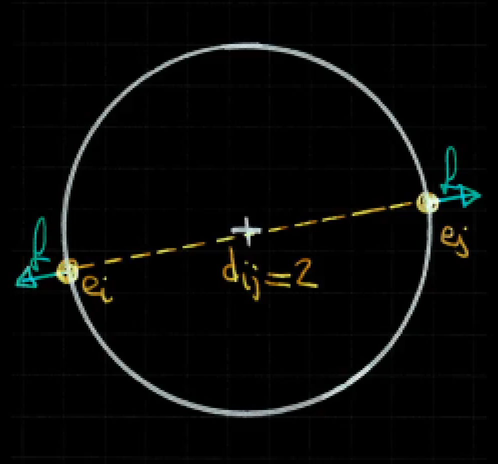
Applied to Orientations: "*Determine the minimum energy configuration of N unit quaternions on the surface of $\mathbb{S}^3$.*"

Electrons



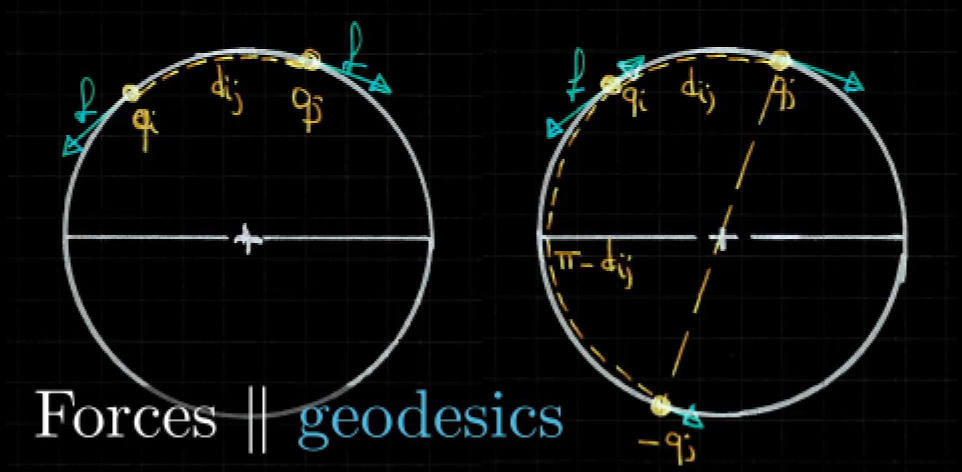
Forces ∥ chords

↓



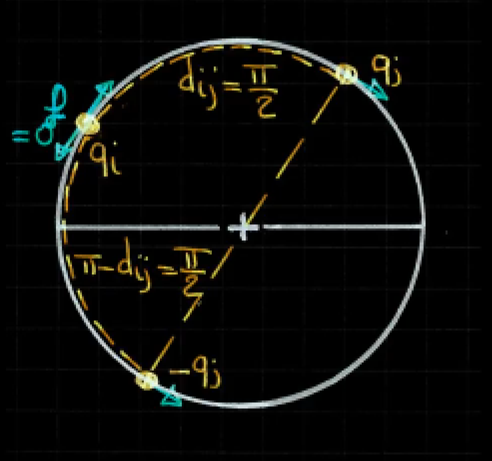
$f \neq 0$

Orientations



Forces ∥ geodesics

↓



$f = 0$

Formulation in tangent space:

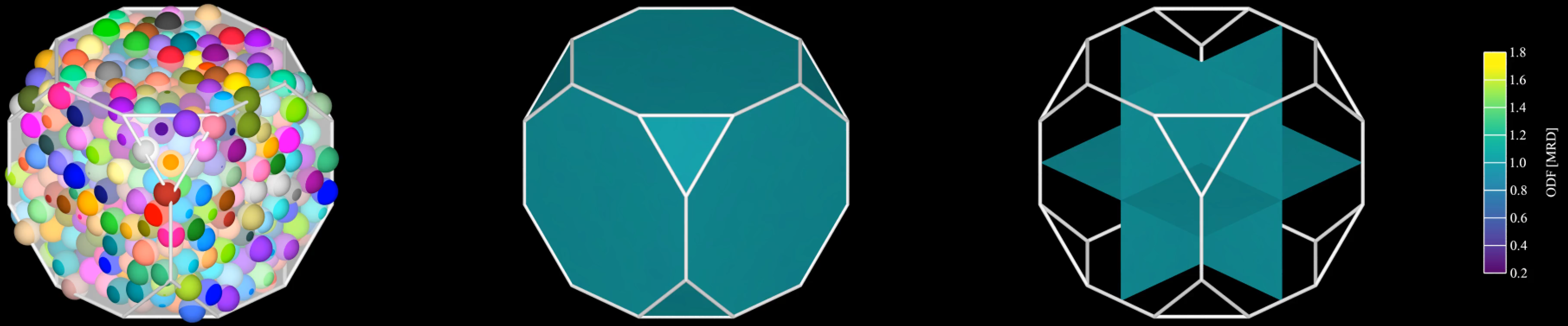
$$\mathbf{f_i} = - \sum_{j=1,\, j\neq i}^{N} \sum_{k=1}^{n_c} \left(\frac{1}{{d_{ij}^k}^2} + \frac{1}{(\pi - d_{ij}^k)^2} \right) \mathbf{r_{ij}}$$

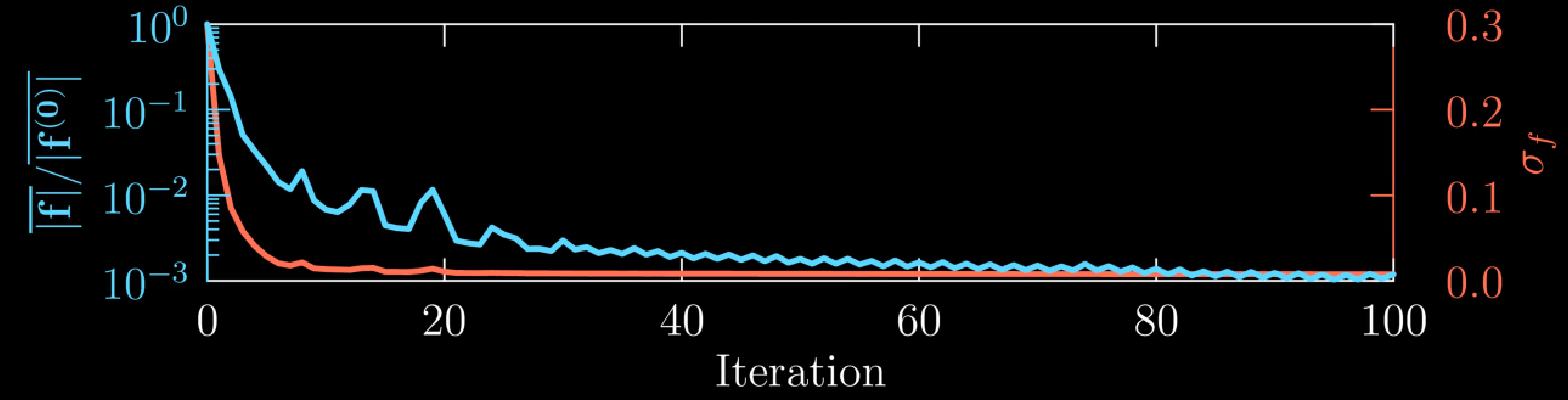
N orientations (cut-off for large $N\,n_c$)

