GM3 2021

A DEM Study on the Effect of Inherent Variability in Assemblies of Spherical Particles

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Sample size & variability in DEM

Barreto & O'Sullivan (2012)…

Undertook parametric simulations of 2000, 4000 & 8000 particles showed identical macroscale results…

But…different microscale results between 2000 compared with 4000 & 8000 particles…

Professor Catherine O'Sullivan

Dr Daniel Barreto

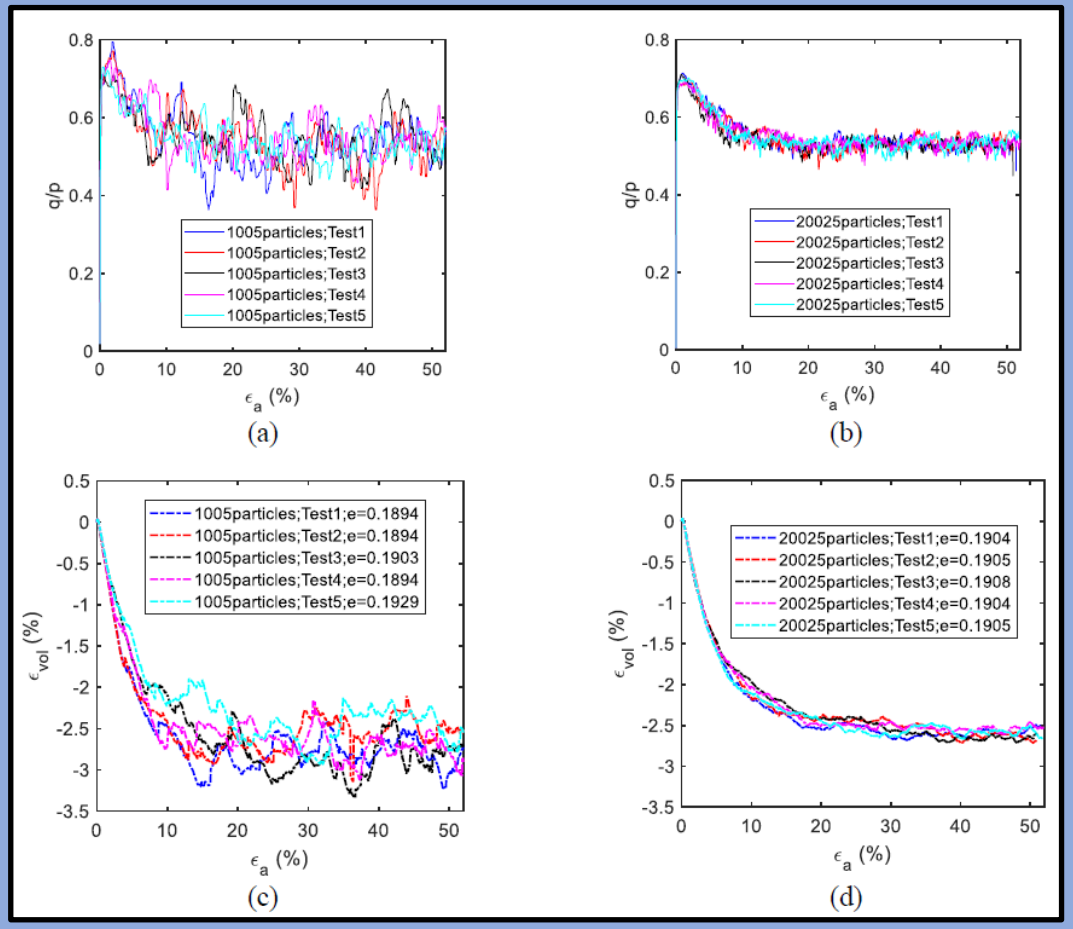
''…fabric revealed differences of up to 31 % between the assemblies with 2,000 particles and the other two specimen sizes….the good agreement in the response of the specimens containing 4,000 and 8,000 spheres meant that simulations of 4,000 particles were used to obtain valid results…''

– Barreto & O'Sullivan (2012)

Sample size & variability in DEM

Adesina et al., (2021) explored variability in 2D DEM simulations with increasing particle count…

Suggesting that a reduction in variability with increasing particle count may a useful metric when determining an appropriate RVE



a) Variation in q/p of 5 simulations of 1005 particles **b**) variation in q/p if 5 tests with 20025 particles **c)** variation in volumetric strain for 5 tests of 1005 particles **d)** variation in volumetric strain for simulations of 20025 particles

Discrete element method & Variability

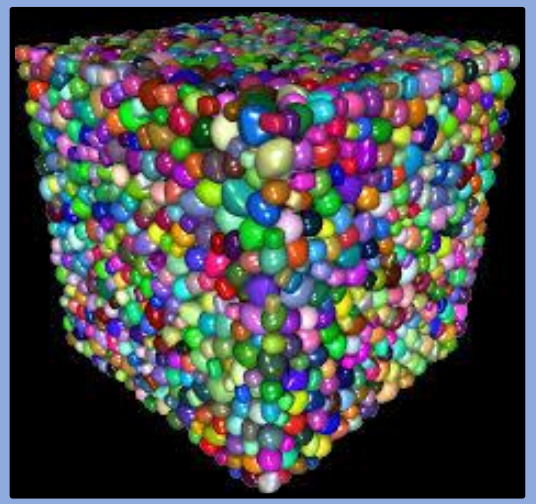
Simulations of 2000 particles (for example) are variable and not ideal RVEs

but are less computationally demanding…

Can we get reliable quantitative measures if we increased the number of simulations?

Is there changes in variation?

If so, how many simulations do we need to perform to reduce variability for different PSDs?



a) Triaxial apparatus used for physical testing can be recreated numerically in DEM **b)** Soil samples are numerically recreated in DEM and drained or undrained tests are undertaken

Description of simulations

- The open source DEM software YADE was used for all simulations
- Spherical particles were generated in a cubical container with periodic boundaries
- Particles were brought into contact through isotropic compression to a confining pressure of 200kPa
- During isotropic compression, boundaries were moved towards the centre of the sample at a constant rate

Confining Stress	200 kPa
Poisson's ratio (ν)	0.22
Particle density (ρ)	2650Kg/m^3
Max strain rate ()	1.e+1
Inter-particle friction (μ)	26.6
Youngs Modulus	70 GPa
Fraction of critical time-step	0.5
Unbalanced force ratio criterion	0.0001

Simulation inventory

Number of Particles	PSD range (mm)	Number of Simulations
500	0.5 - 2	160
1000	0.5 - 2	160
2000	0.5 - 2	160
5000	0.5 - 2	160
8000	0.5 - 2	160

Simulation inventory

Number of Particles	PSD range (mm)	Number of Simulations
500	1 - 2	300
1000	1 - 2	300
2000	1 - 2	300
3000	1 - 2	300
4000	1 - 2	300
5000	1 – 2	300
8000	1 - 2	300
9000	1 - 2	300
10000	1 - 2	300

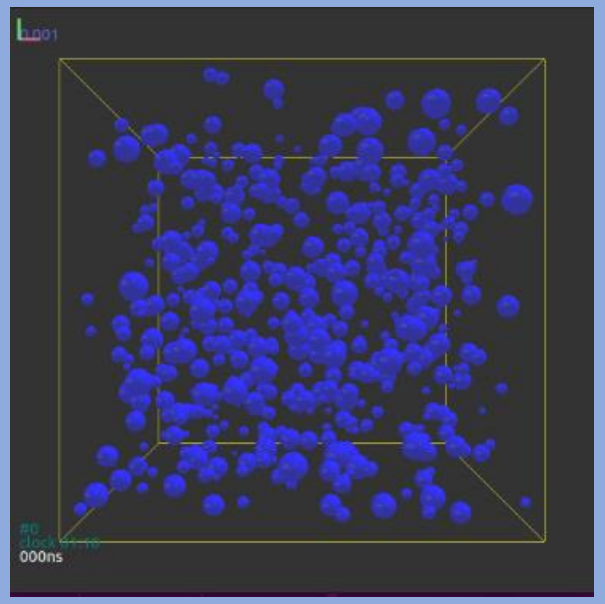
Variability in sample generation

Randomly generated particles may show significant variability over a small number of simulations…

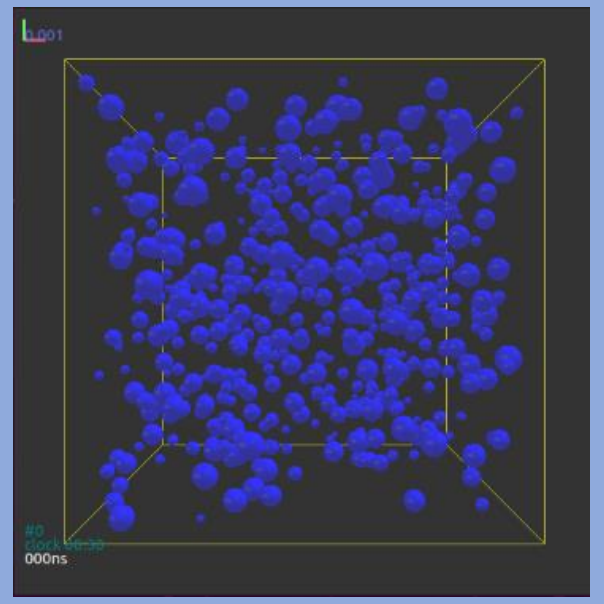
For example randomly generated particles under identical conditions…

