Fractal Growth

Seminar on Computational Physics

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HISKP
Universität Bonn

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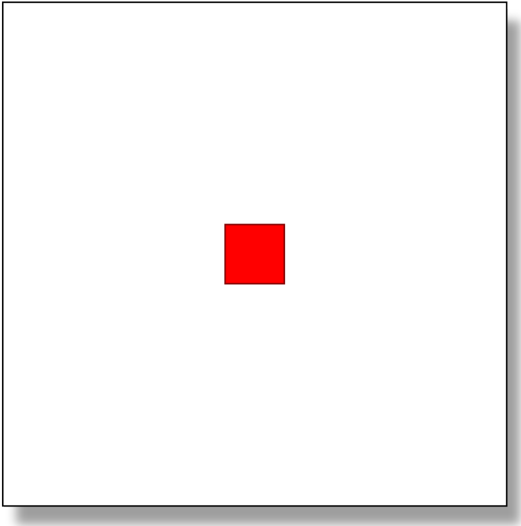

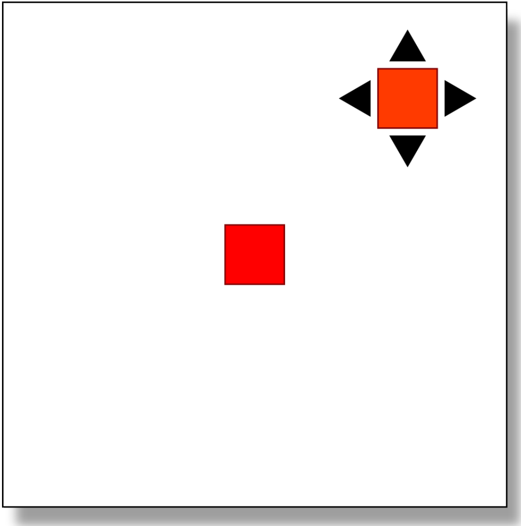

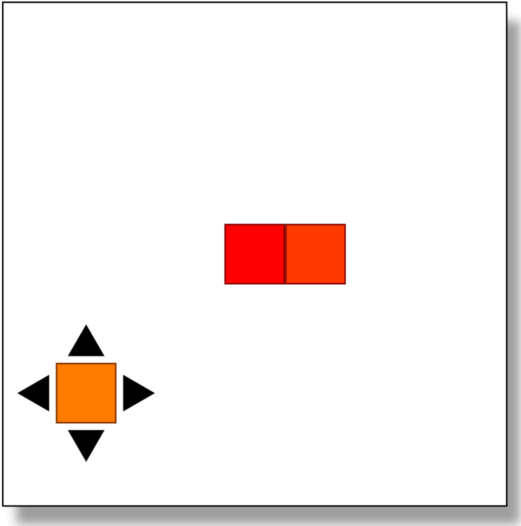

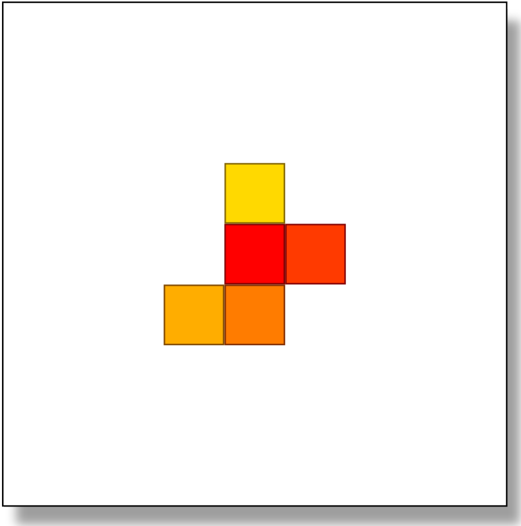

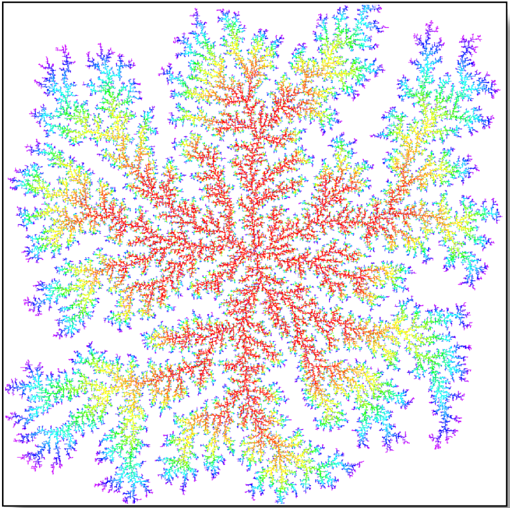

T. A. Witten, L. M. Sander, 1981

Outline

Fractal Dimension

Definition (Hausdorff measure)