Crystal symmetry

$$\mathbf{\Delta q_i}^{(l)} = \alpha^{(l)}\, \mathbf{f_i}^{(l)}$$

(Gradient descent, Barzilai-Borwein step size)





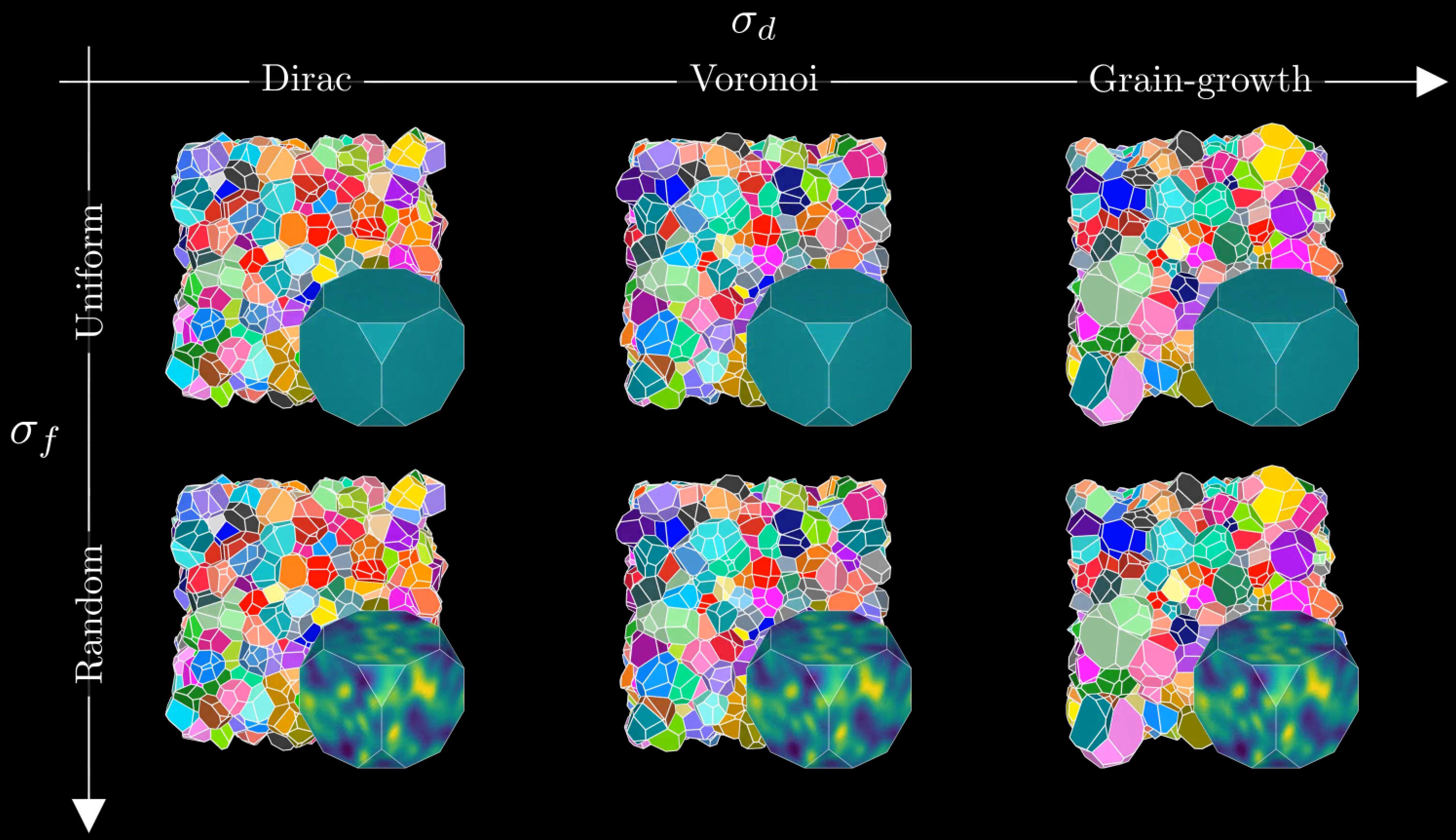
$\sigma_f \simeq 0.007$

1000 orientations, cubic symmetry

$\sigma_f^{bcc} \simeq 0.002$

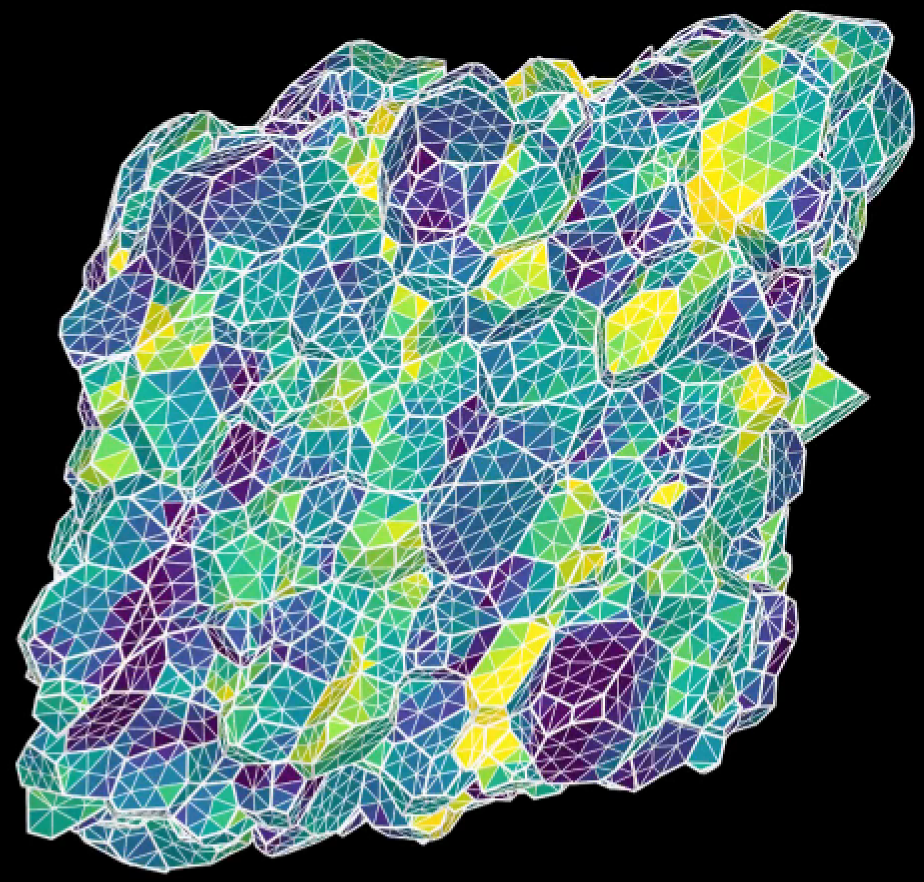
Contents

Microstructural Configurations



Simulations

- Copper in Elasticity
  ($C_{11} = 159$ GPa, $C_{12} = 122$ GPa, $C_{44} = 81$ GPa)
- Periodic polycrystals
- Shear deformation in FE $\to \mu$
  (κ isotropic)

