

CMS 273

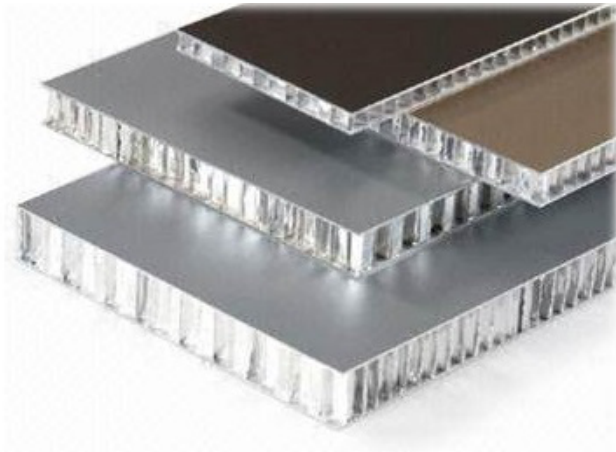
Materials Design By Reinforcement Learning

Chiara Daraio, Ke (Chris) Liu

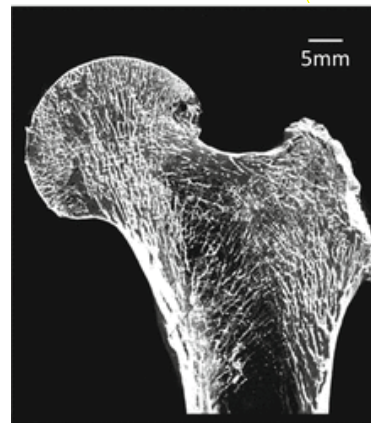
Mechanical and Civil Engineering
Caltech

Structure determines function in materials

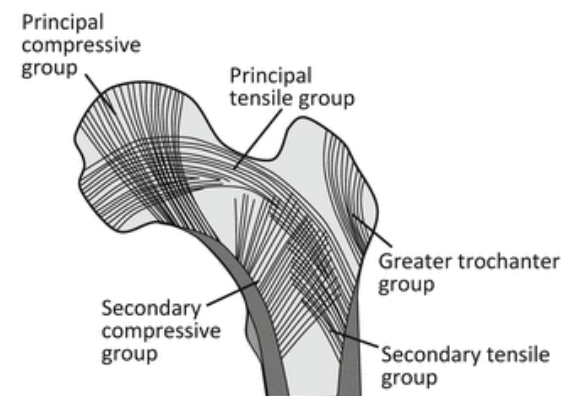
Periodic
(fully ordered)



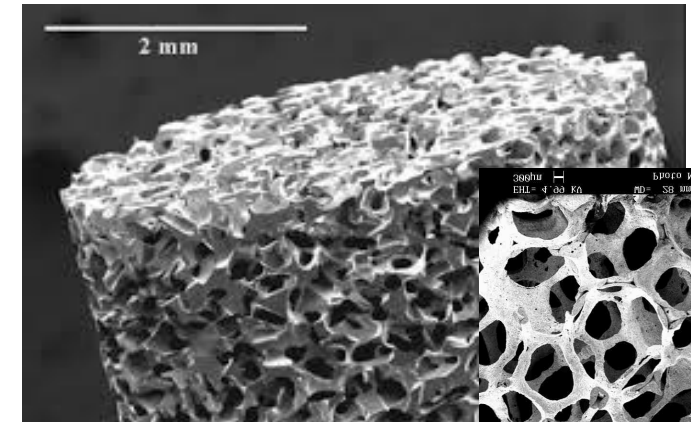
Newcore Global LTD



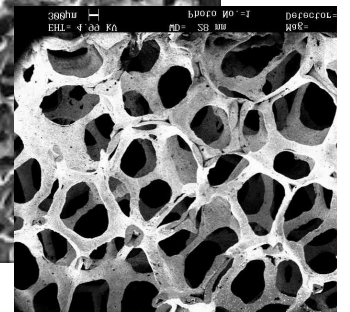
Nakano, 2015.