Tests 1, 2, 3 & 4…

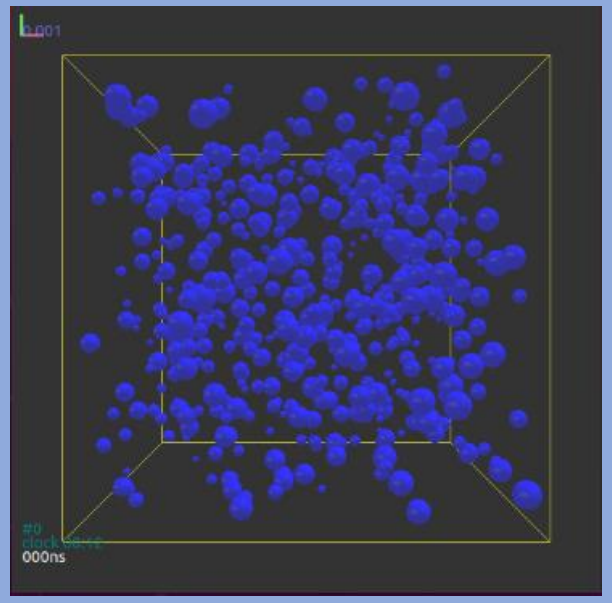
Screenshots of randomly generated particles of identical simulations of 500 particles between 0.5mm - 2mm



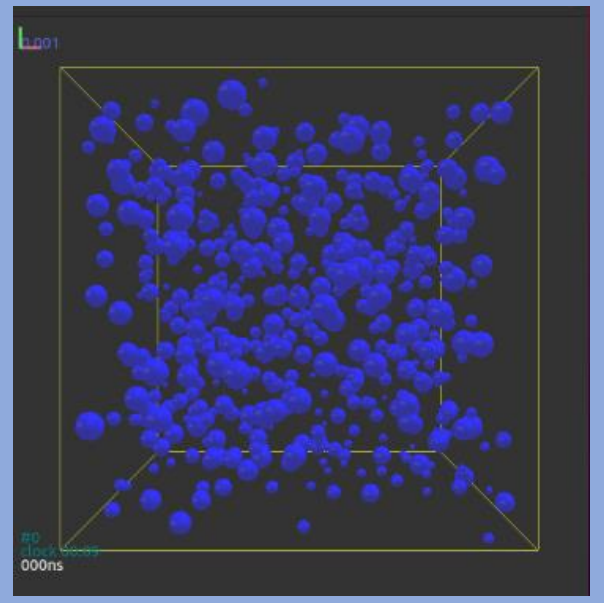
Test 1: 500 particles



Test 2: 500 particles



Test 3: 500 particles



Test 4: 500 particles

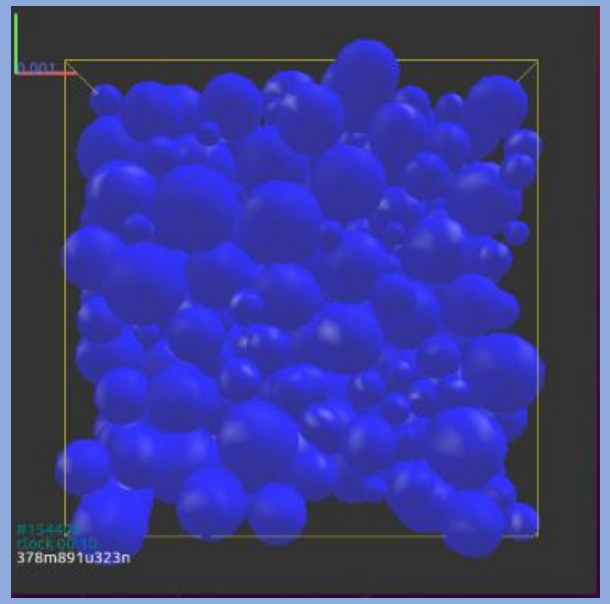
Variability in sample post isotropic compression

The variability in geometry during sample generation effect initial packing and void ratio…

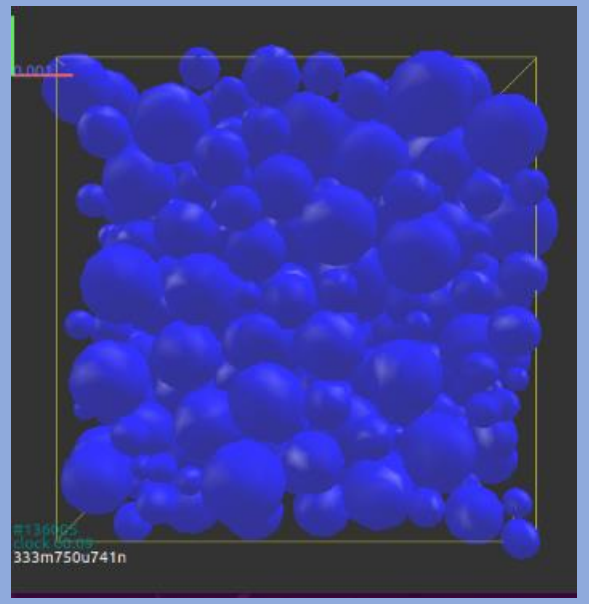
Leading to variation in parameters post isotropic compression…

Tests 1, 2, 3, 4:

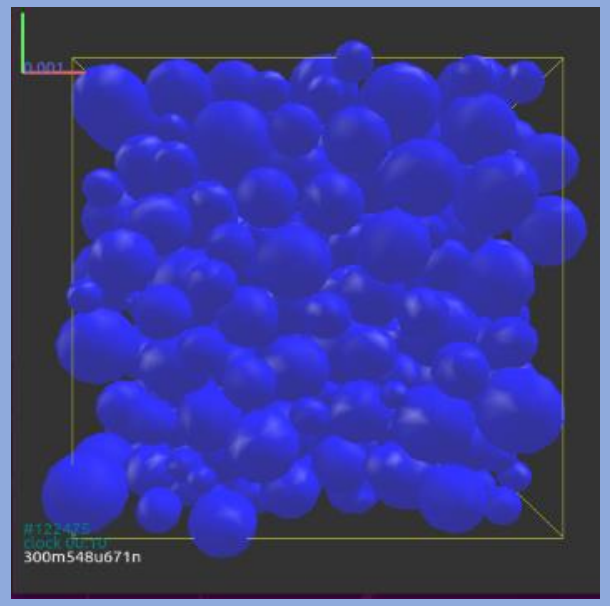
Screenshots of tests post-isotropic compression and before shear for identical simulations of 500 particles between 0.5mm - 2mm