The (outer) *d*-dimensional Hausdorff measure is defined as:

$$H_\varepsilon^d(S) = \inf_{\substack{\bigcup_{i=1}^\infty U_i \supset S \\ \mathrm{diam}(U_i) < \varepsilon}} \sum_{i=1}^\infty \mathrm{diam}(U_i)^d \tag{1}$$

The *d*-dimensional measure is (modulo some measure theory) the limit $\varepsilon \to 0$.

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The Hausdorff dimension of a set is defined as:

$$d_H = \sup\{d \in \mathbb{R}_0^+ \mid H^d(S) = \infty\} \tag{2}$$

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Discrete Calculations

Definition (Simpler working definition)

The fractal dimension of a point set is defined as the following:

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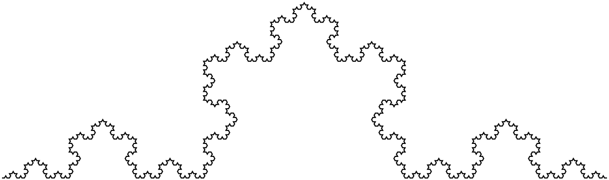
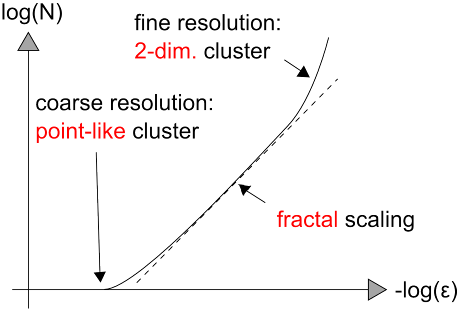


Fractal dimension of finite structures



Box-counting:
$\log(N) = -d \log(\epsilon)$

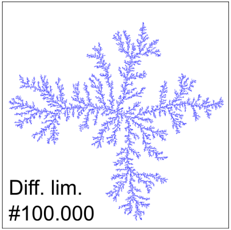
Other scaling power-laws:

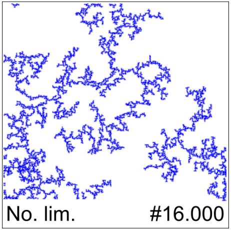
- radius of gyration $R_g \propto N^{1/d}$
- density-density-correlation $C(r) \propto r^{D-d}$
- ...

The Meakin model

1.
- Set seed in the center of the lattice
- Generate particles at $R + 10$ one by one
- Let particle diffuse against the cluster
- Particles further than $2R$ are removed

2.
- Generate many particles once
- Let them diffuse and clump together
- Steady state is reached





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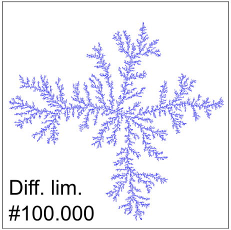

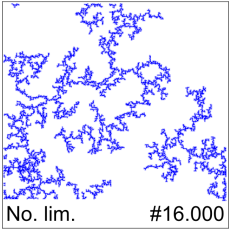

Implementation: Outline

Two types of objects:

- Particles (which carry interaction information)
- Clusters (specialized containers for particles)

The main program step works as follows:

- Update the environment
  - Remove particles that are too far away or to old
  - Create new particles or clusters
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If we want we output graphics or calculate statistics afterwards.