Random
(disordered)



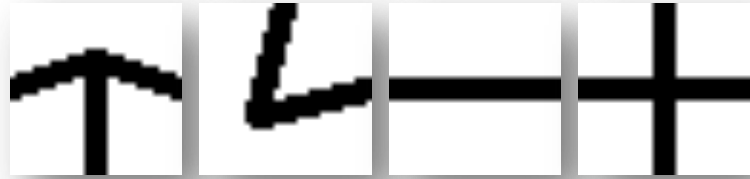
Lakes 1987.



How do we design materials' structure for optimal function?

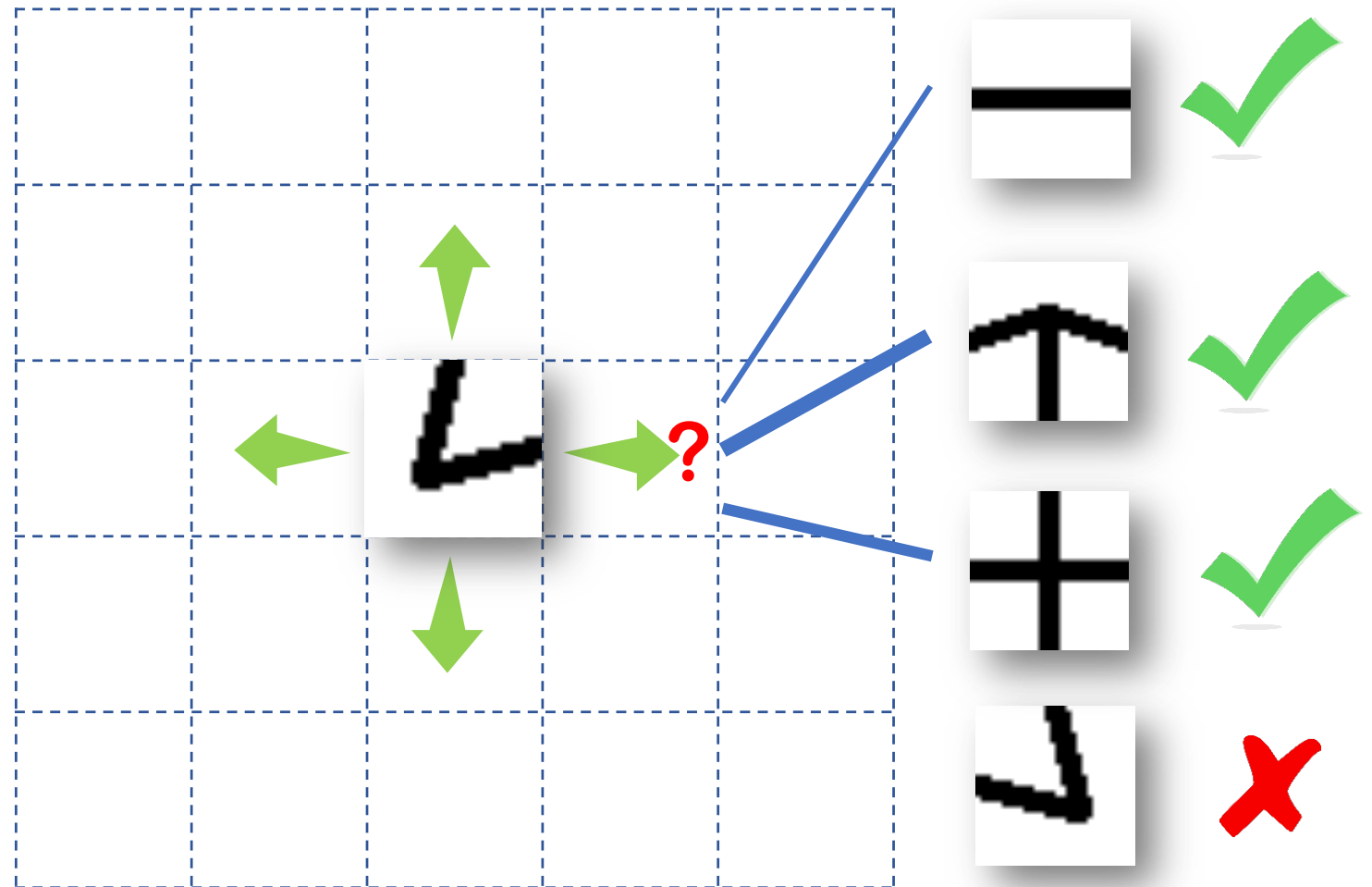
Design material by local growth rules

❖ Building blocks



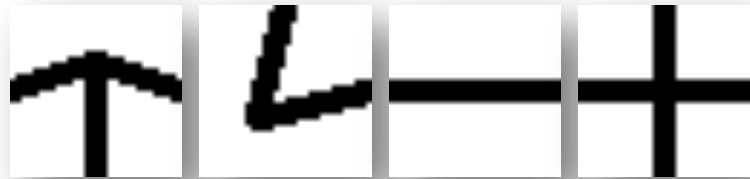
❖ Generation program (growth rules)

- Connectivity rules
- Building blocks availability (marginal frequencies)



