Modelling of physiological and pathological processes

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Lecture 3

The labyrinthine patterns, gyri & sulci, of the cerebral cortex of a human brain:
(a) dorsal view; (b) lateral view.

Reaction–diffusion equations and Turing patterns

To model pattern formation, Turing proposed an interaction between two diffusing biologically active chemical species.

One of the species inhibits growth, and the other enhances it.

At the same time, **they interact to activate and inhibit** each other.

•J. H. E. Cartwright, "Labyrinthine Turing pattern formation in the cerebral cortex", J. Theor. Biol. **217**, 97–103, 2002

•Collected Works of A. M. Turing: Morphogenesis (P. T. Saunders, editor), North-Holland, 1990

A simple reaction-diffusion system:

$$\frac{\partial u}{\partial t} = \nabla^2 u + F(u,v)$$

$$\frac{\partial v}{\partial t} = \delta \nabla^2 v + G(u,v)$$

•u and v are the concentrations of the two diffusing and reacting chemical species (say, u the activator and v the inhibitor)

•F(u, v) and G(u, v) represent the chemical process

•Even if you start from nicely mixed and homogenous solutions, the system may become unstable if δ >1 i.e. when the inhibitor diffuses more rapidly than the enhancer

The chemistry:

$$F(u,v) = \gamma(v - u^3/3 + u)$$

$$G(u,v) = -\gamma^{-1}(u + \lambda + \beta v)$$

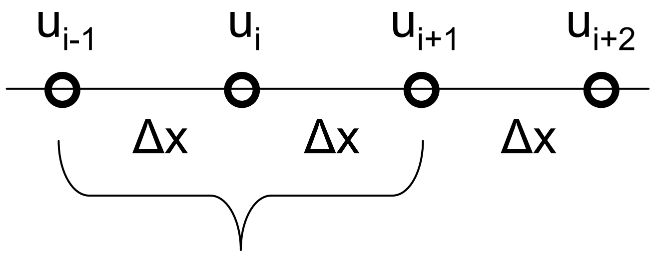
γ determine the interaction kinetics: for $\gamma<1$ inhibition dominates, whereas for $\gamma>1$ activation dominates.

Note that γ is connected with local reaction characteristics whereas δ quantifies how the two species diffuse.

β and λ determine the type of equilibrium states of the local dynamics

$\nabla^2 u$ The Laplacian

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$



$$\frac{\partial u}{\partial x} = \frac{u_{i+1} - u_i}{\Delta x} \ldots as \ldots \Delta x \to 0$$

$$\frac{\partial^2 u}{\partial x^2} = \frac{\left(\frac{u_{i+1} - u_i}{\Delta x}\right) - \left(\frac{u_i - u_{i-1}}{\Delta x}\right)}{\Delta x} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} \ldots as \ldots \Delta x \to 0$$

The temporal derivative:

$$\frac{\partial u}{\partial t} = \frac{u_{t+\Delta T} - u_t}{\Delta T} \ldots as \ldots \Delta T \rightarrow 0$$

Issues to consider:

Let us think about the 1D case for a second:

$$\frac{u_{t+\Delta T} - u_t}{\Delta T} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2}$$

WHERE IS u_t and WHEN is u_i ???

Option 1: Explicit scheme

$$\frac{u_i^{t+\Delta T} - u_i^t}{\Delta T} = \frac{u_{i+1}^t - 2u_i^t + u_{i-1}^t}{\Delta x^2}$$

Intuitive consideration:
What do they mean
as far as my choice
for time step?

Option 2: Implicit scheme

$$\frac{u_i^{t+\Delta T} - u_i^t}{\Delta T} = \frac{u_{i+1}^{t+\Delta T} - 2u_i^{t+\Delta T} + u_{i-1}^{t+\Delta T}}{\Delta x^2}$$

Implications:

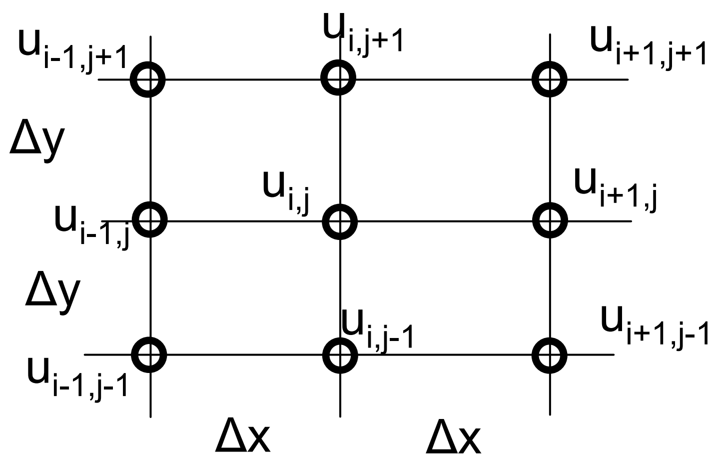
- Stability
  - Implicit schemes are much more stable (often unconditionally stable)

- Simplicity
  - Explicit schemes are often very easy to program
  - Implicit schemes require the solution of a linear system
  - Implicit schemes for non-linear problems require the solution of a linear system many many times!