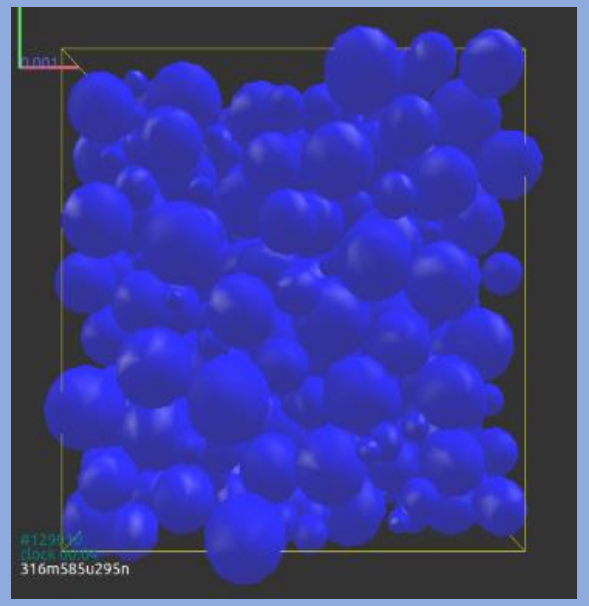
Test 1: 500 particles



Test 2: 500 particles

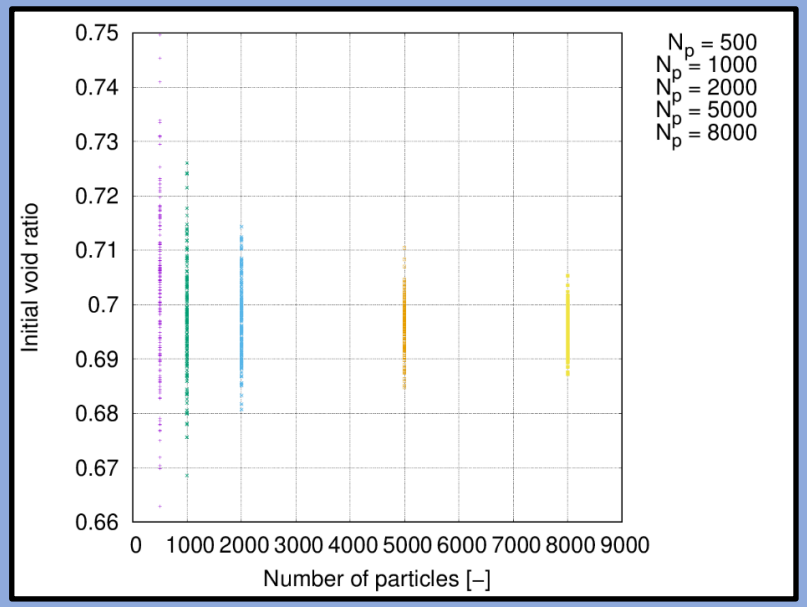


Test 3: 500 particles

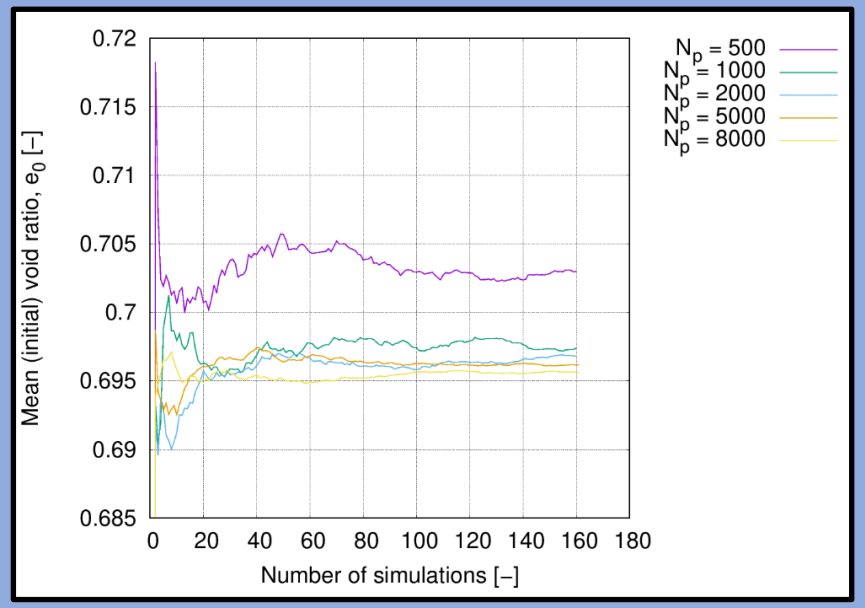


Test 4: 500 particles

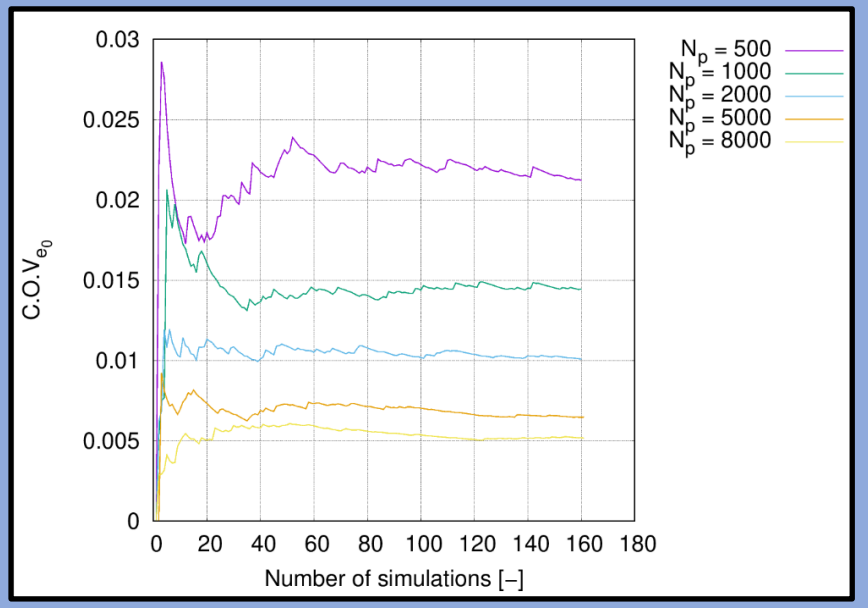
Results-Variability in initial void ratio (0.5mm - 2mm)



a)



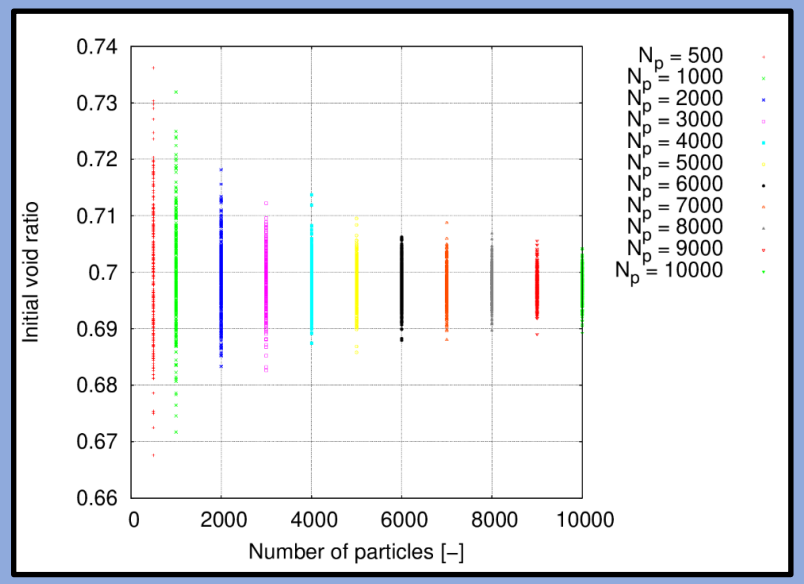
b)



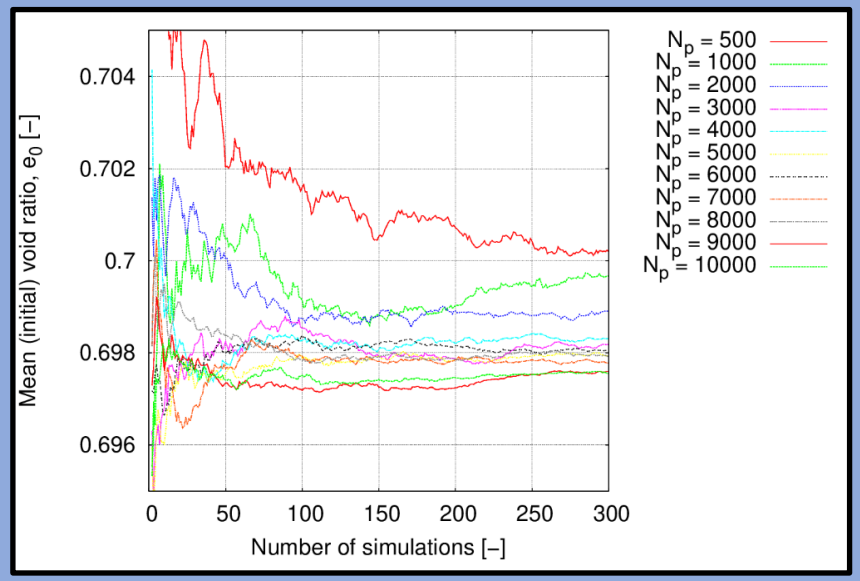
c)

a) Initial void ratio **b)** Mean (initial) void ratio **c)** Coefficient of variation for initial void ratio

Results-Variability in initial void ratio (1mm - 2mm)



a)



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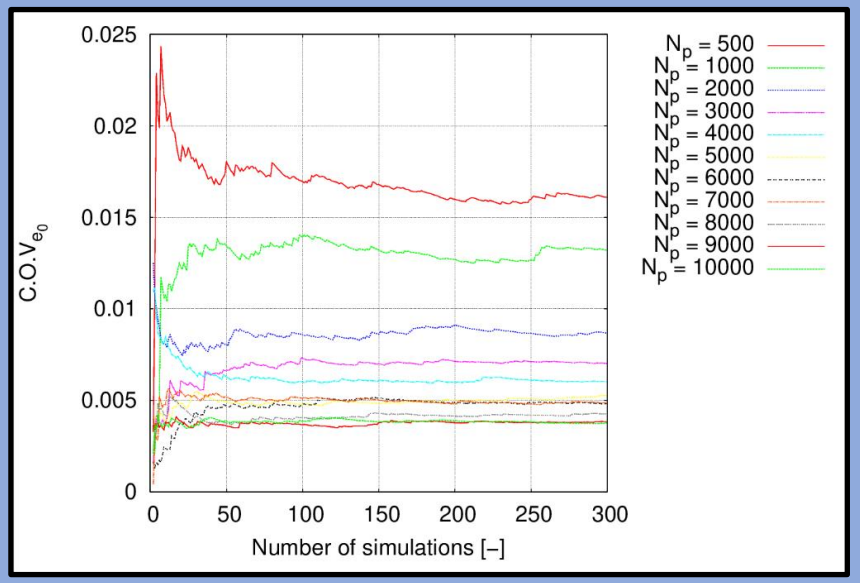
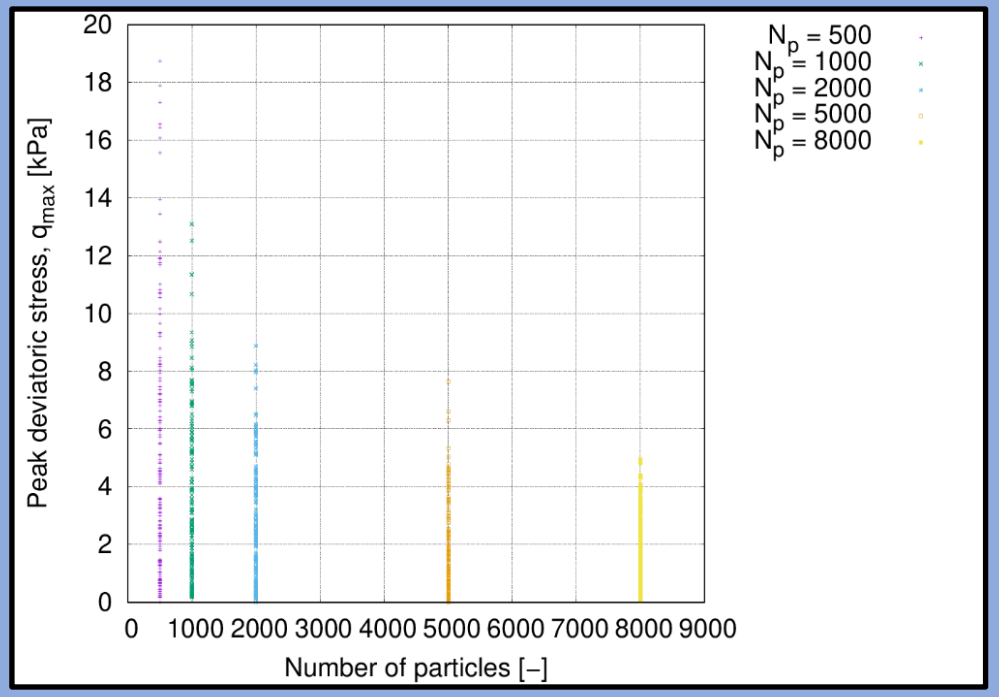
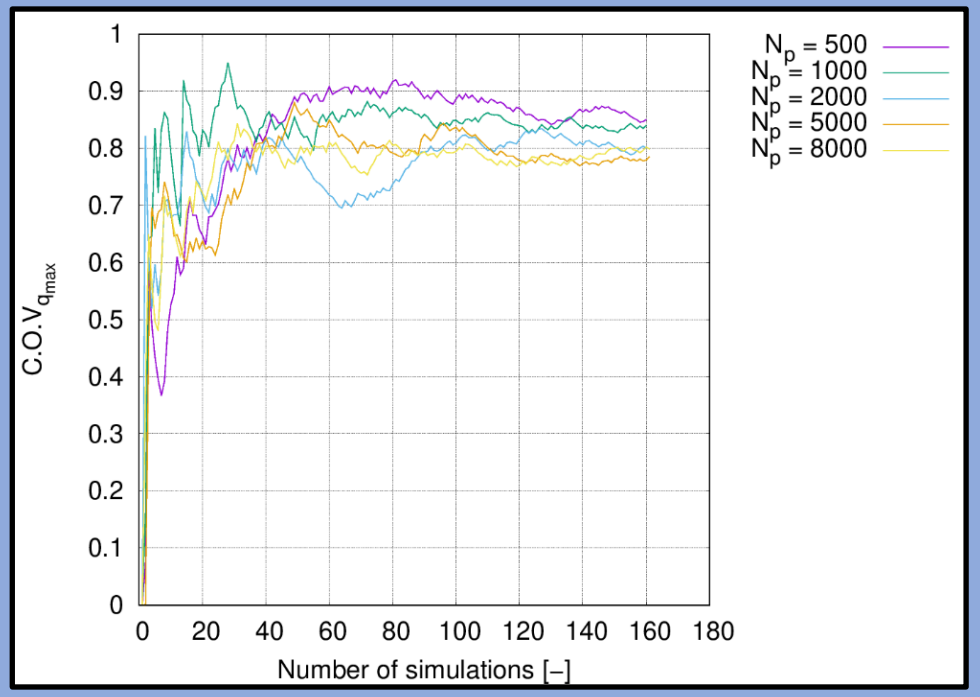