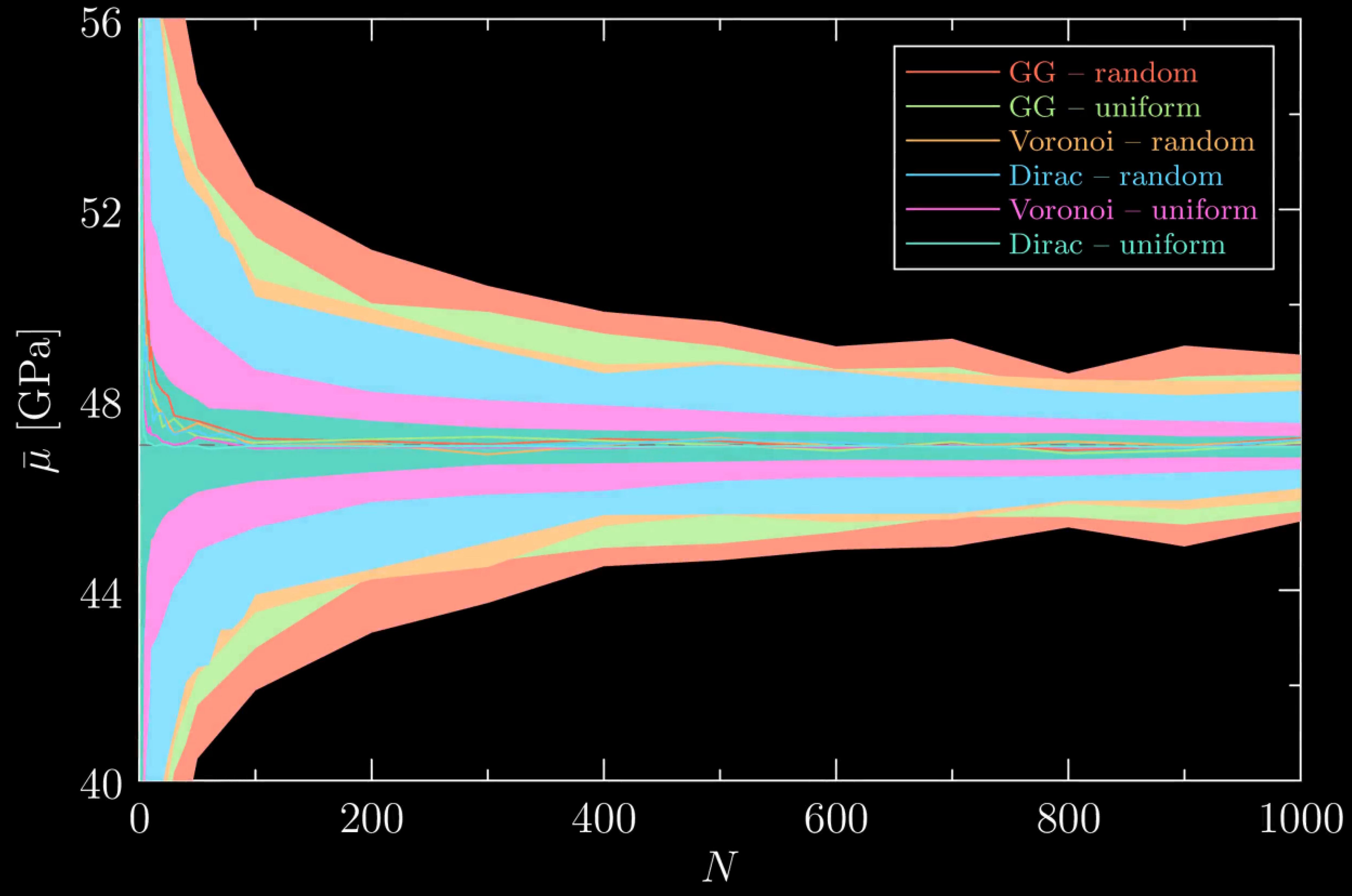


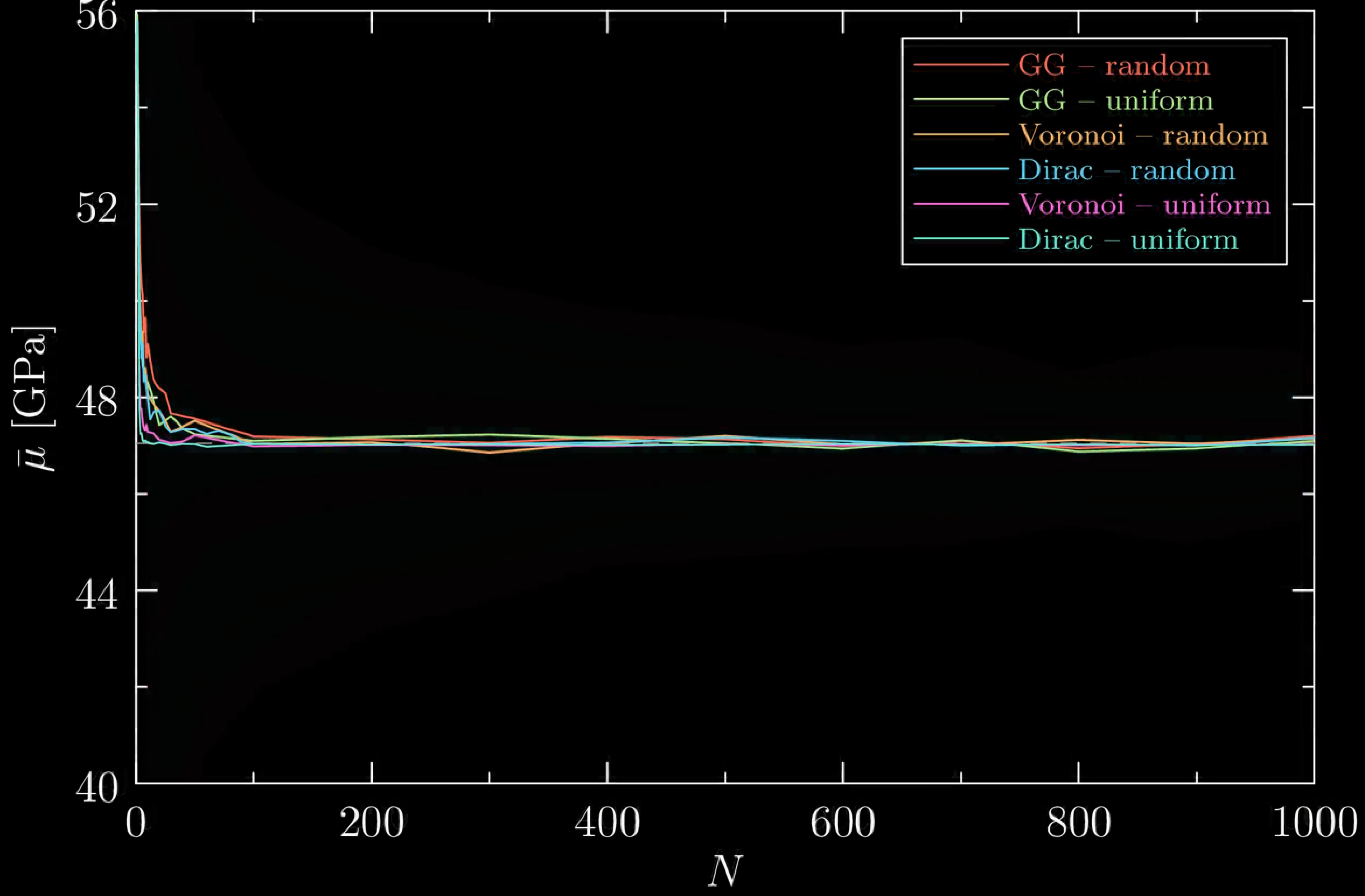
For each microstructural configuration

For $N = 3, 4, 5, \ldots, 10, 20, 30, 40, 50, \ldots, 100, 200, 300, 400, 500, \ldots, 1000$