- Speed & Memory
  - Implicit schemes require more memory
  - Explicit schemes are much easier to parallelise

- Accuracy
  - The two often have different requirements in terms of discretization, attention to detail is important

In our case the explicit scheme would read:



$$\frac{u_{i,j}^{t+\Delta T} - u_{i,j}^{t}}{\Delta T} = \frac{u_{i+1,j}^{t} - 2u_{i,j}^{t} + u_{i-1,j}^{t}}{\Delta x^2} + \frac{u_{i,j+1}^{t} - 2u_{i,j}^{t} + u_{i,j-1}^{t}}{\Delta y^2}$$

Exercise: do the algebra and get the unknown explicitly.

Other issues:

•Boundary conditions

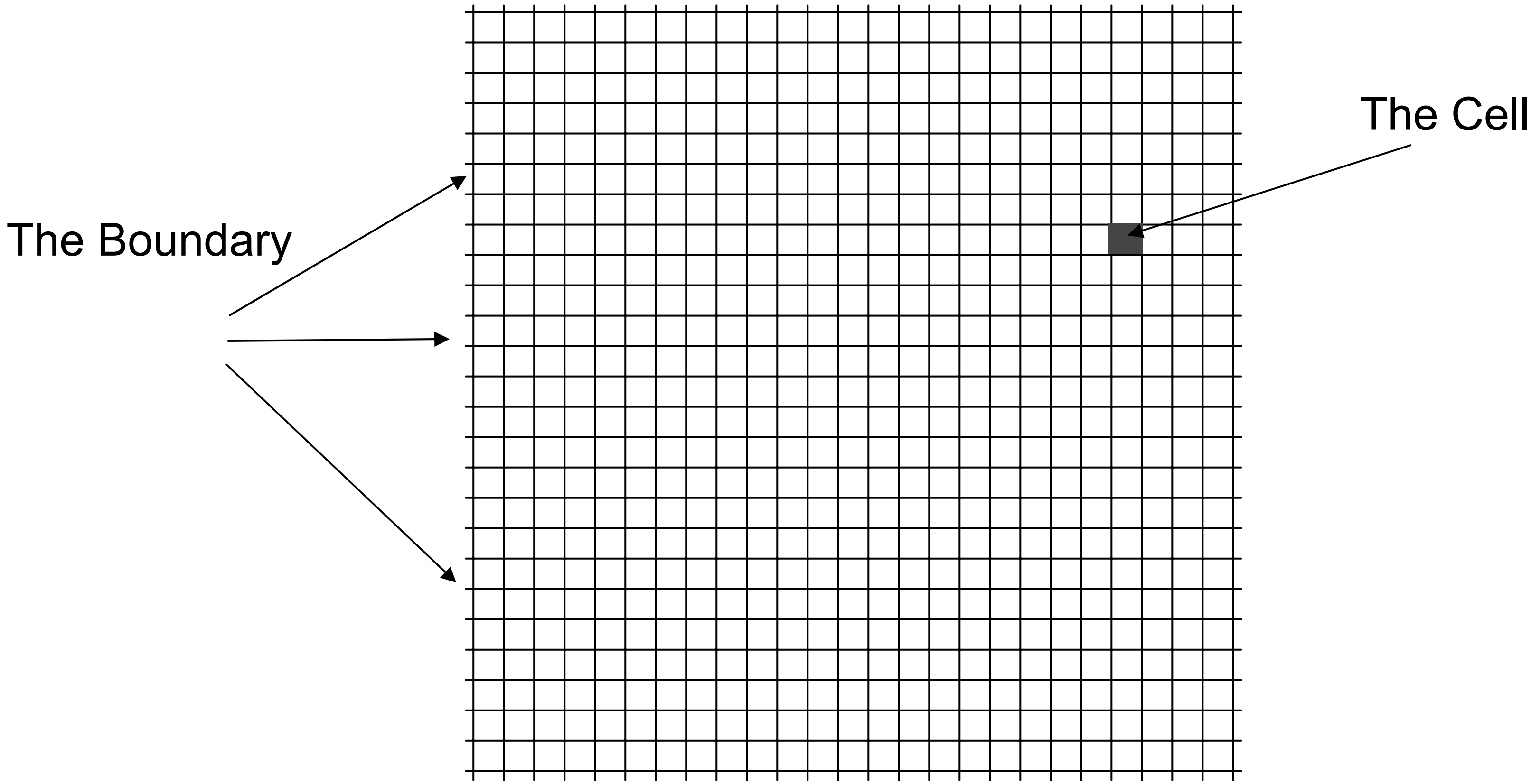
•Initial conditions

•Other difference schemes

•Different topologies

•Different equations

“The Grid”

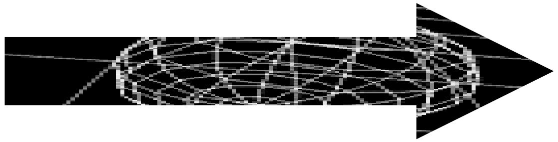


Grids and Computing: a Tangent in the storyline

The American Whirlwind, built in the mid-1940s. Based on thermionic tubes - valves, used to solve problems of aircraft flight performance. The switch from tubes to transistors (1950s), reduced the size of state-of-the-art computers from 2 huge rooms to 1.