c)

Results-variability in peak deviatoric stress (0.5mm – 2mm)

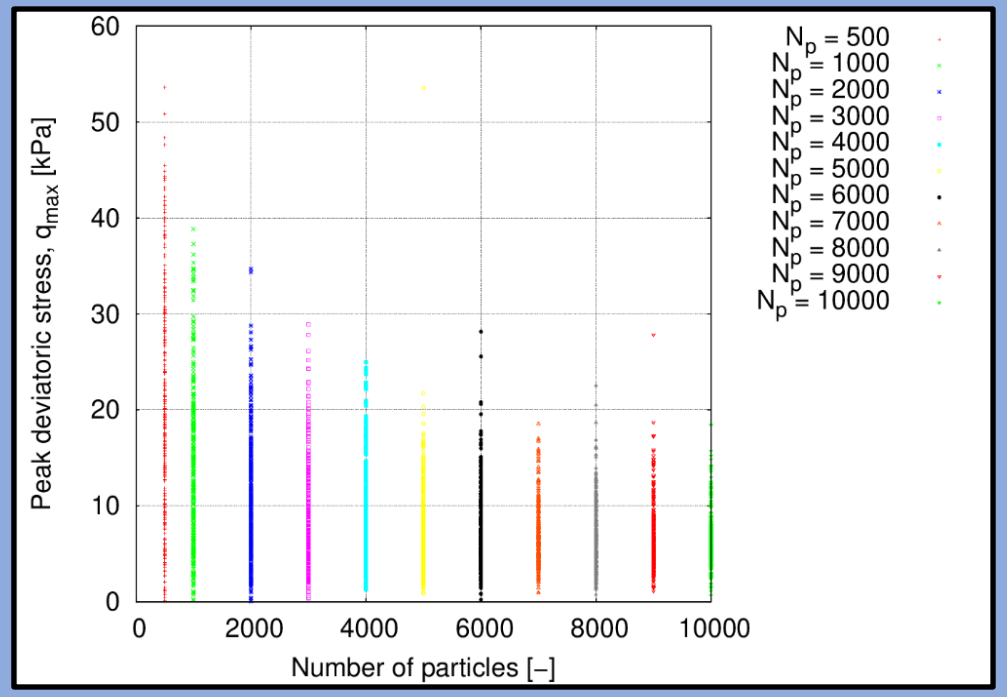


a)

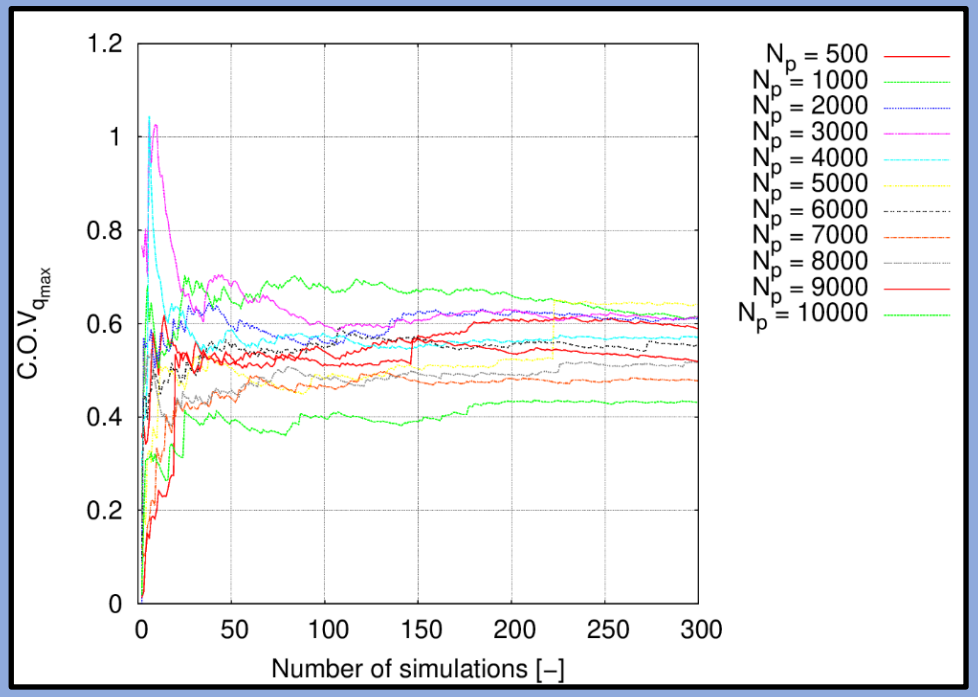


b)

Results-variability in peak deviatoric stress (1mm – 2mm)

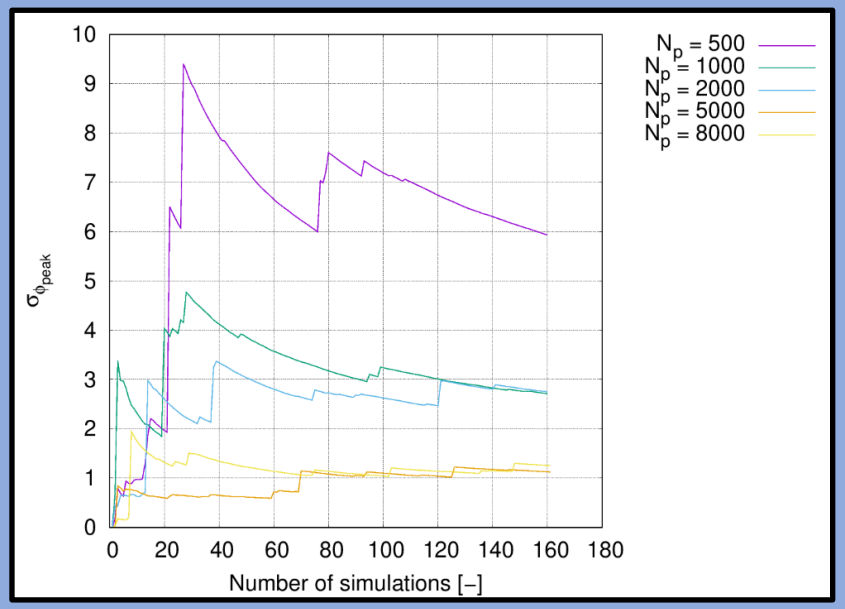


a)

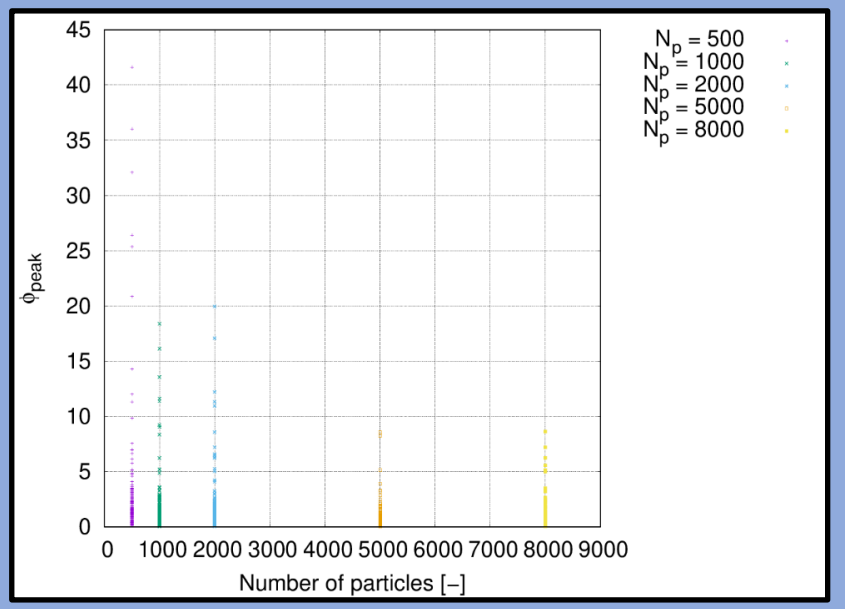


b)