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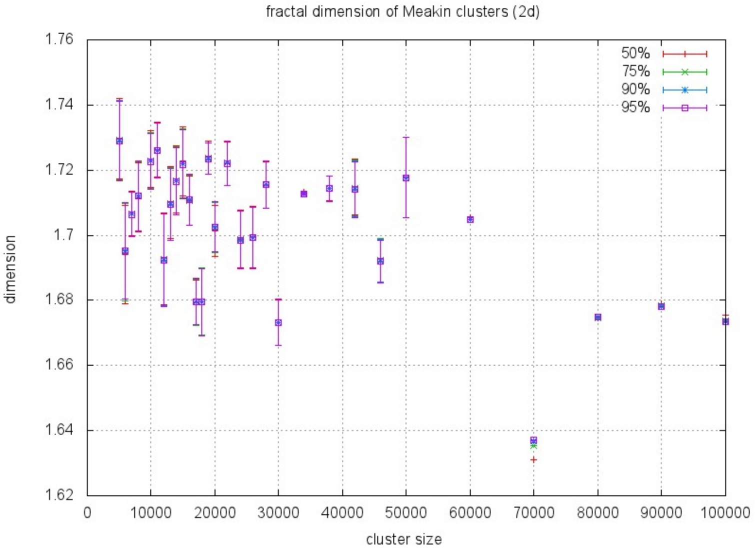
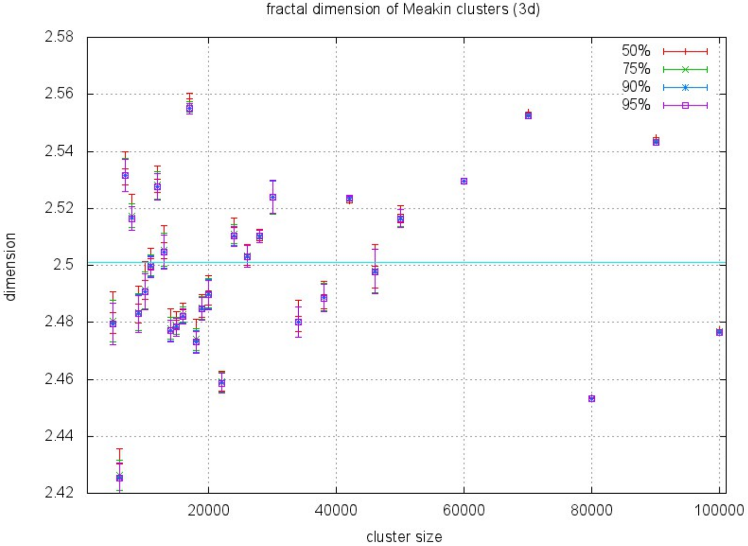
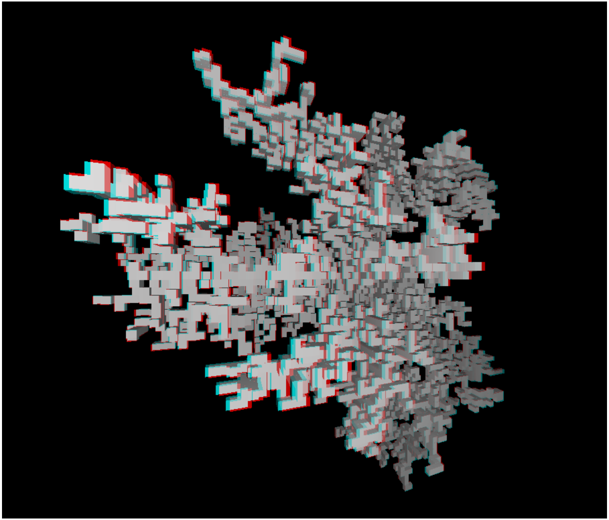
Fractal dimension of 2-d Meakin clusters



Fractal dimension of 3-d Meakin clusters

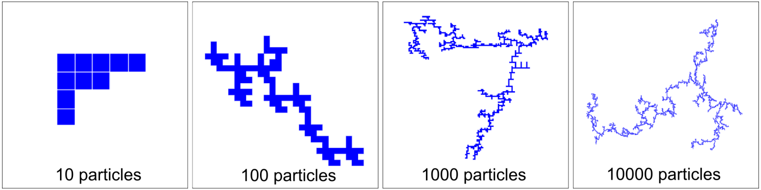


Anaglyph of 3-d Meakin cluster (8000 particles)



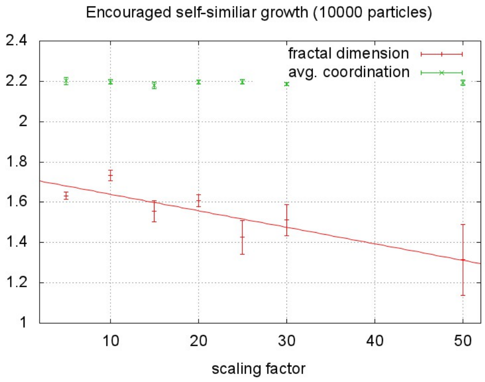
Encouraged self-similar growth

- Want to create structures with tailor-made dimensionality while maintaining basic building principle (physically motivated!)
- Idea: Encourage certain scaling behaviour (remember $D \approx -\frac{\log N}{\log \epsilon}$)
- Diffuse clusters instead of particles