Grids and Computing: a Tangent in the storyline

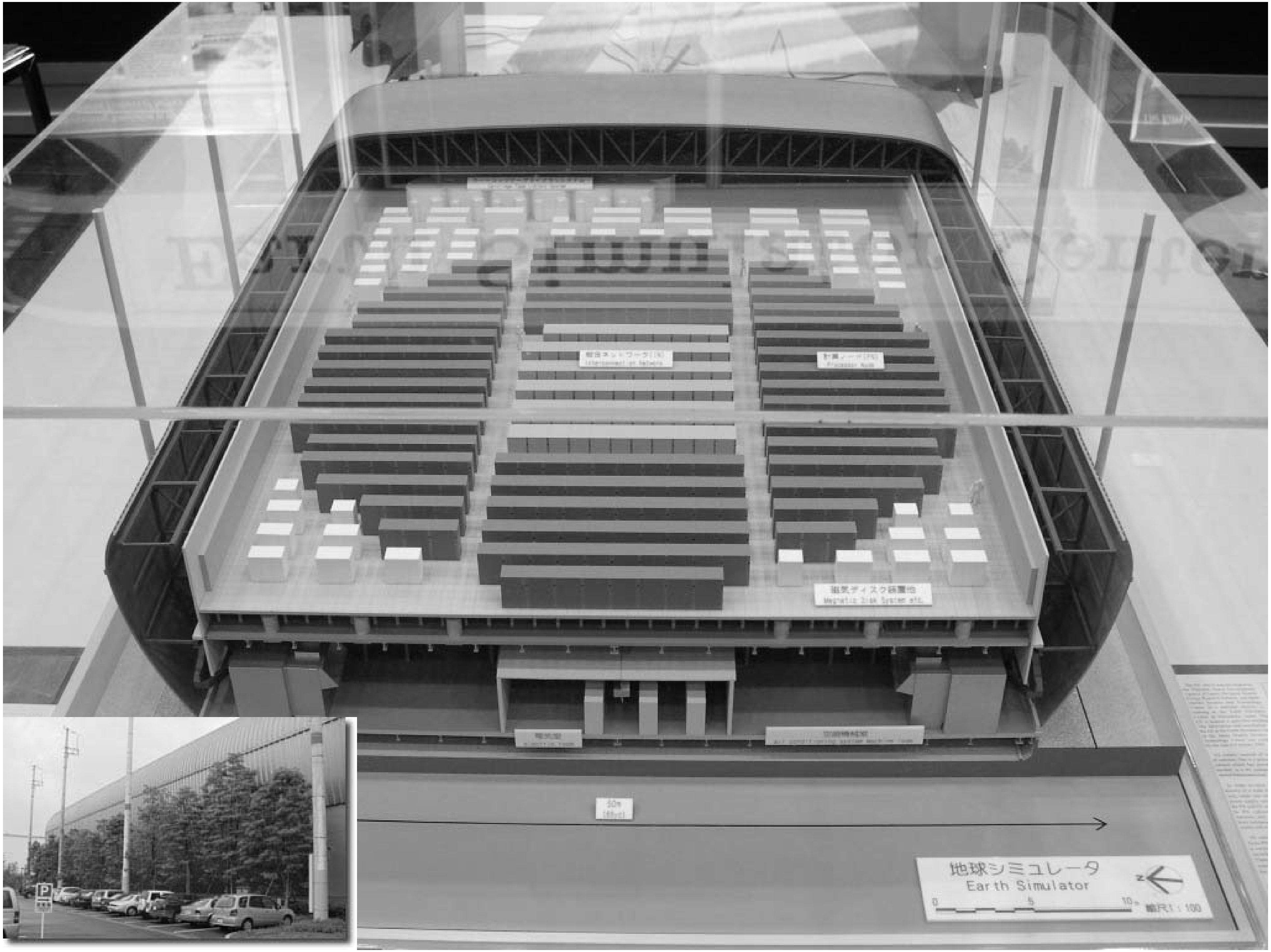
Thousands of times faster,
hundreds of times cheaper



Grids and Computing: a Tangent in the storyline

Hundreds of times faster,
ten times cheaper

The Earth Simulator, parallel computing, outrageous grids and the mother of all DNSs:


磁気ディスク装置他
地球シミュレータ
Earth Simulator
縮尺1：100

The Earth Simulator, parallel computing, outrageous grids and the mother of all DNSs:

"Nodes"
NI=NJ=NK=4096

Total Nodes=NI x NJ x NK
68518346688 (68 billion nodes)