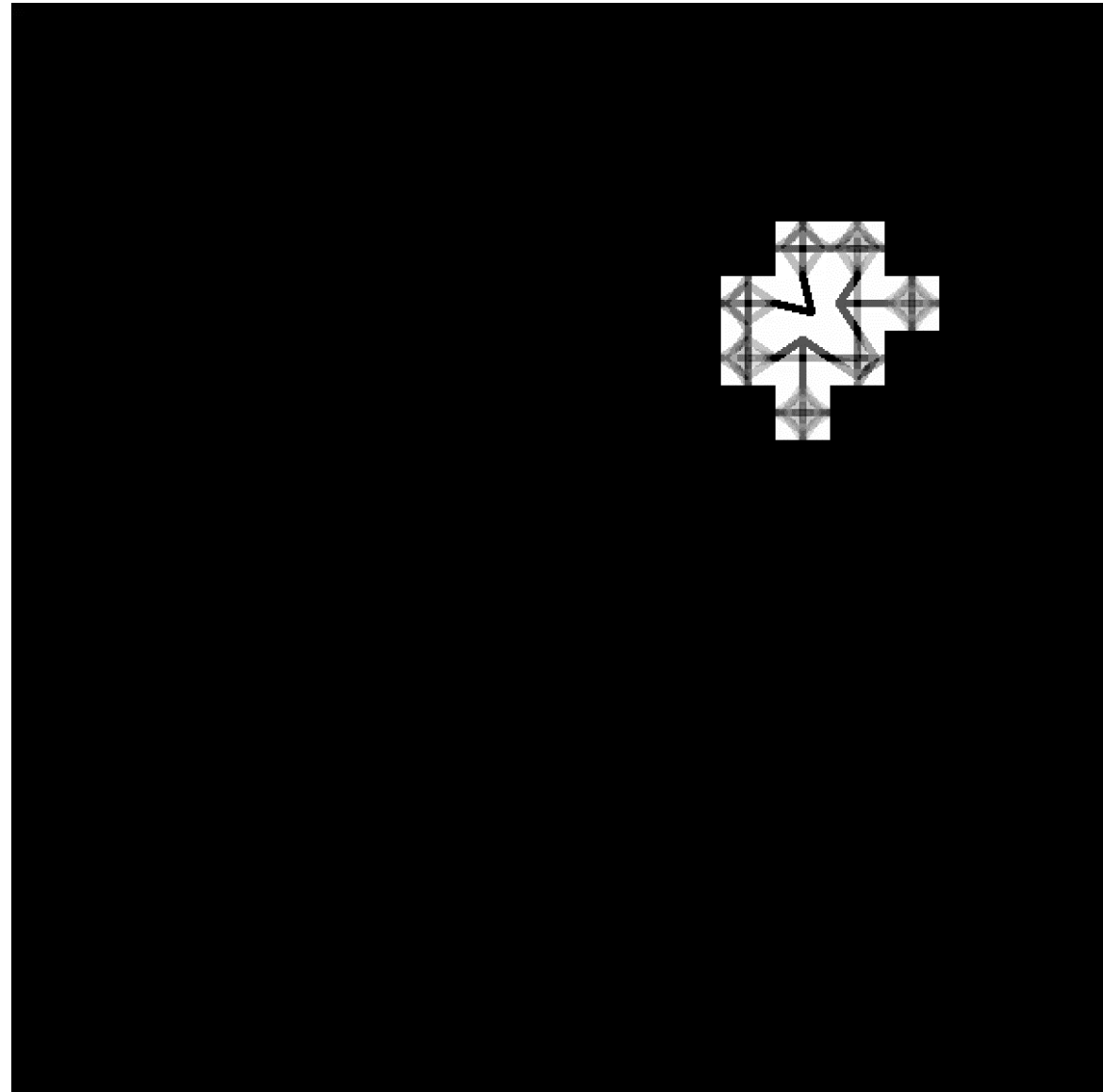
Design material by local growth rules

❖ Building blocks