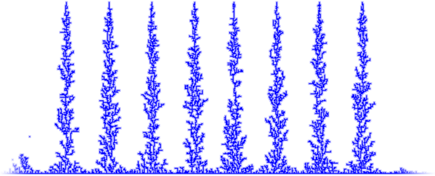
A theoretical treatment is difficult:

- Hybridization of IFS and statistical process, so no simple scaling law
- Non-negligible finite-size effects

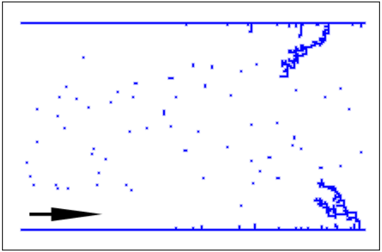


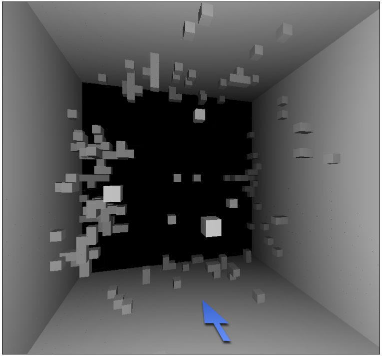
Dendrites

Pyrolusite
Jonathan Zander, 2008

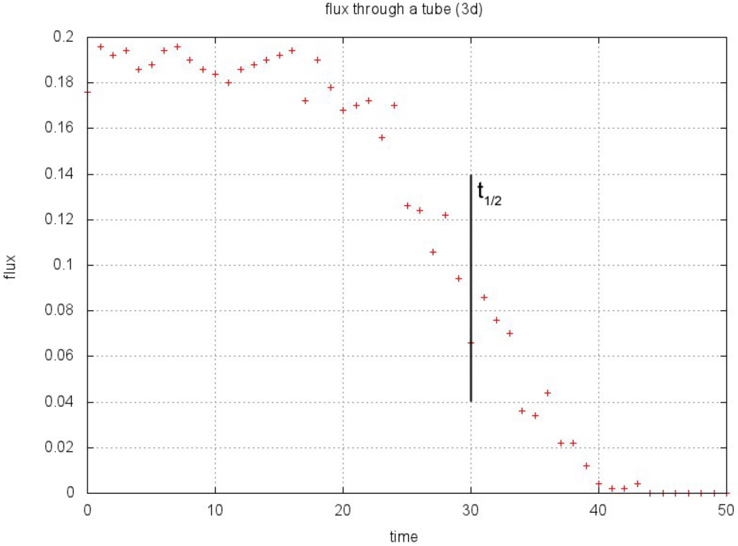


Tubes

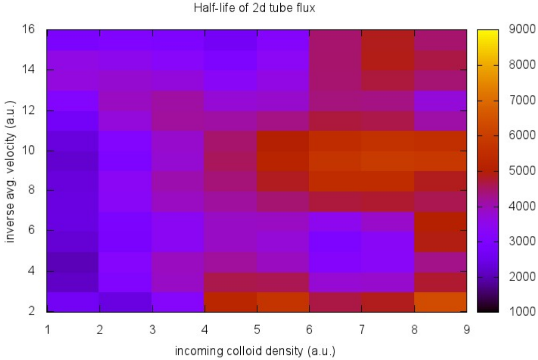




Tubes: flux


flux through a tube (3d)
0.2
0.18
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
flux
0
10
20
30
40
50
time
$t_{1/2}$

Tubes: flux

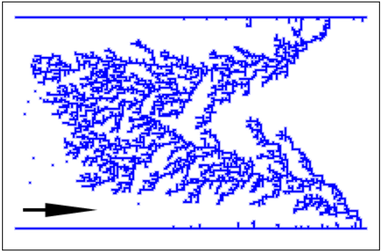


2-dimensional simulation, length/radius: 10

Tubes: real-world physics?