Timesteps
200000

Write 1 in 100

Snapshots
2000

The Earth Simulator, parallel computing, outrageous grids and the mother of all DNSs:

Total Nodes x Snapshots
1.37037E+14

U,V,W,P = 4 variables per node

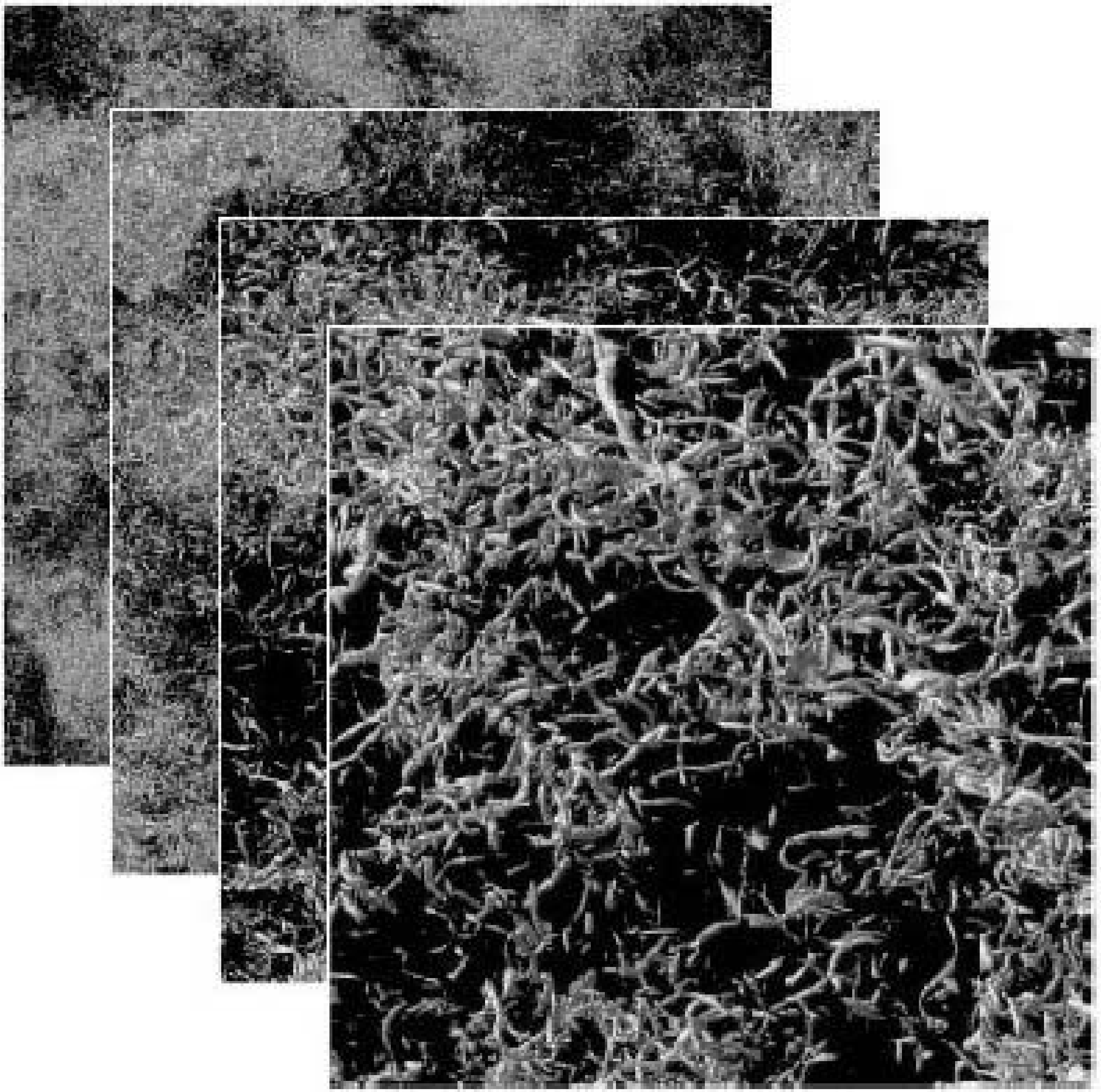
Variables x Total Nodes x Snapshots
5.48147E+14