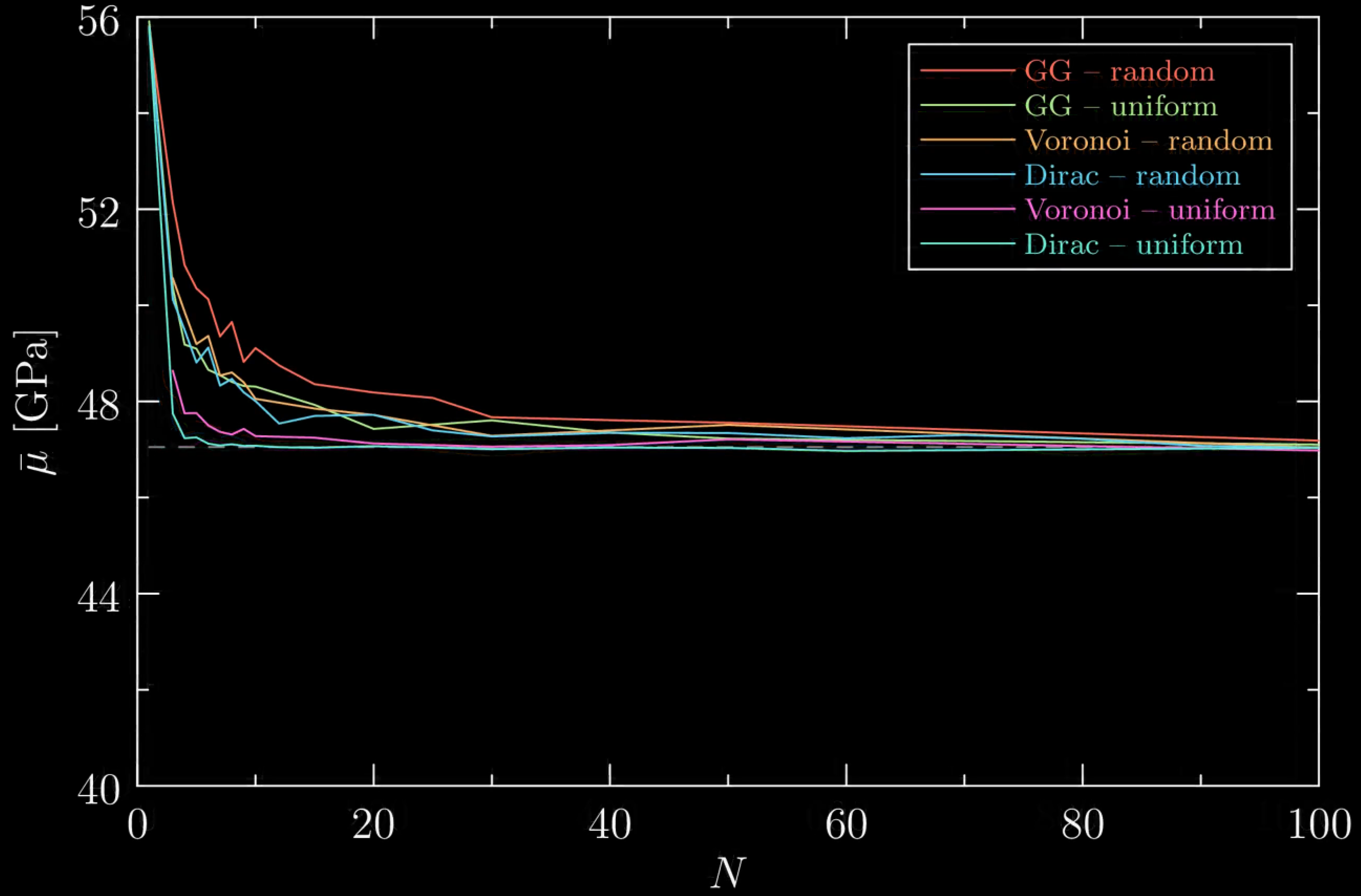
Consider 100s different microstructures to get $\{\mu_1, \mu_2, \mu_3, \ldots\}$

Compute $\bar{\mu}(N)$ and $e_\mu(N)$

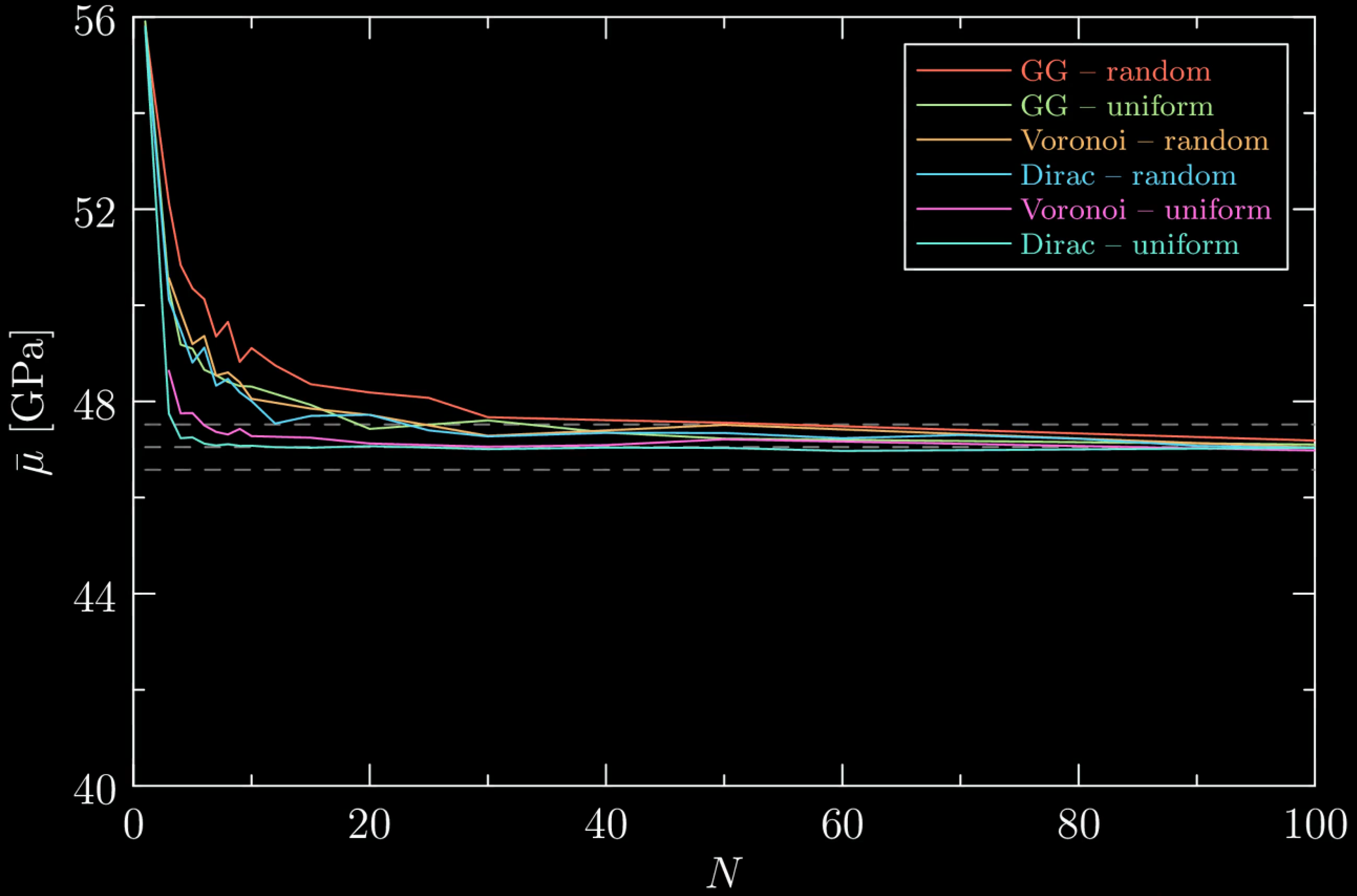

56
52
48
44
40
$\bar{\mu}$ [GPa]
0
200
400
600
800
1000
N
GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform