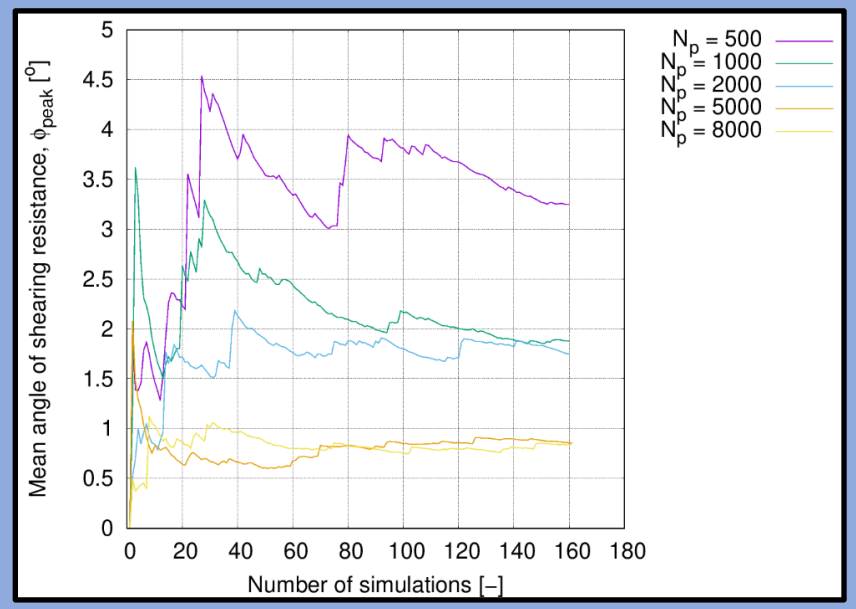
Results-variability in angle of shearing resistance (0.5mm – 2mm)



a)

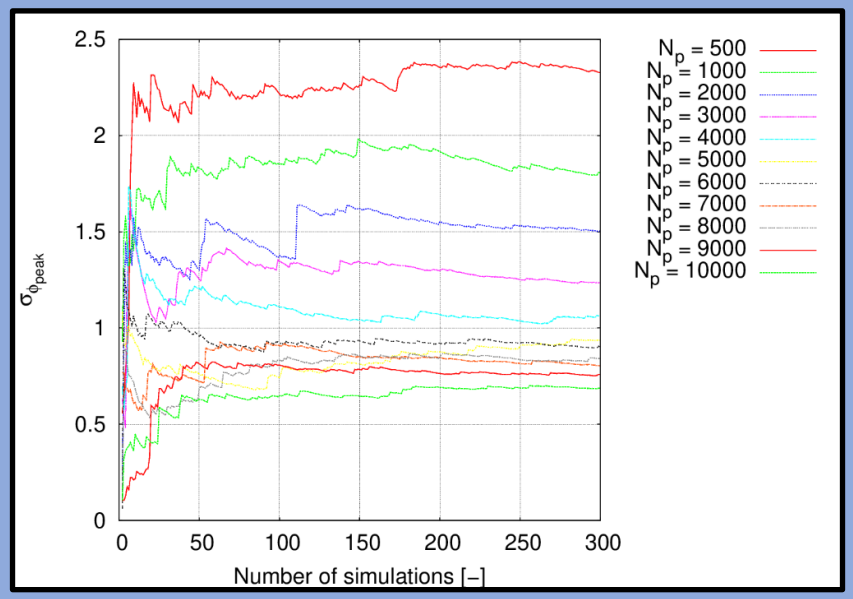


b)

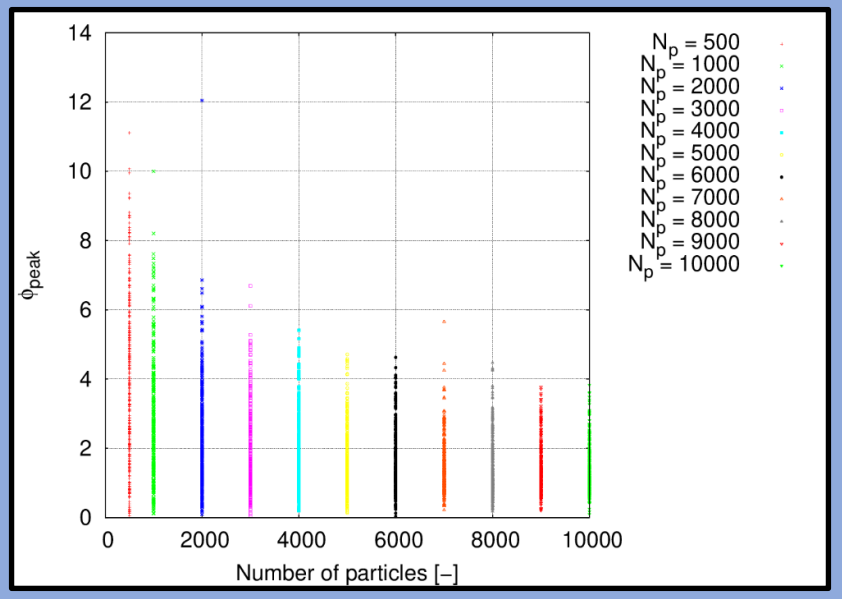


c)

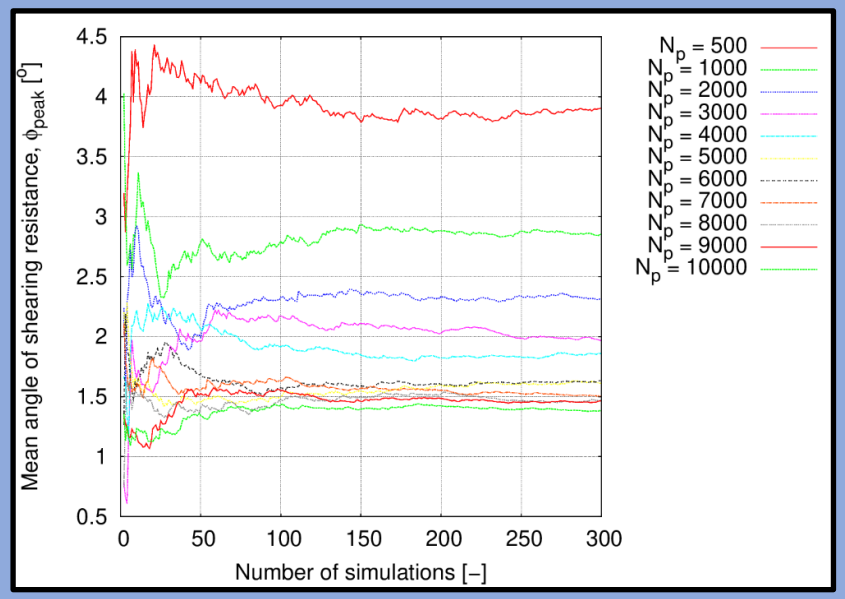
Results-variability in angle of shearing resistance (1mm – 2mm)



a)



b)



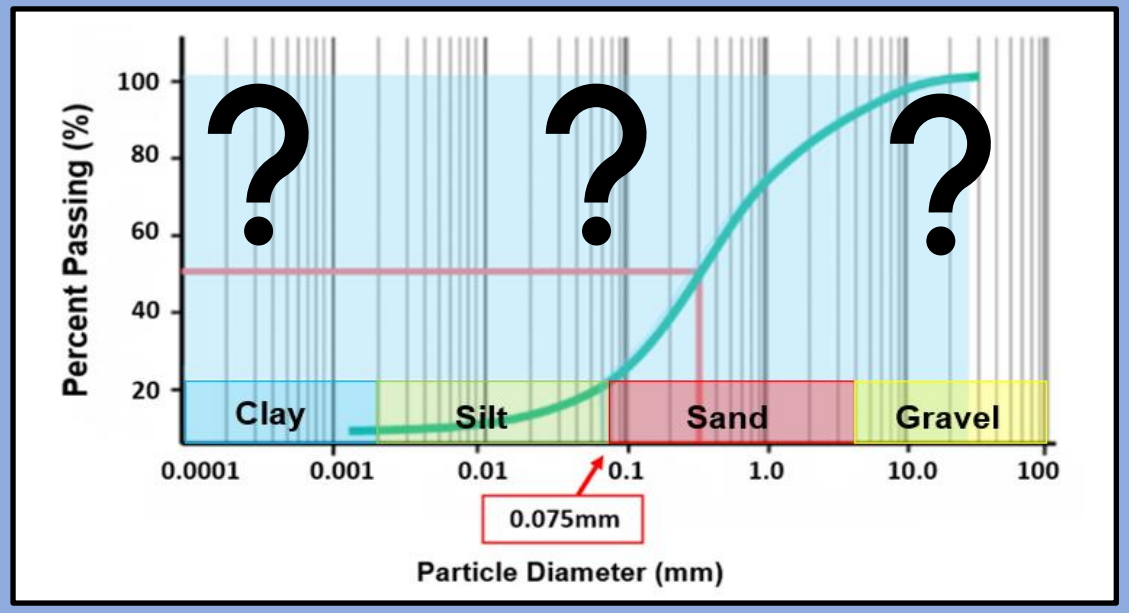
c)

Effects of PSD?