Double Precision (8 bytes)
4.38517E+15 bytes

Convert to Petabytes: /(1024*1024*1024*1024*1024)
3.89481708 Pbytes

Its reasonable to assume an 1:3 compression (/3)
1.29827236 Pbytes

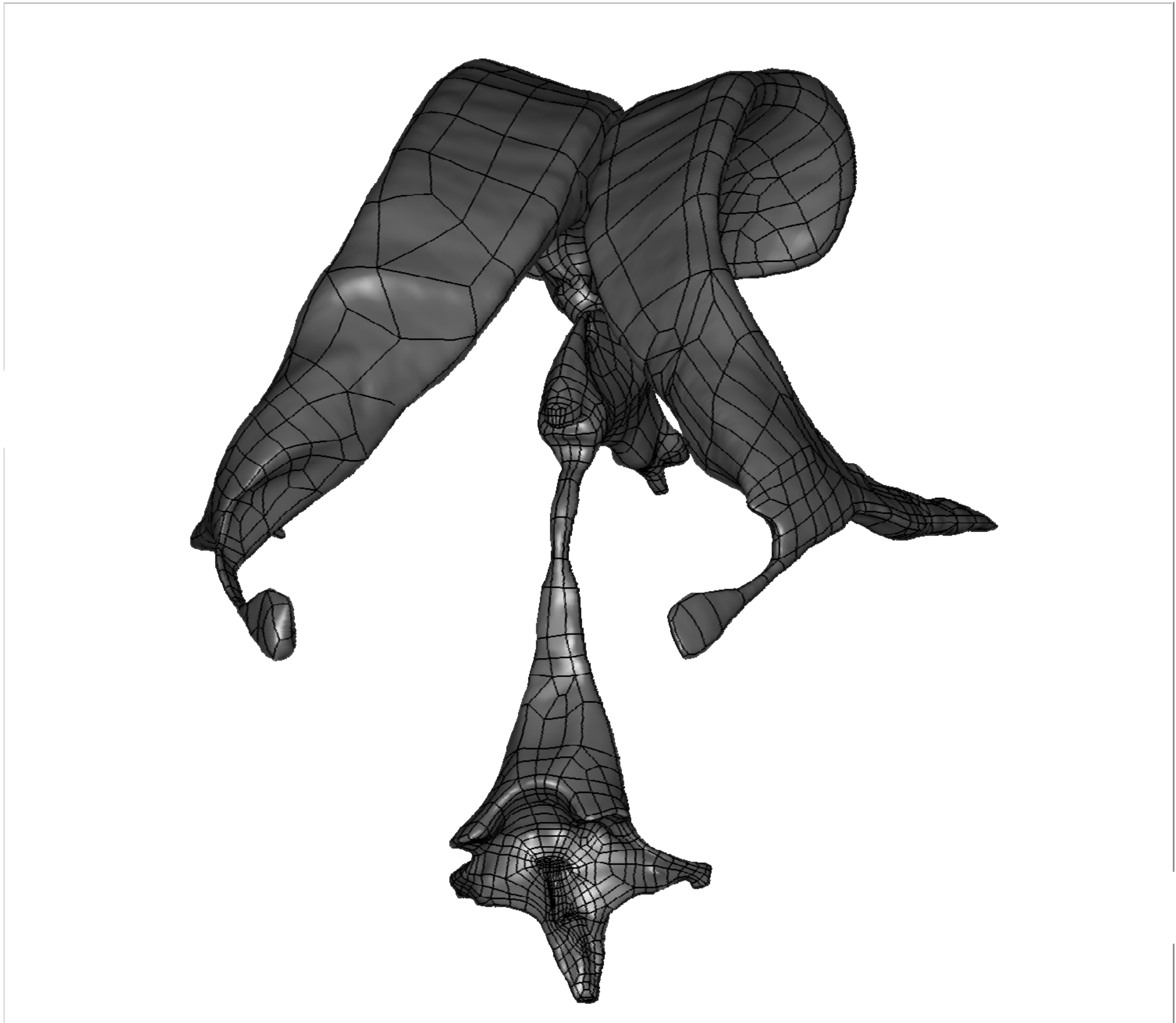
The Earth Simulator, parallel computing, outrageous grids and the mother of all DNSs:



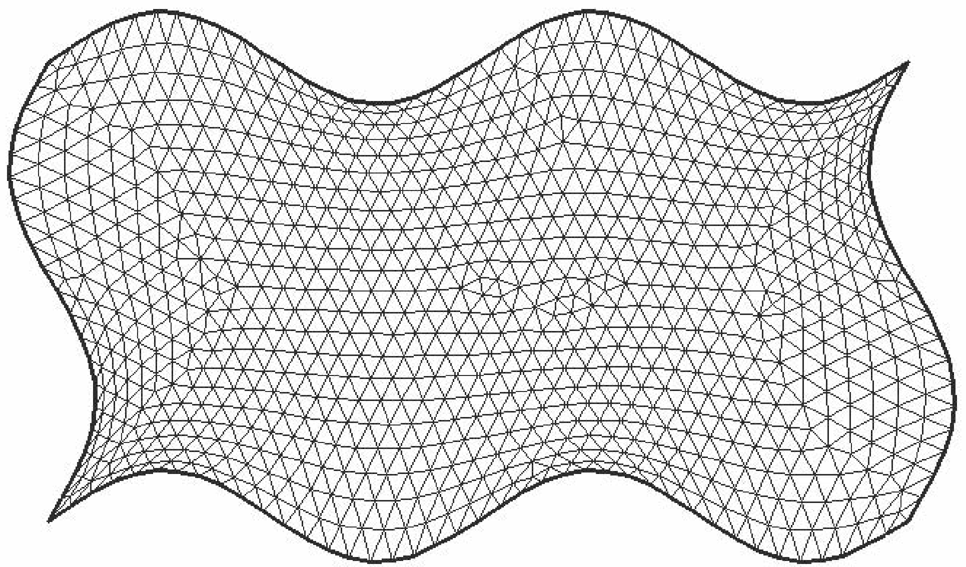
Yukio Kaneda, “Reynolds Number Dependence of the Statistics in High Resolution DNS of Turbulence with up to Re~1130”