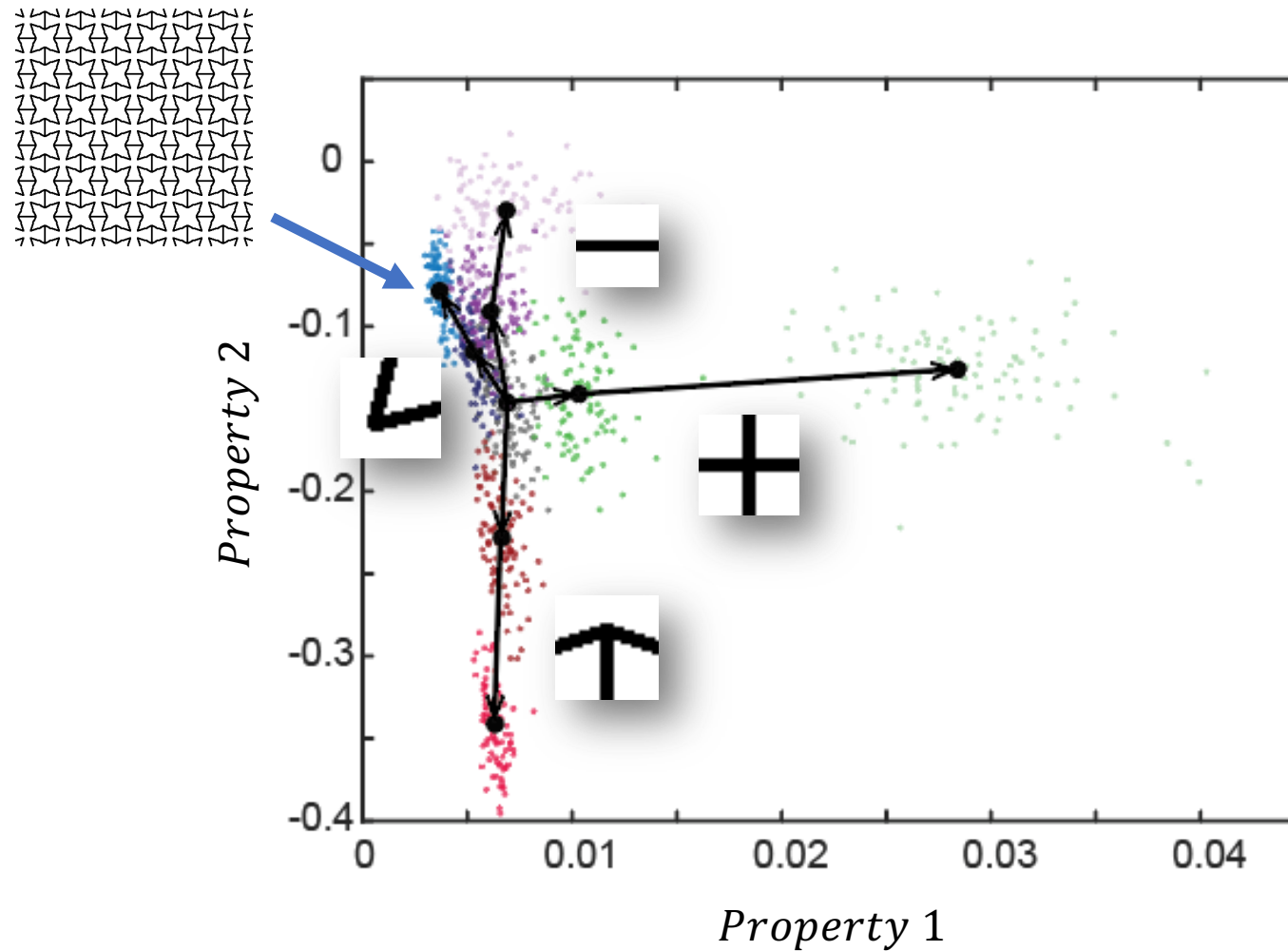


❖ Generation program (growth rules)