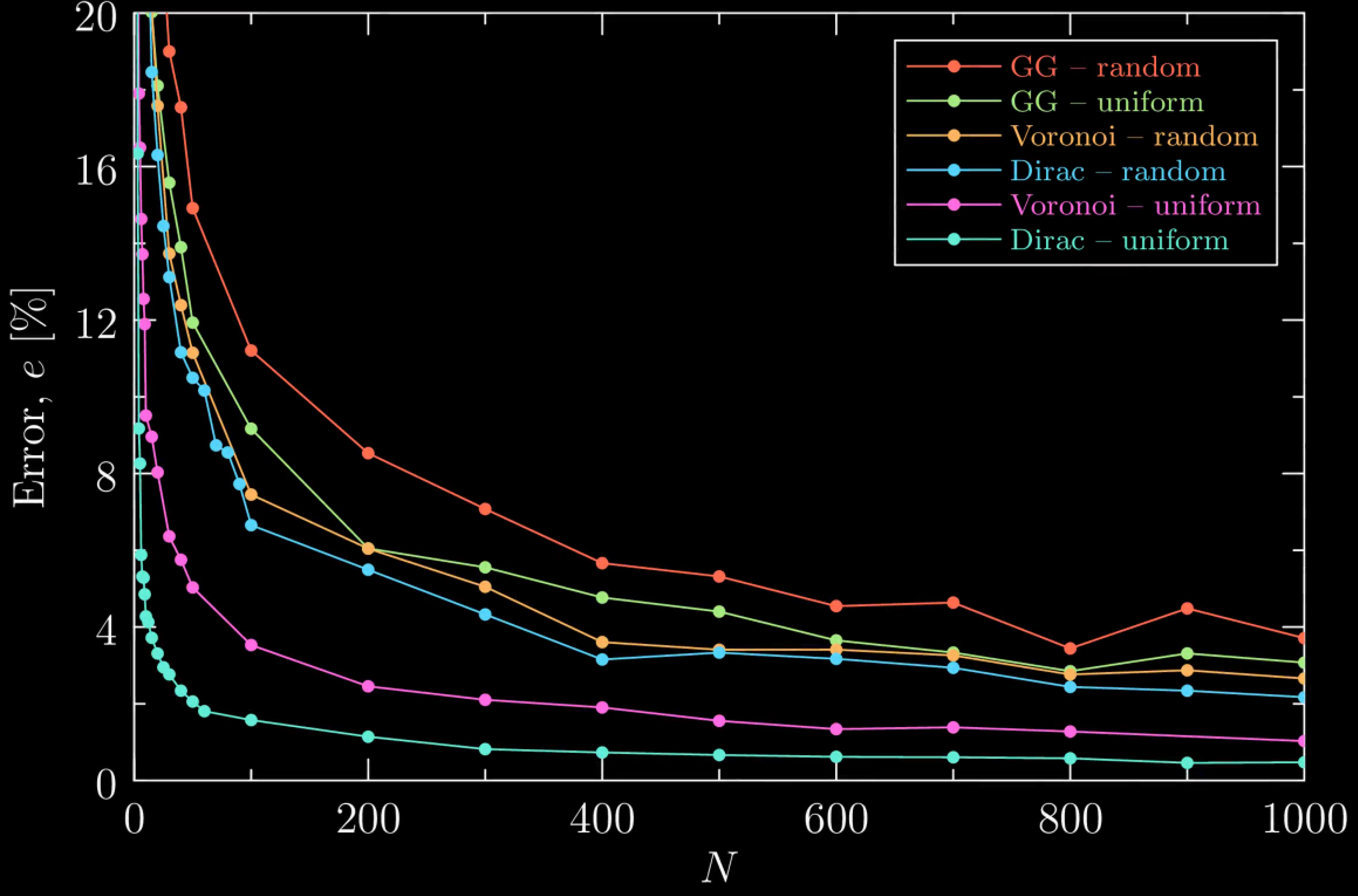
GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform
56
52
48
44
40
0
200
400
600
800
1000
$\bar{\mu}$ [GPa]
N