Obstacles are fixed unphysically:

- require breaking of bonds
- leads to MD-like simulations

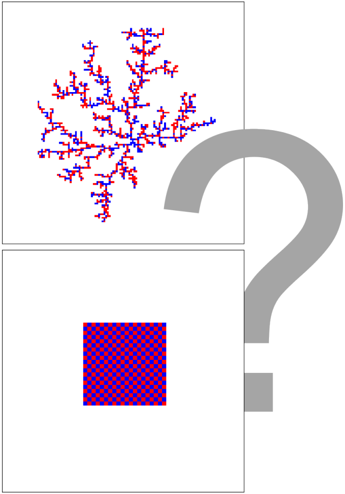


Crystals vs. Dendrites

Idea: Add Coulomb-like interaction

- Introduce particle charge
- Set preferred directions in random walk depending on other particles
- Try to observe a transition from $D = 1.6$ to $D = 2$

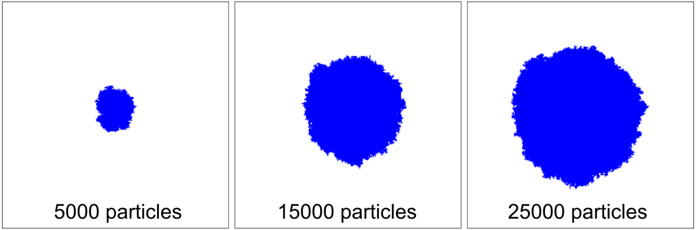
This is work in progress.



The Eden-Meakin model

Idea

Describe organic growth (rather than anorganic):
Add new clusters size at nearest neighbours

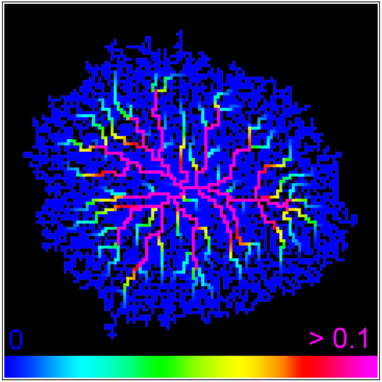


M. Eden, 1961, P. Meakin, 1991

The Eden-Meakin model

Scoring system:

- For each new particle, randomly choose an adjacent "parent"
- Add a score $\Delta S = (1 + l)^{-\eta}$ to each of the l ancestors
- Reduce all scores S_i by $1/N_m$
- Remove particles of non-positive score

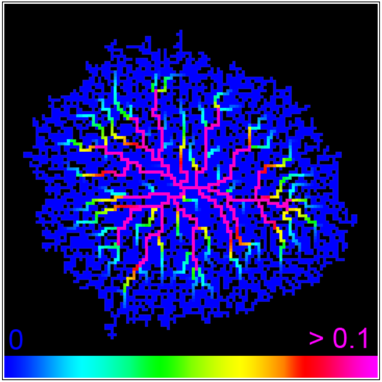


$\eta = 1$, $N_m = 102400$

The Eden-Meakin model

Features:

- fractal backbone with $D = D(S_{\text{thres}})$
- finite "equilibrium" size
- adaptivity, memory



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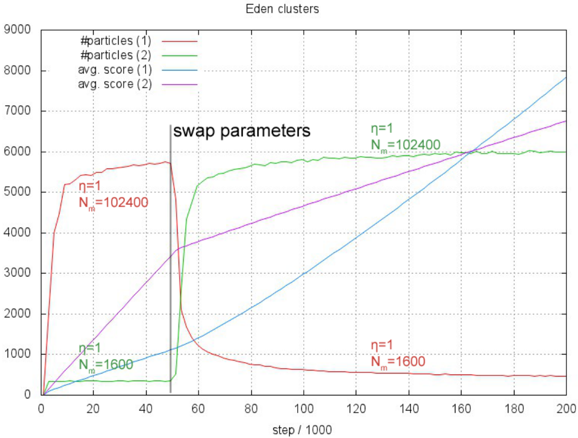
The Eden-Meakin model: examples



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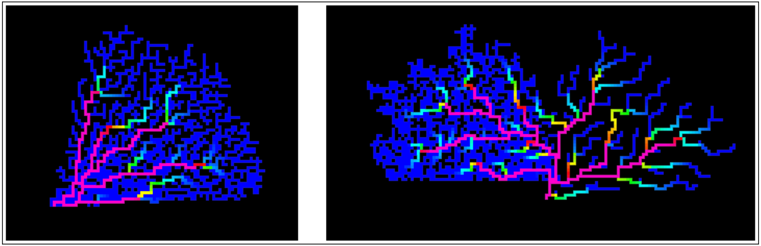


Geometrical scoring: $\Delta S \propto \frac{\vec{x} \cdot \hat{e}_{\text{sun}}}{|\vec{x}|}$

Summary

- Combining simple methods motivated by natural processes generates fractal structures, e.g. Brownian motion and molecular adhesion.
- It is possible to simulate these efficiently on a lattice
- The fractal dimension can be calculated as $D = -\frac{\log N}{\log \epsilon}$ or estimated on discretized structures via the radius of gyration.
- Fractal structures describe anorganic and organic real world phenomena.

