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# Optimized Wang Cubes for reconstruction of heterogeneous materials

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The term (re)construction of either 2D or 3D random heterogeneous material models used to be linked with the traditional concept of the Periodic Unit Cell (PUC). Unfortunately principles of the PUC approach with periodic boundary conditions are in direct conflict with definitions of randomness and heterogeneity. Few years ago a group of researches started to reduce consequences of this approach by utilization of the Wang tiling concept [3], which allows us to create aperiodic planes/spaces with relative small set of Wang Tiles/Cubes. This contribution deals with an upgrade of methods for generation of Wang tiles based on molecular dynamic algorithms. We will focus on 3D material samples representing domains with impenetrable hard spherical particles of identical radii in a matrix.

The main building block for tiling in 3D, Wang cube, can be described as a cube with different codes (information) on walls allowing compatibility within tiling process. The stochastic CSHD algorithm [1] is applied, since for material engineering there is no need to create strictly aperiodic samples. We consider the smallest set of Wang cubes based on two possible types of codes on walls for each of axis *x*, *y*, *z* in coordinate system. This assumption together with stochastic principles of tiling form basic set of sixteen Wang Cubes, Fig. 1.

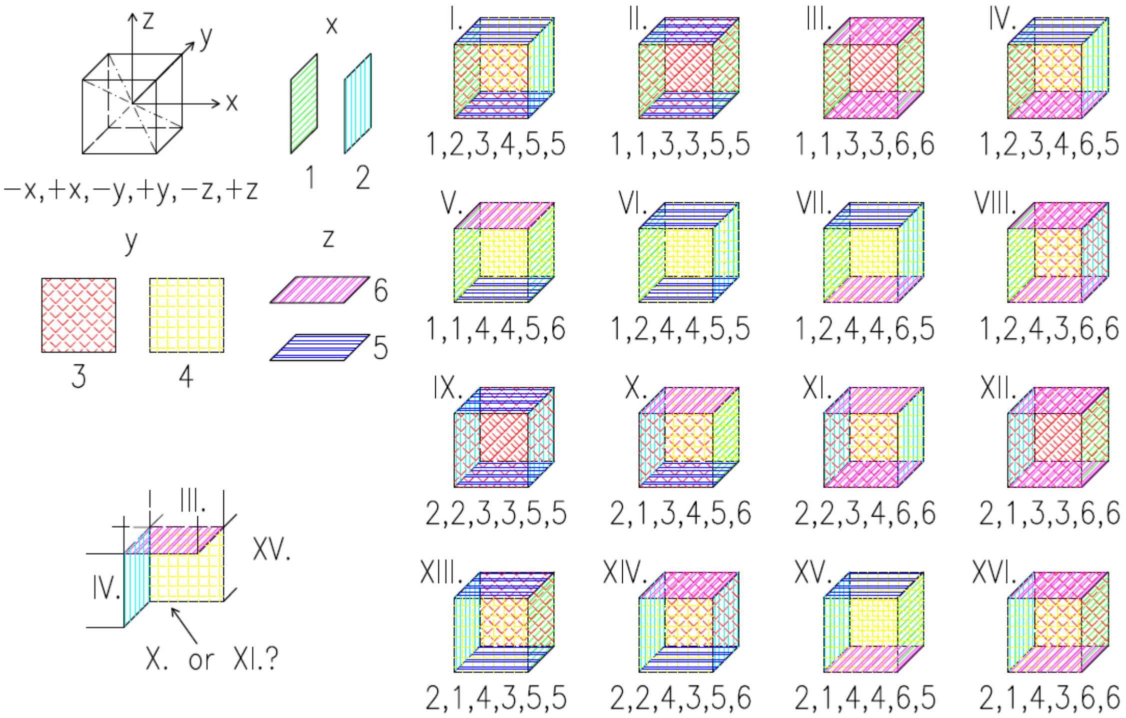


Fig. 1. Principles of stochastic tiling, basic set of 16 Wang Cubes

In previous works [2] a dynamic algorithm was used for generation of Wang cubes in order to efficiently prevent particles overlapping. Here particles collide from each other and rebound from walls of Wang cube volume border parts. Every single cube of the set was divided into six border and one central box to meet requirements for both tiling principles and particle volume fraction. Despite the reduction of unwanted periodicity in comparison with the PUC concept, approach with the cube volume division leads to secondary periodic peaks in lower order statistic description. In this contribution we present a significant upgrade of dynamic algorithm based on adaptive walls, Fig. 2.

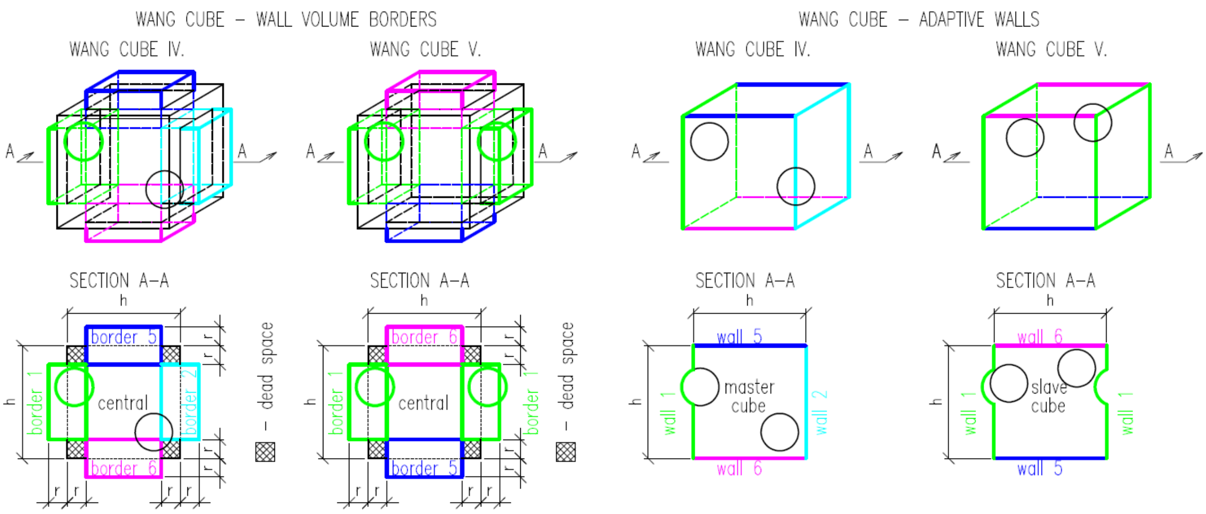


Fig. 2. Simplified comparison of algorithms for Wang Cubes generation: Wall volume borders vs Adaptive Walls

In Fig. 2 are shown only two representatives of the set with just codes in *x*, *z* axis and with only two particles to keep visual comparison clear for the reader. In the first case particles in border volume parts have to be copied to all cubes with appropriate code on wall. On the other hand with adaptive walls there is a master cube, where the particle forms the wall deformation. The walls on slave cubes with the same code then only follow the deformation without copying particles from the master cube, which increase heterogeneity of the tiling.
This contribution briefly introduced Wang tiling for reconstruction of 3D random heterogeneous material domains. Described modification of algorithm for Wang cubes generation together with particle swarm optimization method reduce unwanted secondary artefacts in lower order statistical descriptors. All of these improvements represent promising ways how to get closer to heterogeneous material models of required properties as fundamentals for various fields of material engineering.

## Acknowledgements

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## References


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