Special Purpose Parallel Supercomputer Based on the Dynamic Lattice Liquid Model

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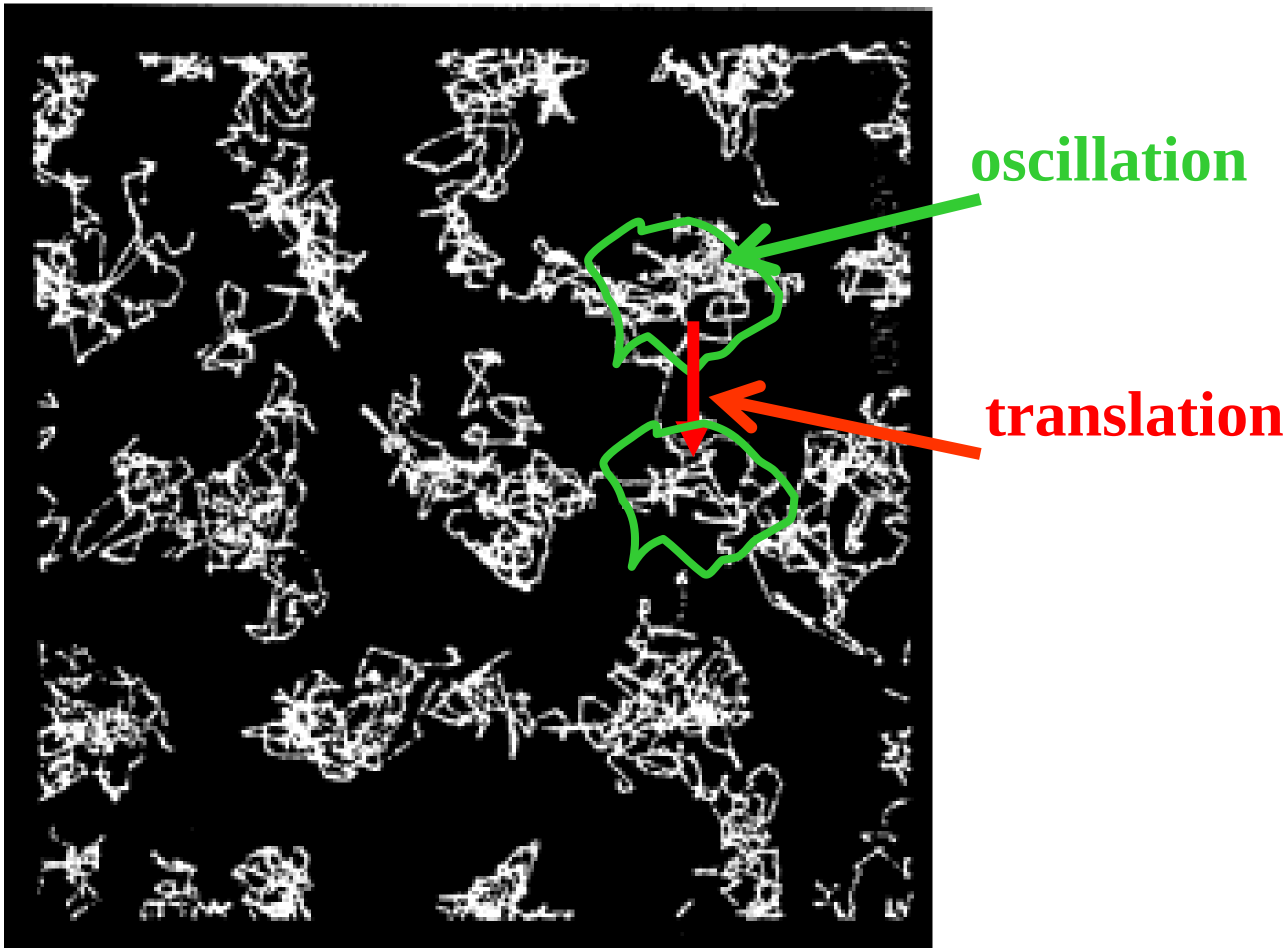
1