References

- T. A. Witten and L. M. Sander, Phys. Rev. Lett. 47, 1400 (1981)
- H. E. Stanley, J. Phys. A 10, L211 (1977)
- P. Meakin, Phys. Rev. A 27, 1495 (1983)
- P. Meakin, Phys. Rev. Lett. 51, 13 (1983)
- M. Eden, Proc. 4th Berkeley Symp. on Mathematics, Statistics and Probability, vol. 4, F. Neyman, ed., (1961)
- P. Meakin, Physica A, 179 (1991)

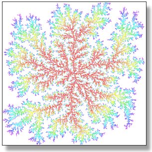
Fractal growth is fun!

source code

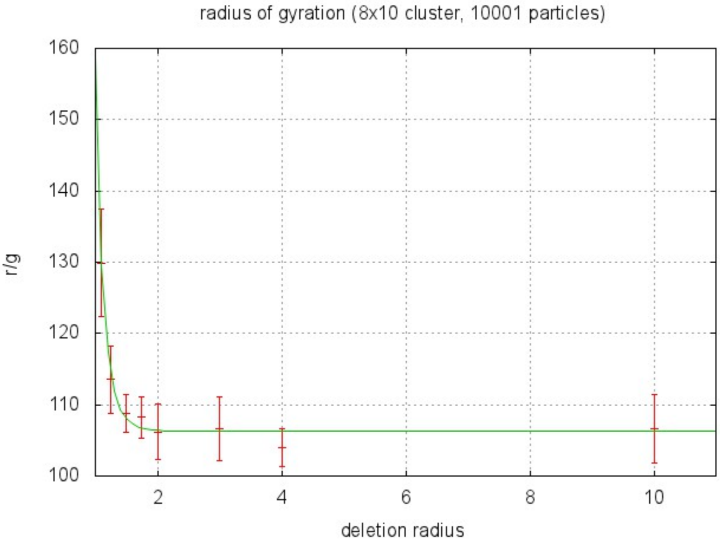
`http://github.com/filmor` or `http://github.com/palmstroem`

(may not always be in working state, requires gcc $\geq$ 4.5.2)

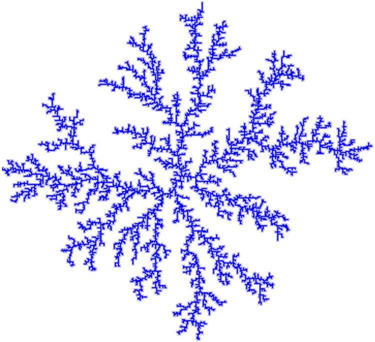
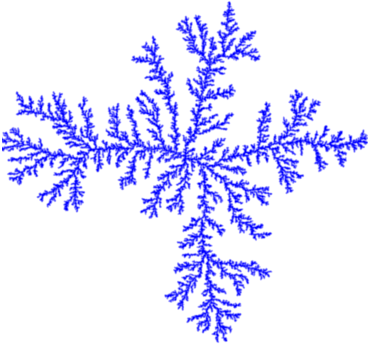
Thank you for listening!



"Diffusion from infinity"



Self-similiarity

Clusters

Cluster objects need to do some tricks to be efficient.

- Memory efficiency:
  - Save only a cube surrounding the cluster, not a full lattice
  - Let this cube grow on purpose (in 2^d steps) and reset its center
- Runtime efficiency:
  - Save also a vector of all particles
  - Save a radius (for fast collision checks)

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Additional Notes

- The whole program is build of templates (compile-time polymorphy)
    - Gives similar flexibility as runtime-polymorphy (virtual functions)
    - Greatly improves performace on good compilers (ca. handcoded C)
    - Lets us use the same framework for Meakin and Eden
- In a later version will unify clusters and particles
    - They have similar movement and interaction characteristics
    - $\Rightarrow$ Implementation of the above is currently tedious
- Sadly we haven't found a method to parallelize, if someone finds one, tell us :)

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