Department of Computational Science and Engineering
Graduate School of Engineering, Nagoya University, Japan

Grids

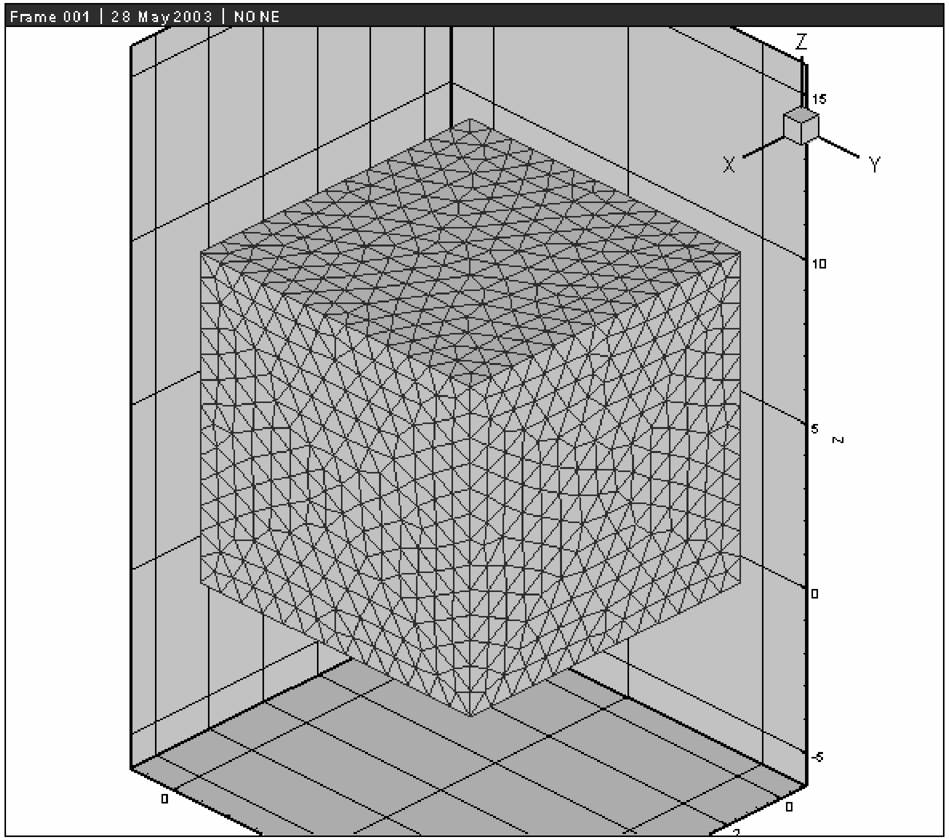