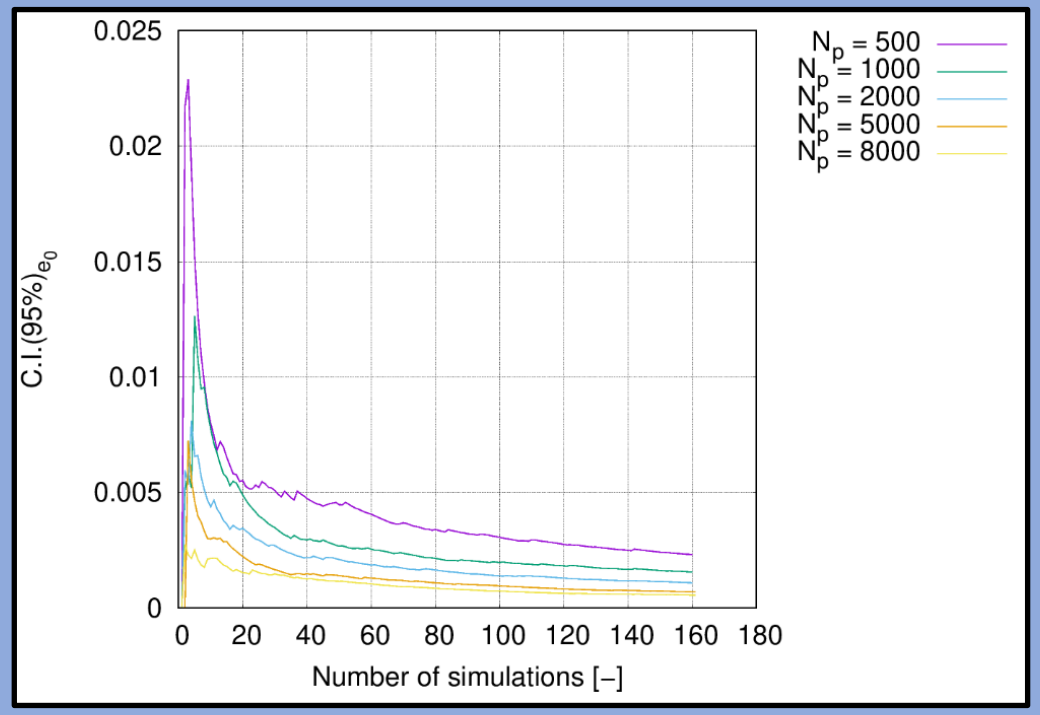
Like increasing particle count…

Increasing the PSD reduces the variability…

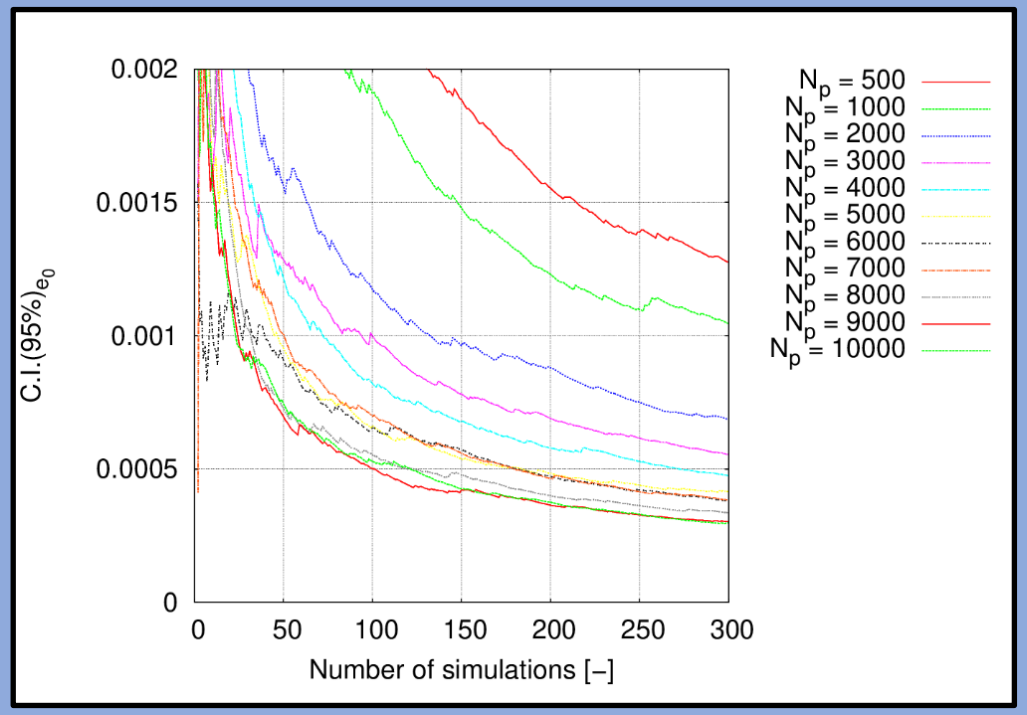
Simulations of 1mm – 2 mm show later ‘convergence’ than simulations of 0.5mm – 2mm…



Results-variability & PSD confidence interval (95%)

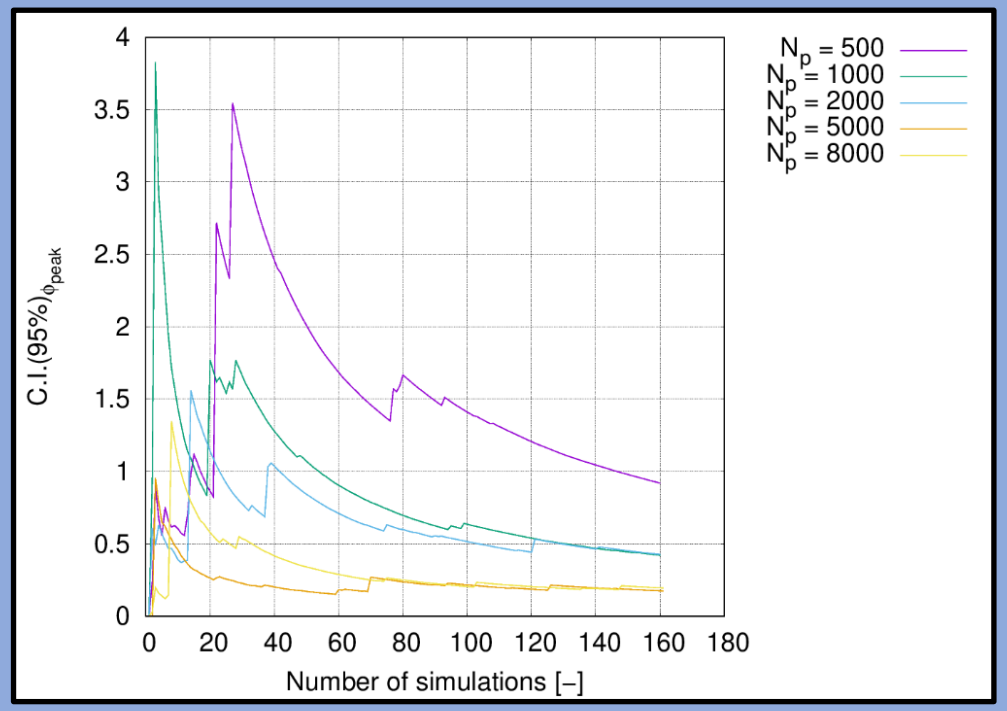


a)

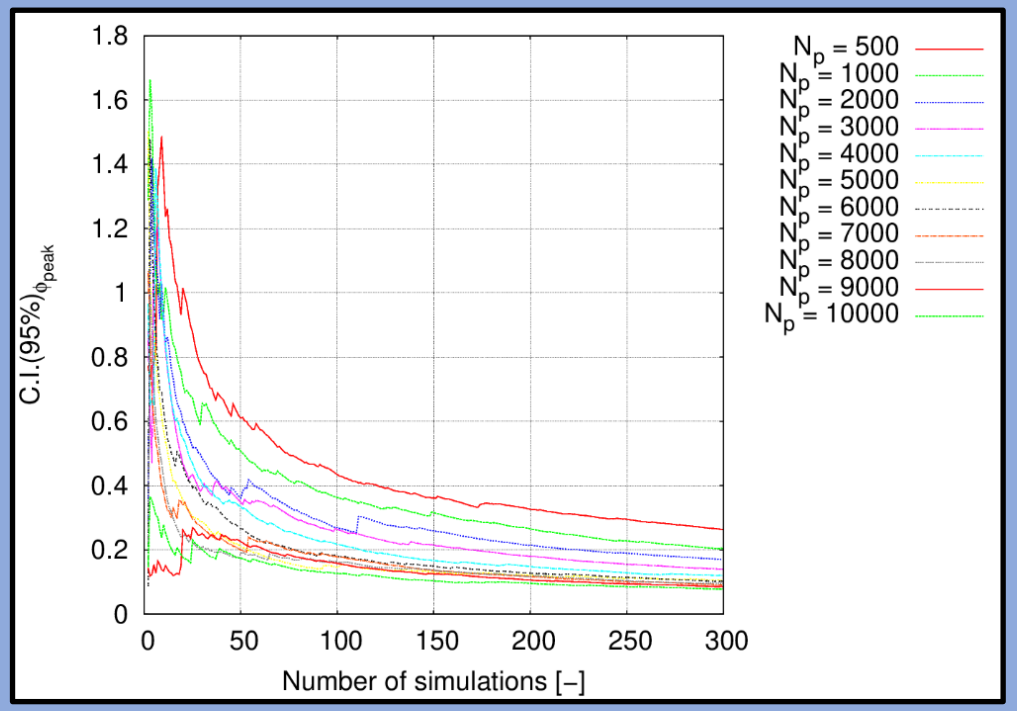


b)

Results-variability & PSD confidence interval (95%)



a)