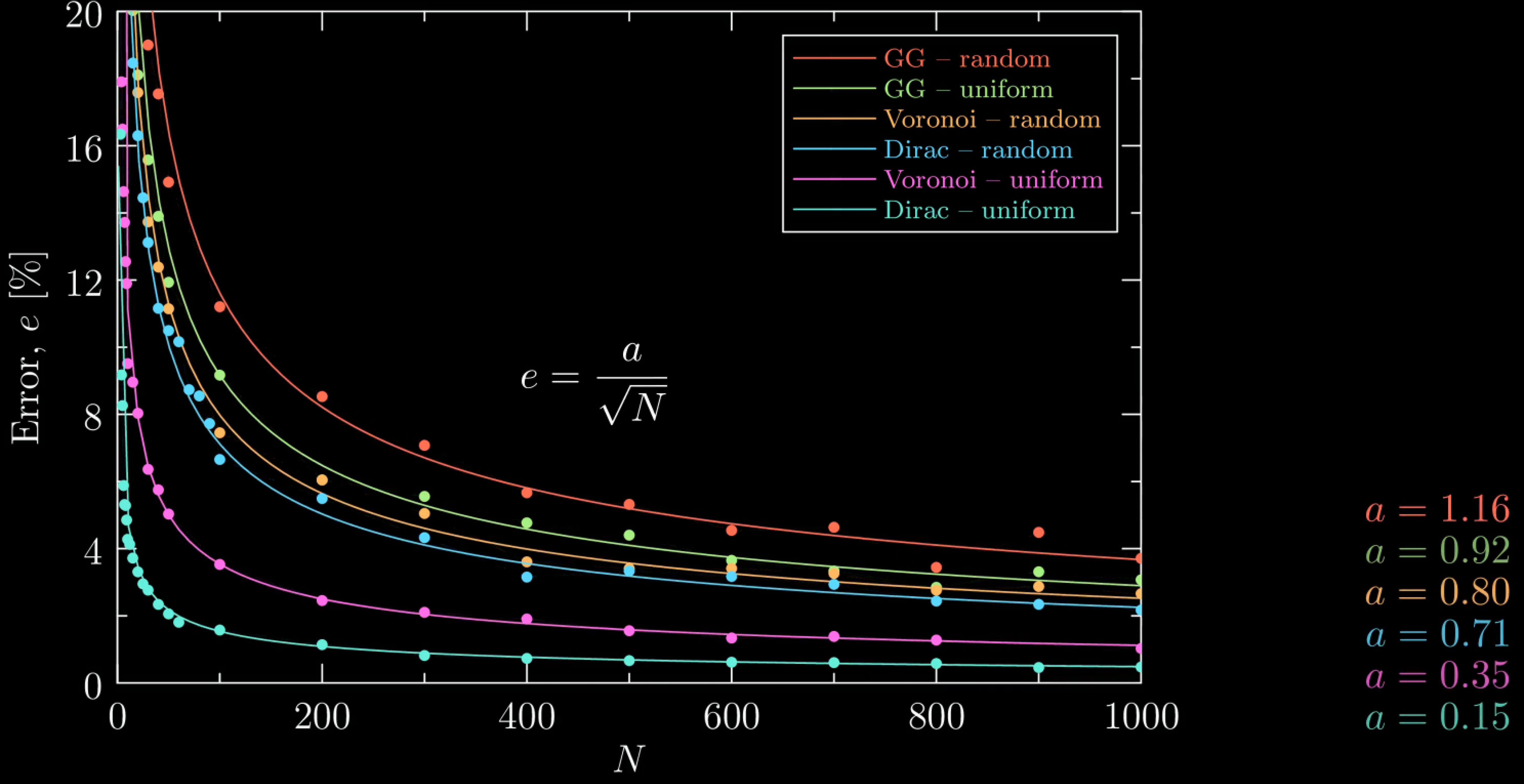


56
52
48
44
40
$\bar{\mu}$ [GPa]
0
20
40
60
80
100
N
GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform



"Gray area" (1%): "Grain-growth – random": $N \leq 50$, "Dirac – uniform": $N \leq 4$(!)


GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform
Error, e [%]
N
0
4
8
12
16