Grids

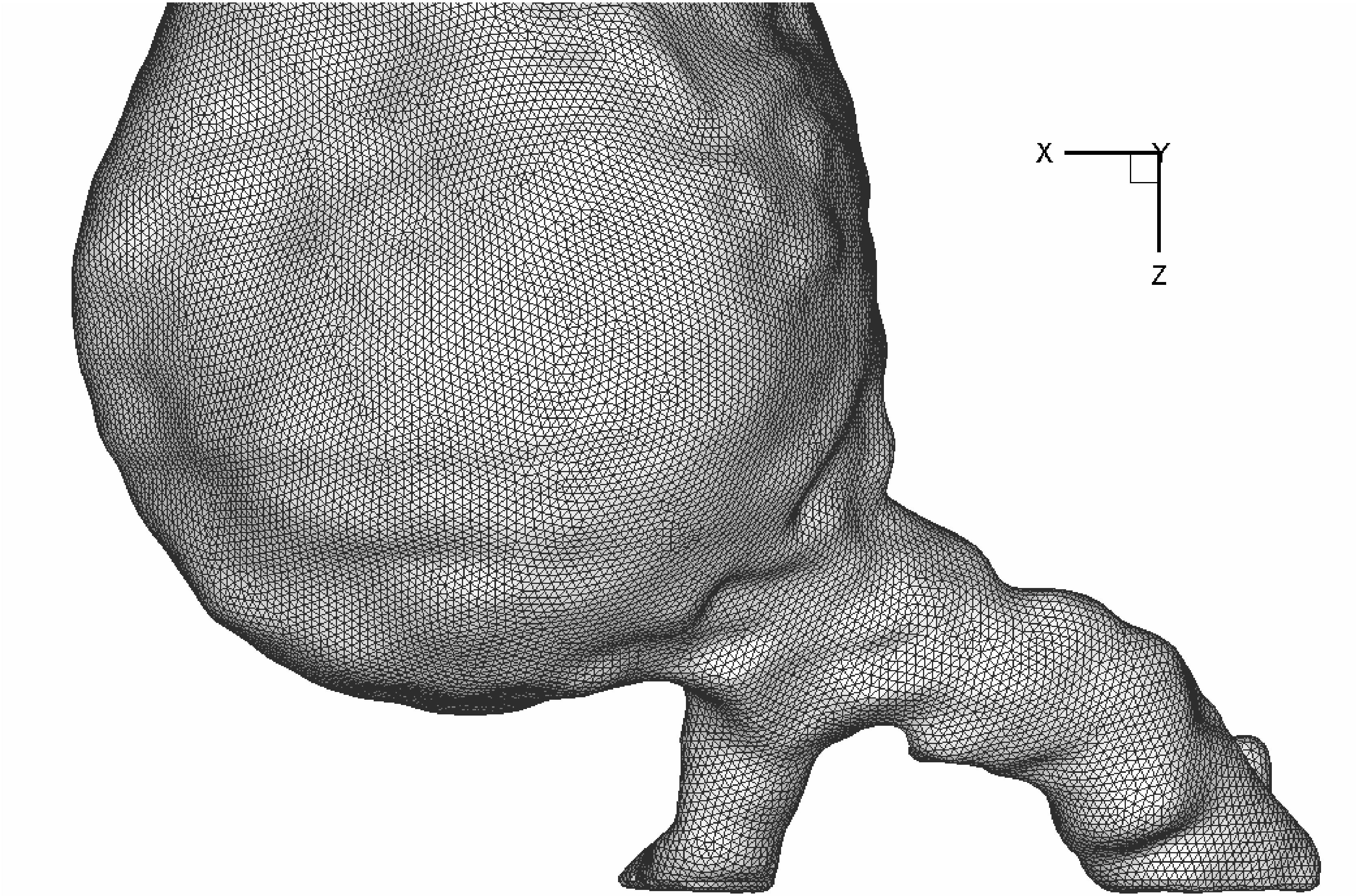


Unstructured: think of connectivity issues & relating storage

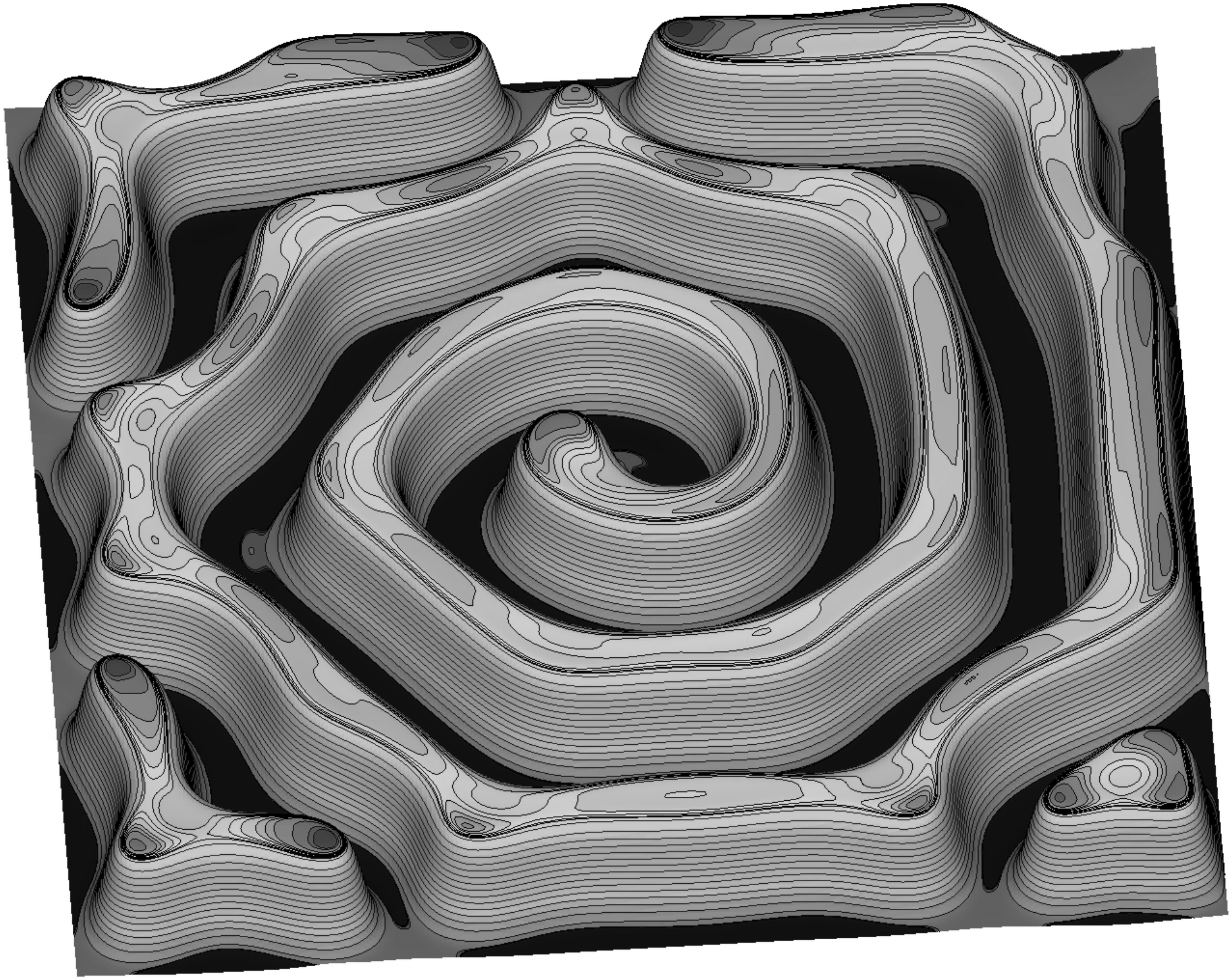