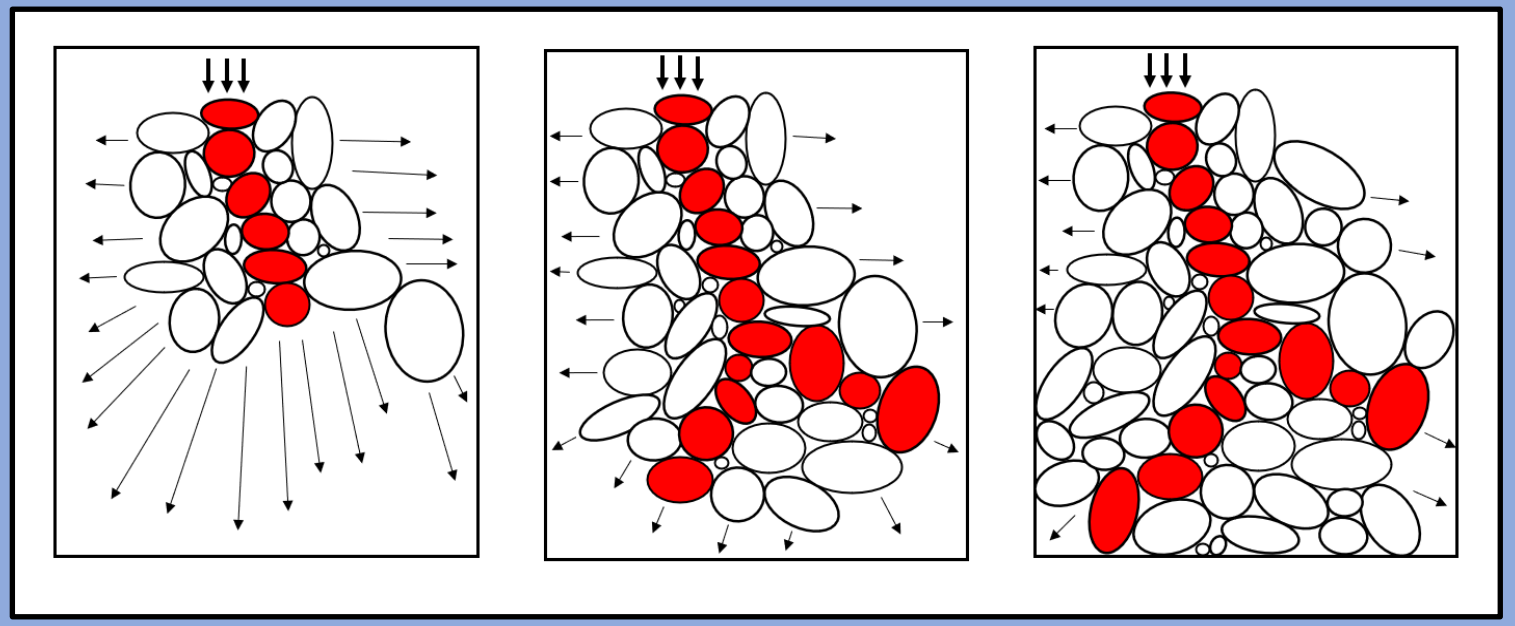
b)

Increasing particle count & decreasing variability

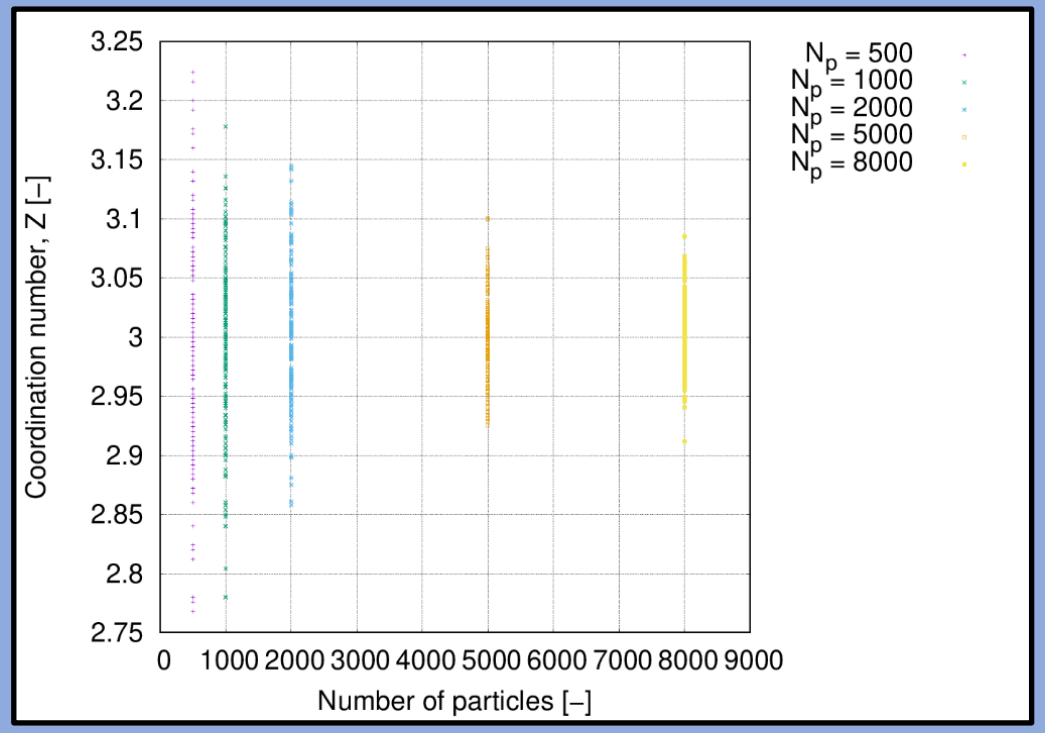
As PSD increases variability decreases…

Simulations with lower particle count and smaller PSDs may enable greater ‘movement’ within the sample…

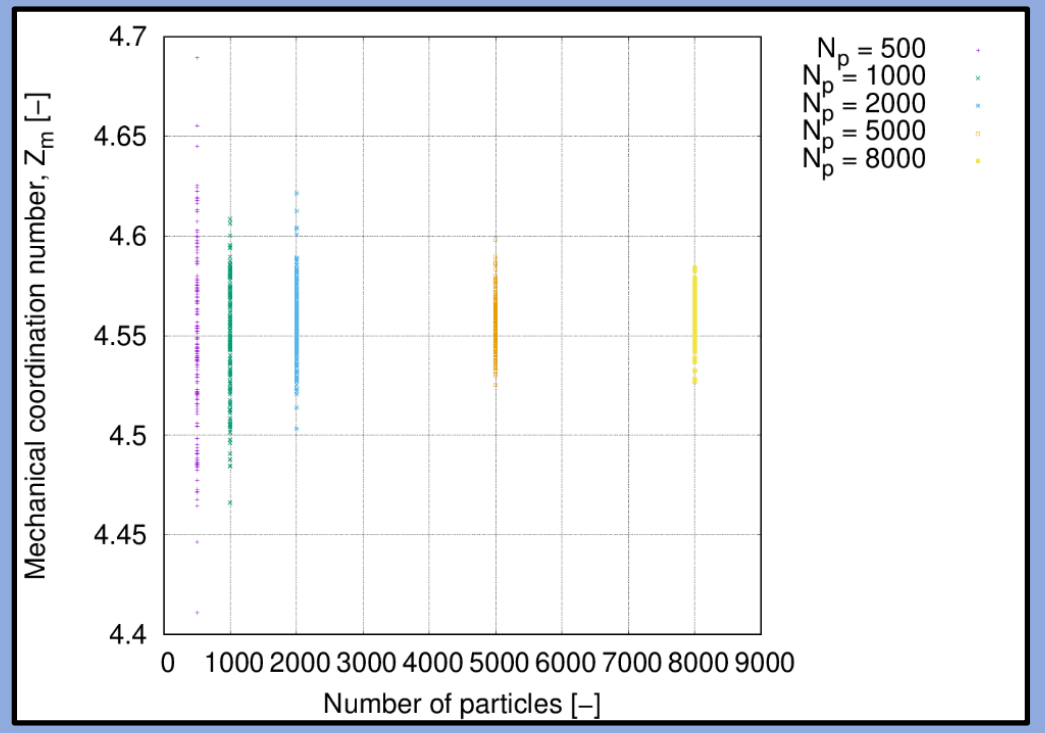
Samples with larger particle counts and PSD’s likely limits the amount of movement under deformation..



Results-variability in coordination numbers (0.5mm – 2mm)

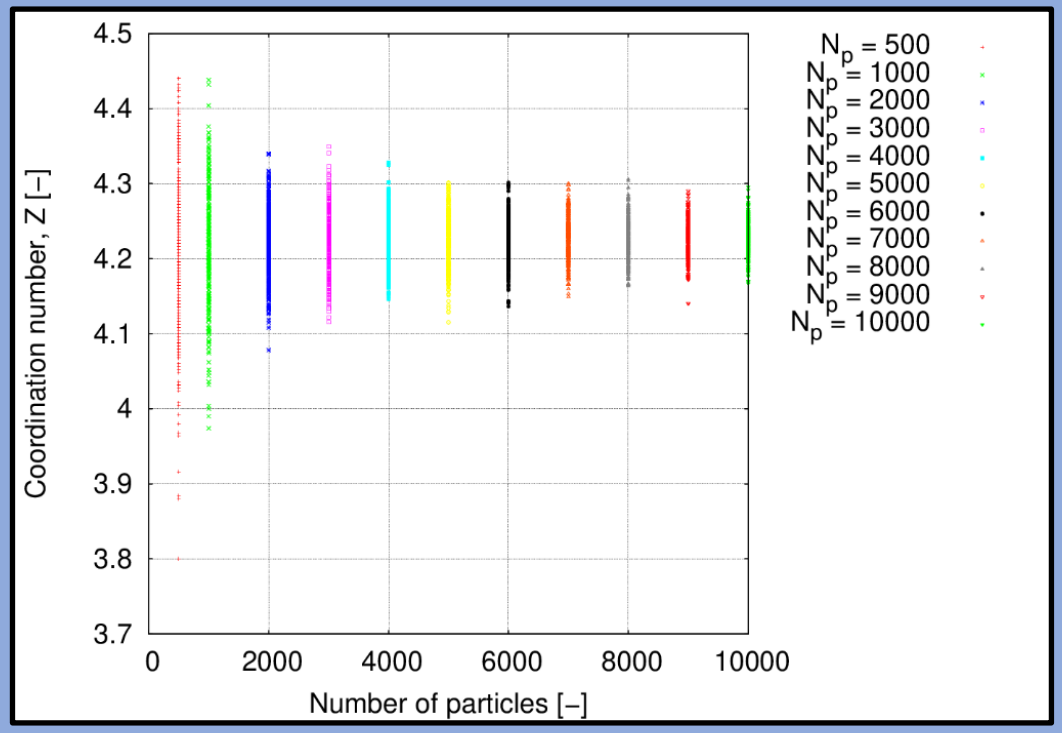


a)