20
0
200
400
600
800
1000



From "Grain-growth – random" to "Dirac – uniform": e divided by 7.7, N divided by $7.7^2 = 60$

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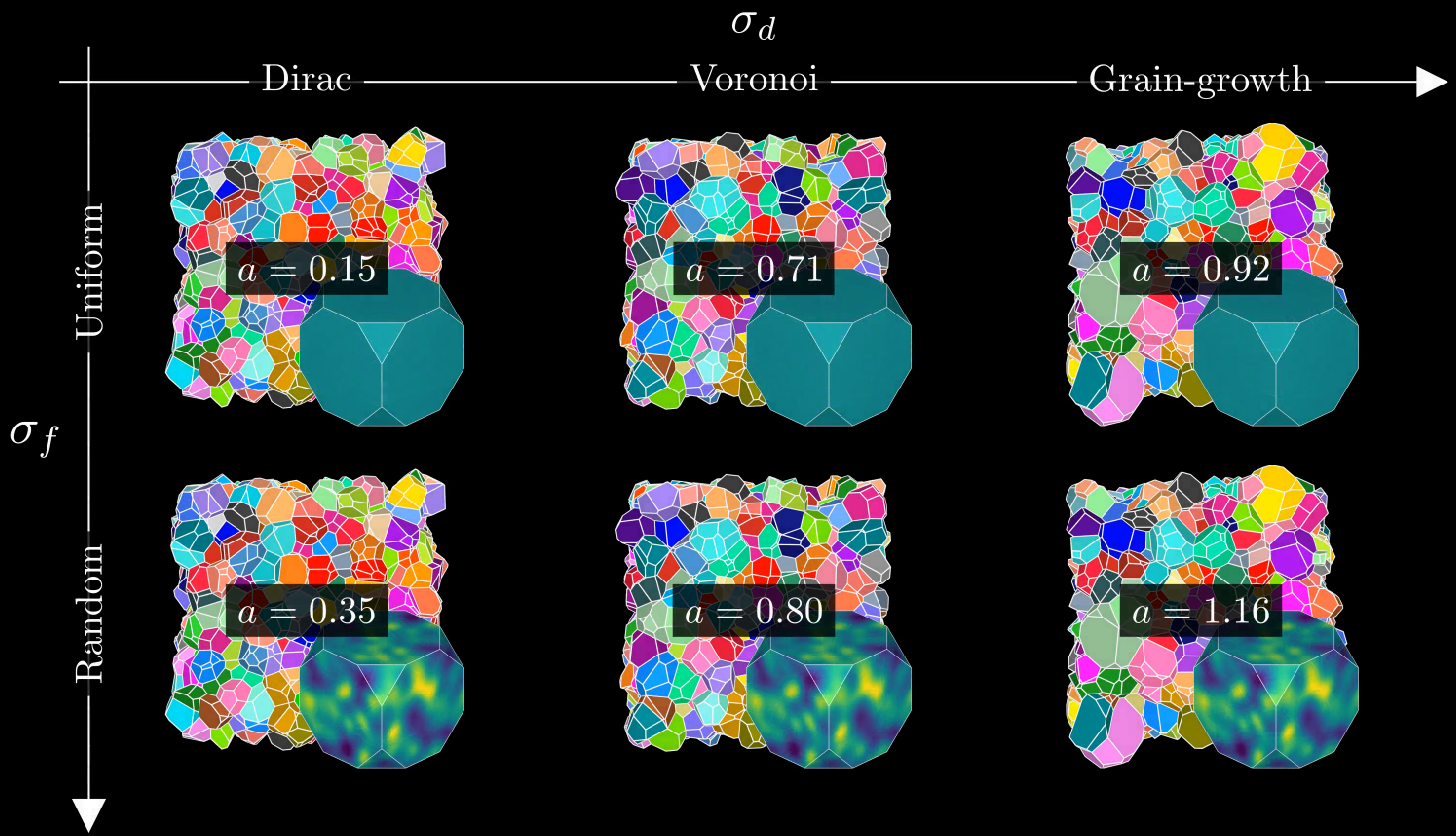
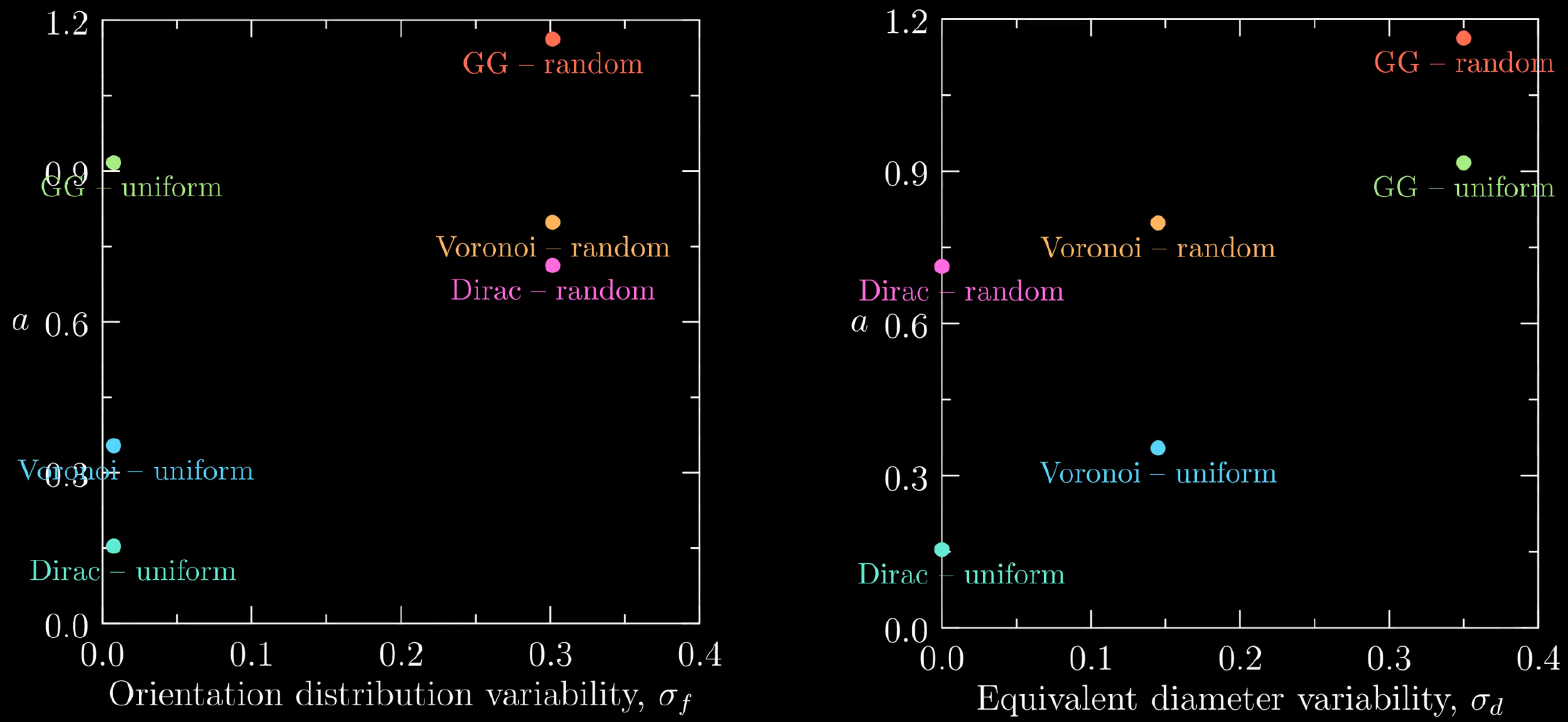
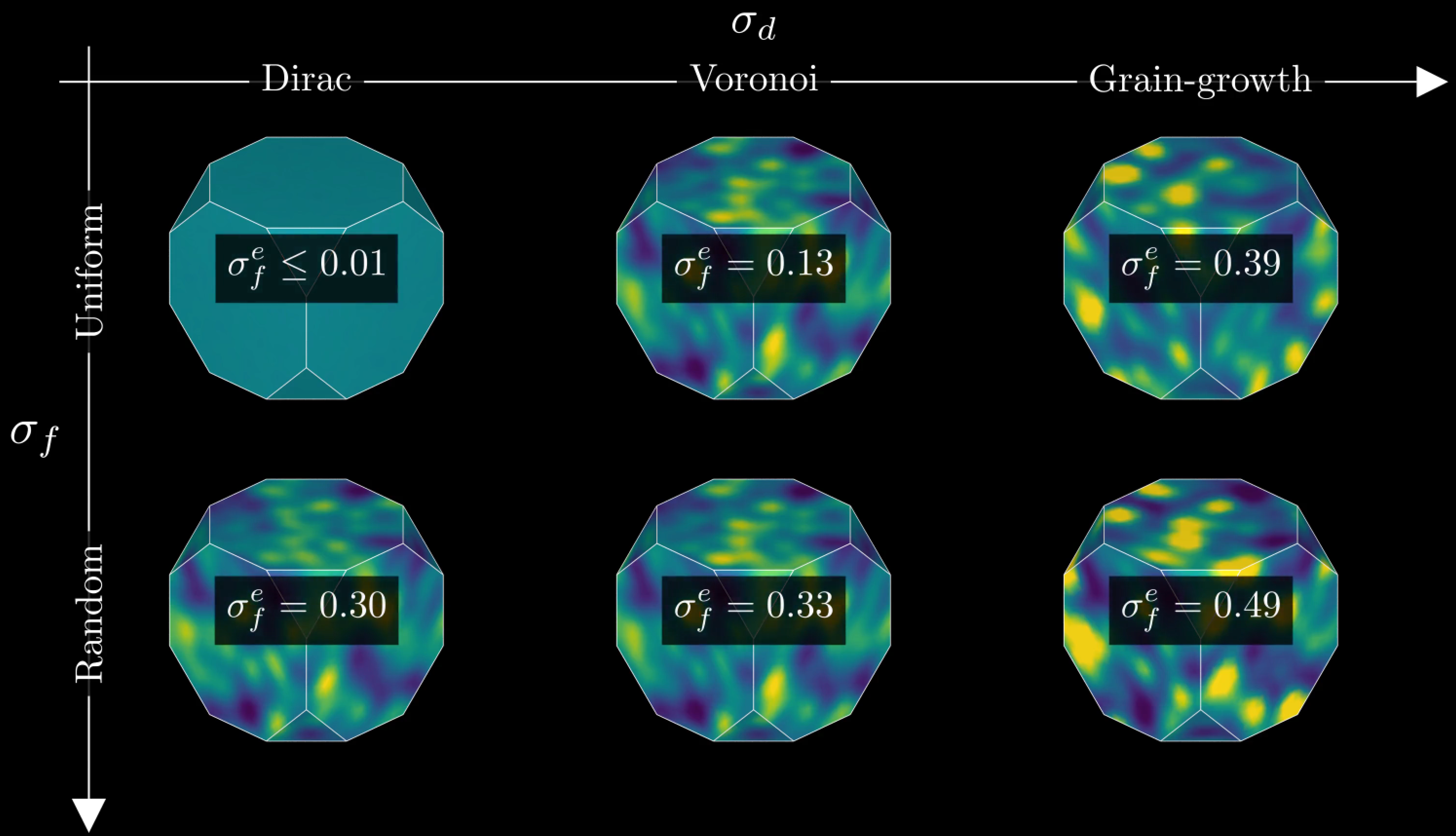
Microstructural Configurations