Grids

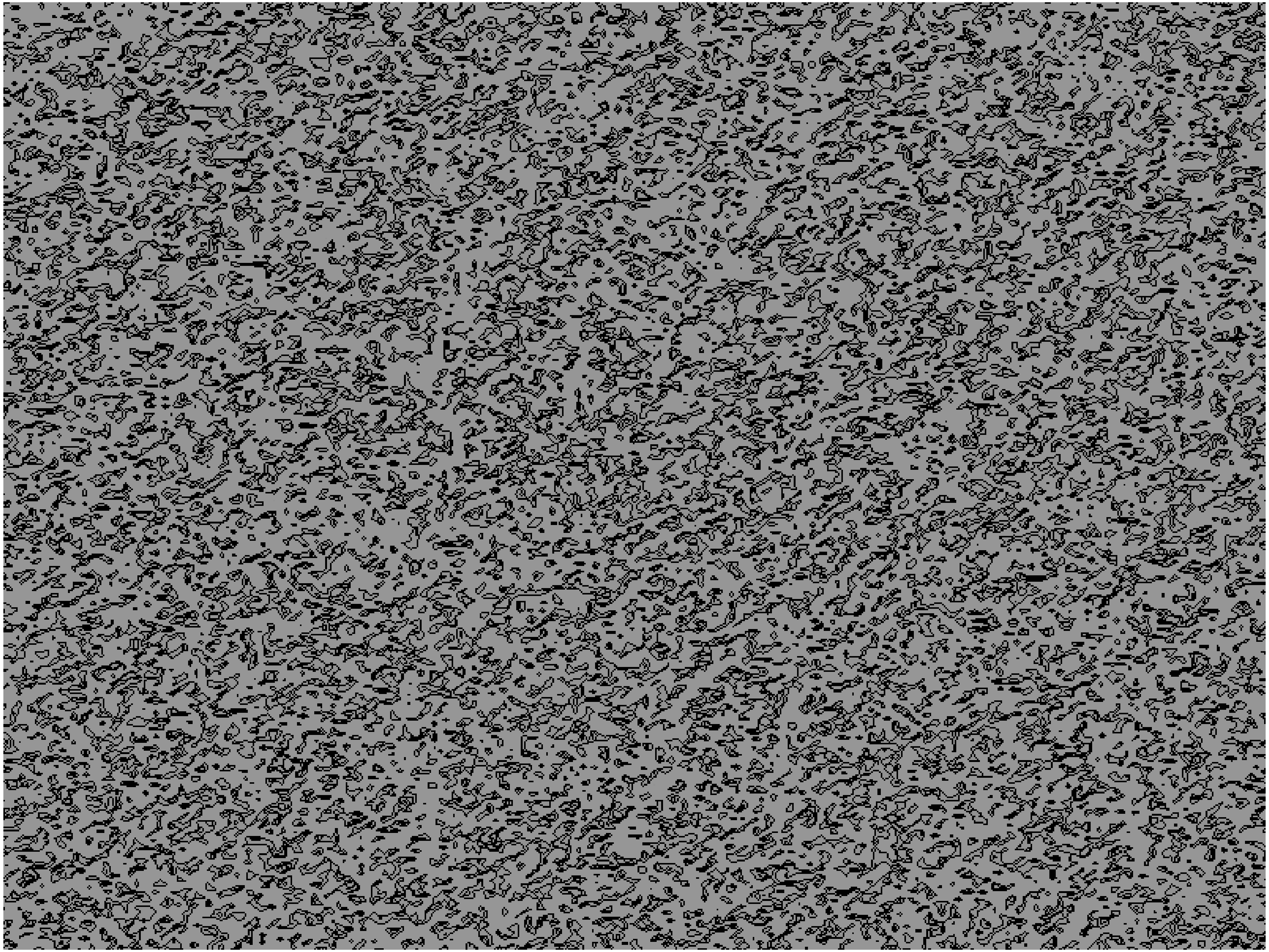


Grids



Reaction-diffusion system seeded in a spiral fashion





Is it similar ???