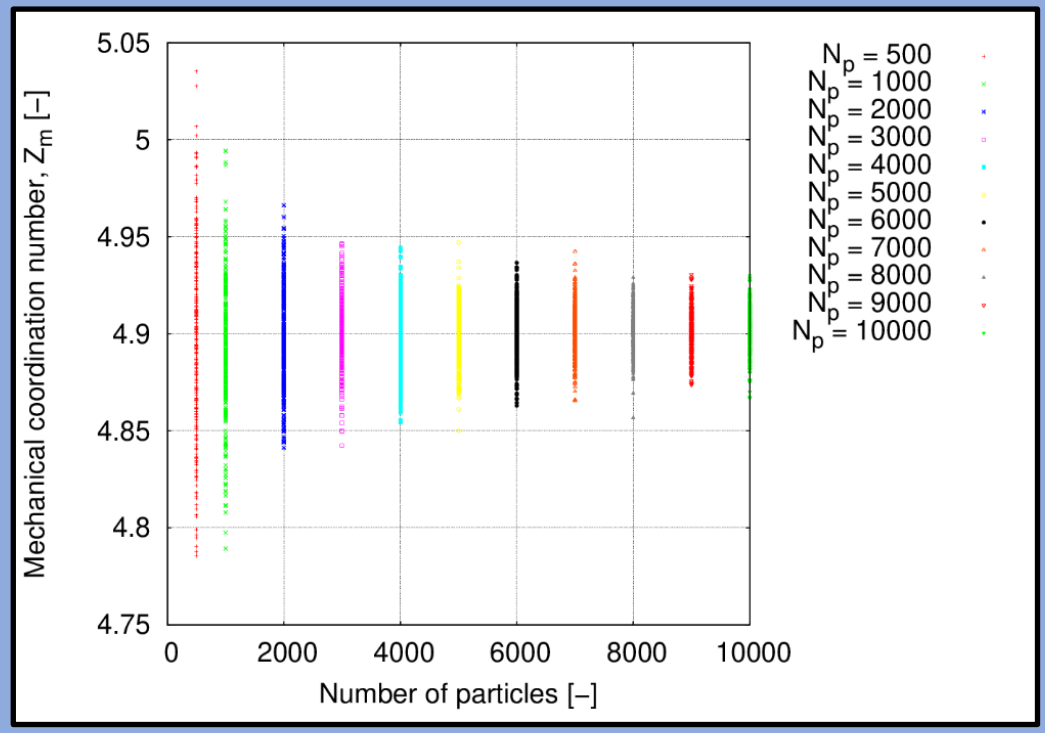


b)

Results-variability in coordination numbers (1mm – 2mm)

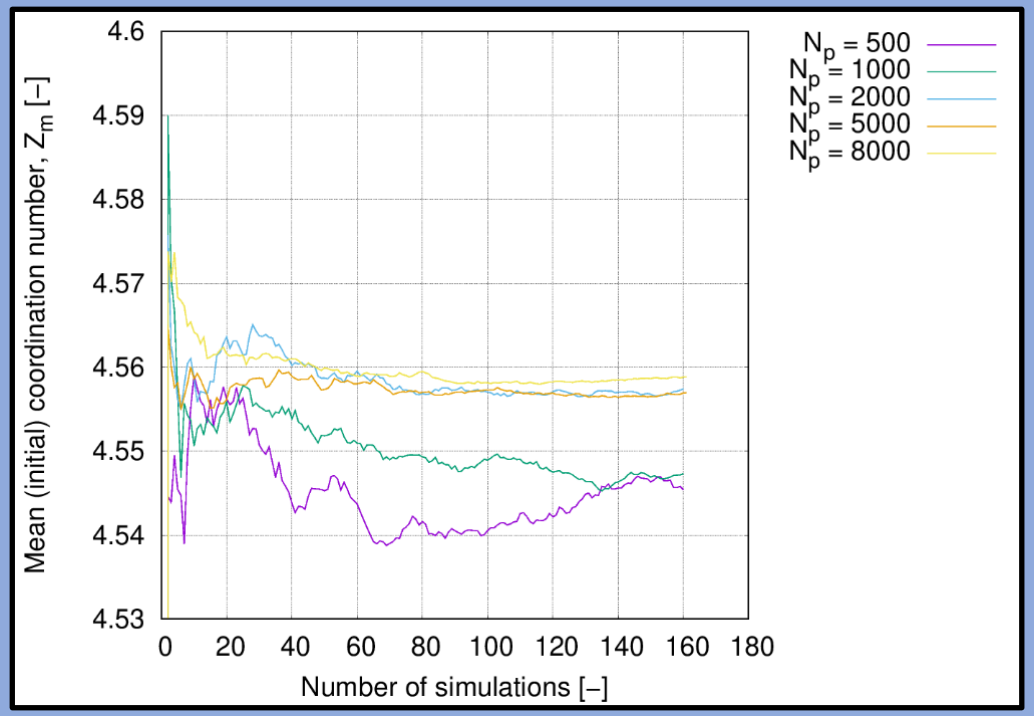


a)

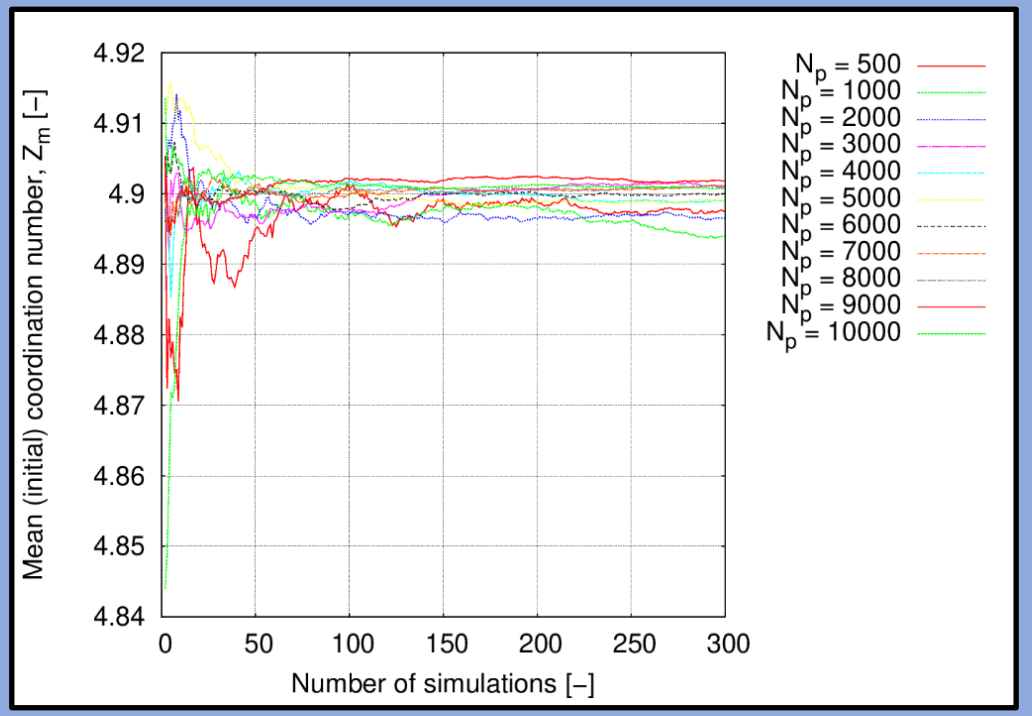


b)

Results-variability in coordination numbers



a)



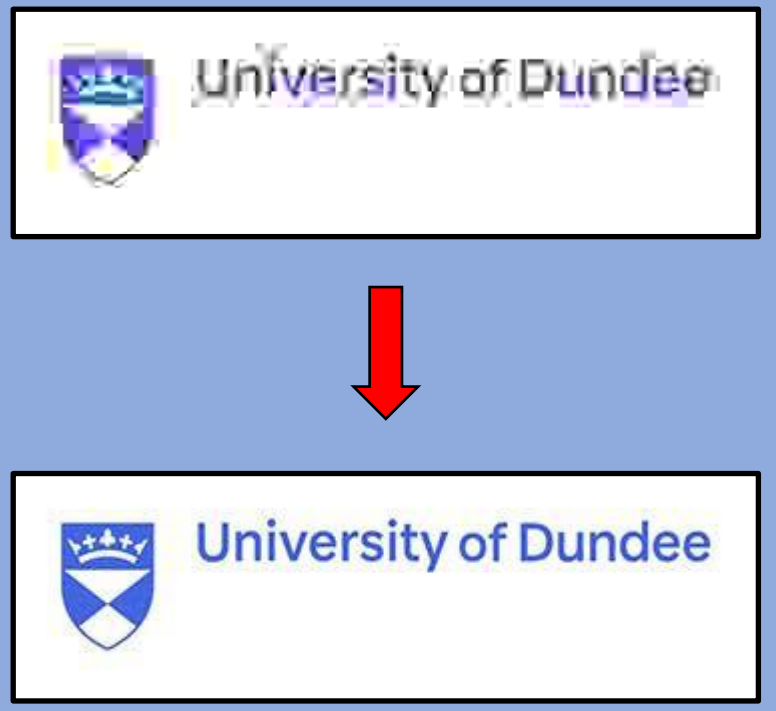
b)

Variability & number of simulations

A small number of repeated tests may only give us part of the ‘’answer’’…

Variability may be a result of a lack in statistical homogeneity in the random sample distribution…

Increasing the number of simulations may decreases the heterogeneity



a) A limited number of pixels creates low resolution, similarly a low number of simulations may create variability in output **b)** Many pixels give high resolution, an increased number of simulations may give statistically more homogenous outputs**.**

Conclusions

Key findings:

- Increasing the number of repeated simulations reduces variability in output
- Between 160-200 simulations needed for reliable RVE
- Repeated simulations offer a more statistically accurate representation of DEM simulations- independent of the particle count
- Larger PSD's produce increase statistical heterogeneity and may require less tests to reach convergence

Contributing Researchers

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Dr Vasiliki Dimitriadi

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School of Engineering & the Built Environment

Thank you

If you have any questions, I would be happy to answer them

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