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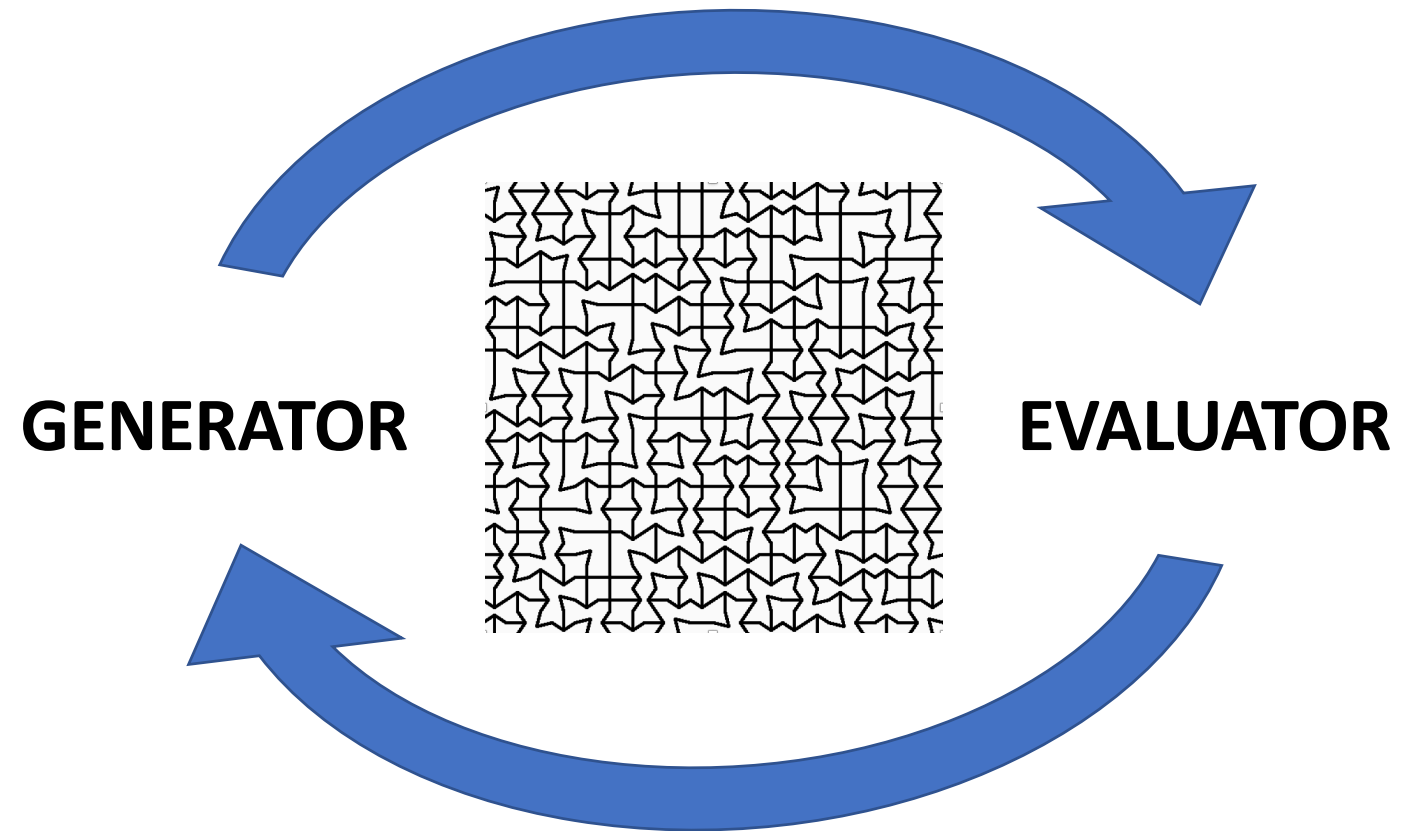