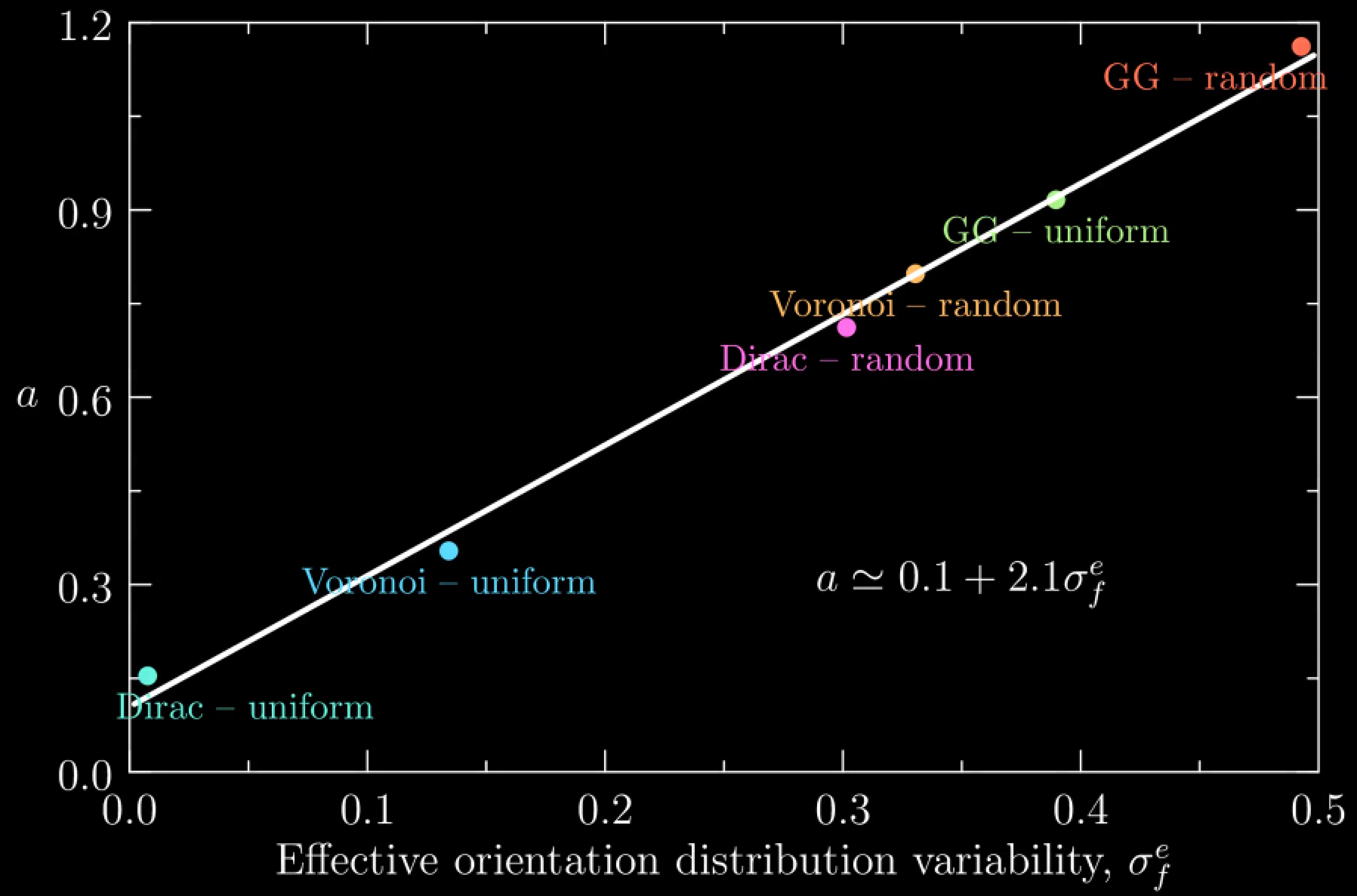



1.2
0.9
0.6
0.3
0.0
a
0.0
0.1
0.2
0.3
0.4
Orientation distribution variability, σ_f
GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform
1.2
0.9
0.6
0.3
0.0
a
0.0
0.1
0.2
0.3
0.4
Equivalent diameter variability, σ_d
GG – random
GG – uniform
Voronoi – random
Dirac – random
Voronoi – uniform
Dirac – uniform

Microstructural Configurations



$$e = \frac{0.1 + 2.1\,\sigma_f^e}{\sqrt{N}}$$



$$\sigma_f^e = \sqrt{{\sigma_f}^2 + f(\sigma_d)^2}$$

σ_f: orientation distribution effect

$f(\sigma_d)$: size distribution effect

	Dirac	Voronoi	Grain-growth
a	0.73	0.79	1.13
$f(\sigma_d)$	0.00 (0%)	0.13 (13%)	0.39 (57%)
σ_f	0.30 (86%)	0.30 (74%)	0.30 (33%)
constant	0.10 (14%)	0.10 (13%)	0.10 (10%)

Conclusions (for Copper / Grain-growth)

- "Uniformized" polycrystals can be used ($\bar{\mu}^{uni} \simeq \bar{\mu}^{exp}$)

  1% deviation on μ for $N \leq 50$ for "experimental" vs $N \leq 4$ for "uniformized"

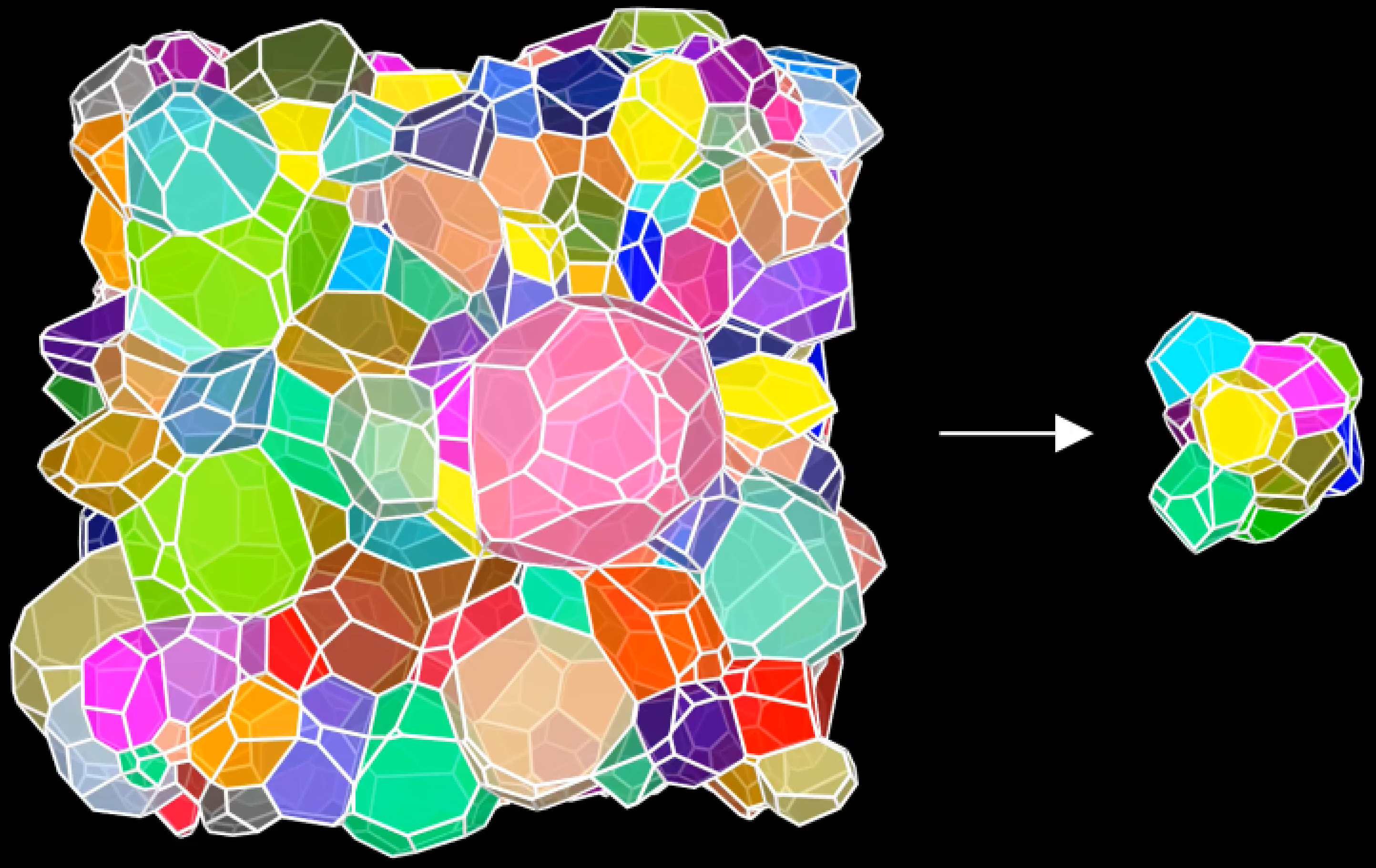
  (for PBCs, deviation related to the uniformity rather than the size)

- Error (e_μ) divided by 7.7, RVE size divided by 60

- Error (e_μ) related to N, σ_d and σ_f by

$$e_\mu = \frac{0.1 + 2.1\,\sigma_f^e}{\sqrt{N}}$$

$$e_\mu = \frac{f_1(C_{ij}) + f_2(C_{ij})\,\sigma_f^e}{\sqrt{N}}$$



$e_\mu = 2\%$