Virtual evaluation of properties (FEM)



Influence of growth rules on properties

Closed loop virtual lab



Project goals

1. Use reinforcement learning to associate the design information in the “growth” process to resultant material properties;
2. Optimize for target properties.

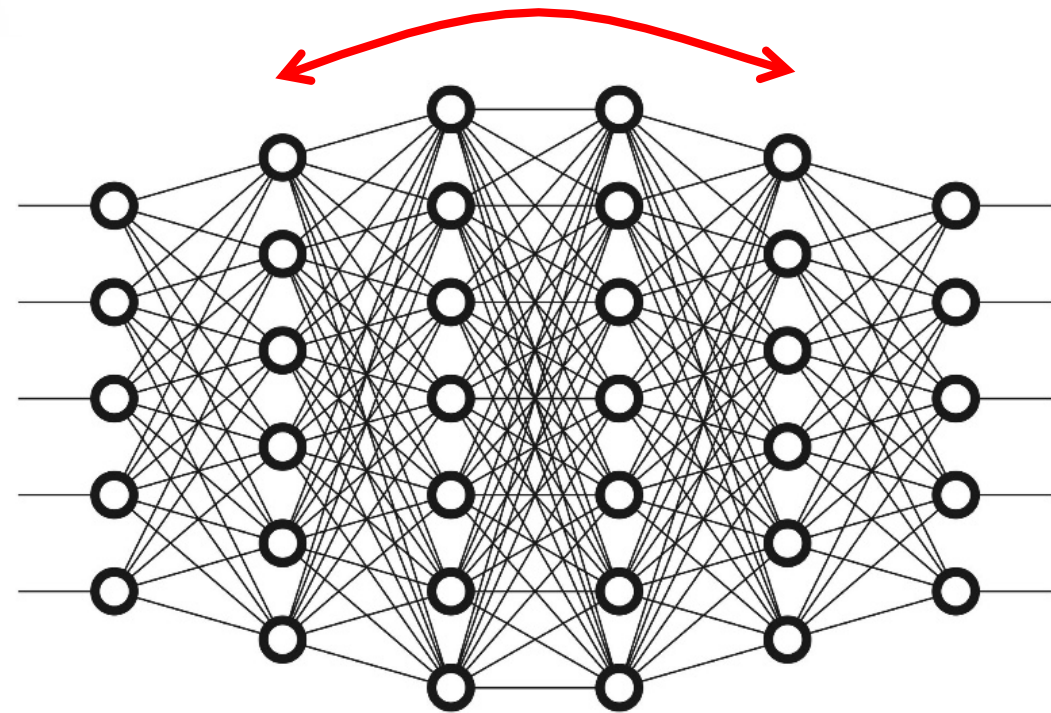


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Experimental validation