Movement of discs on the plane, without the friction

$$\sum_i E_i = const$$

$$\sum_i \vec{p}_i = const$$

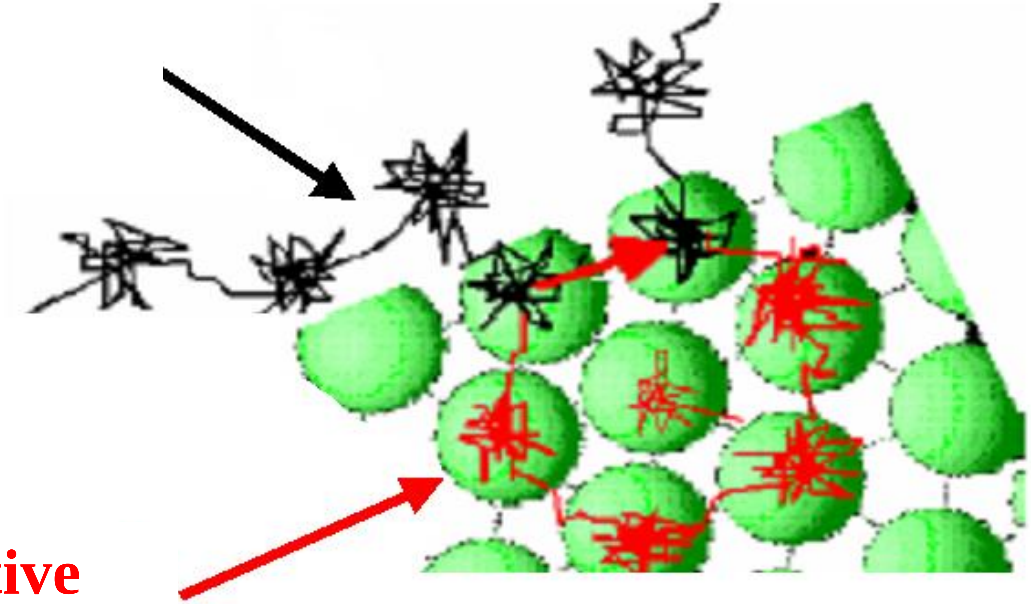
Computer Simulation
B. J. Alder i T. E. Wainwright, 1959



Studies in Molecular Dynamics B. J. Alder, T. E. Wainwright
J. Chem. Phys. 31, 459, (1959).

DLL model
T. Pakuła, 1997

Single molecule trajectory



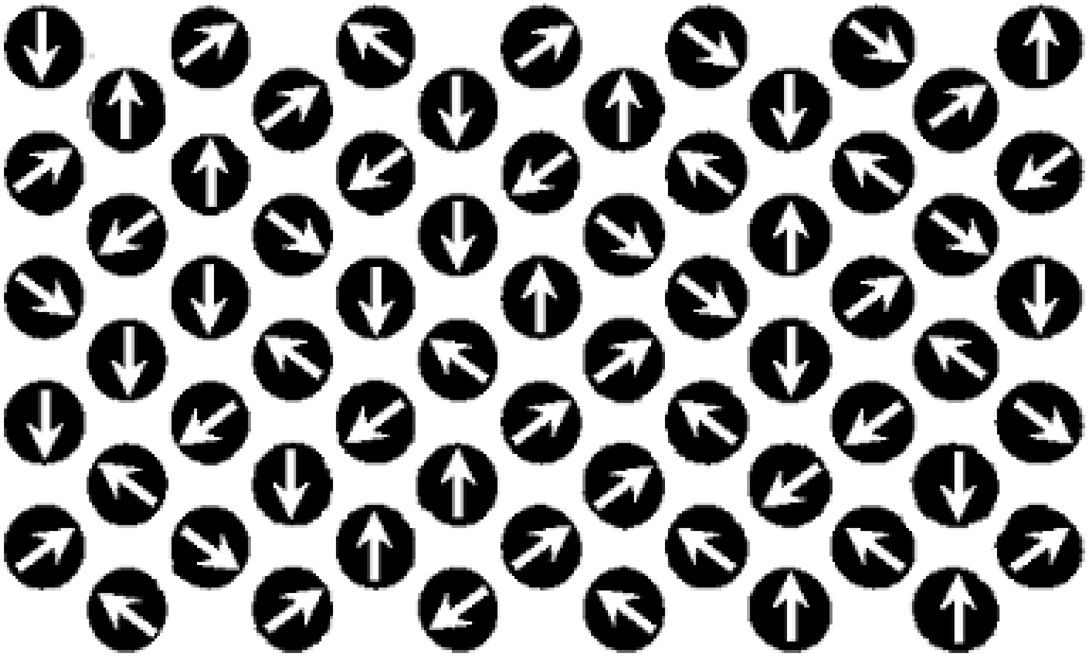
Cooperative movement

One simulation is a three steps' cycle

2

Step one

Randomising attempt of movements (oscillation)



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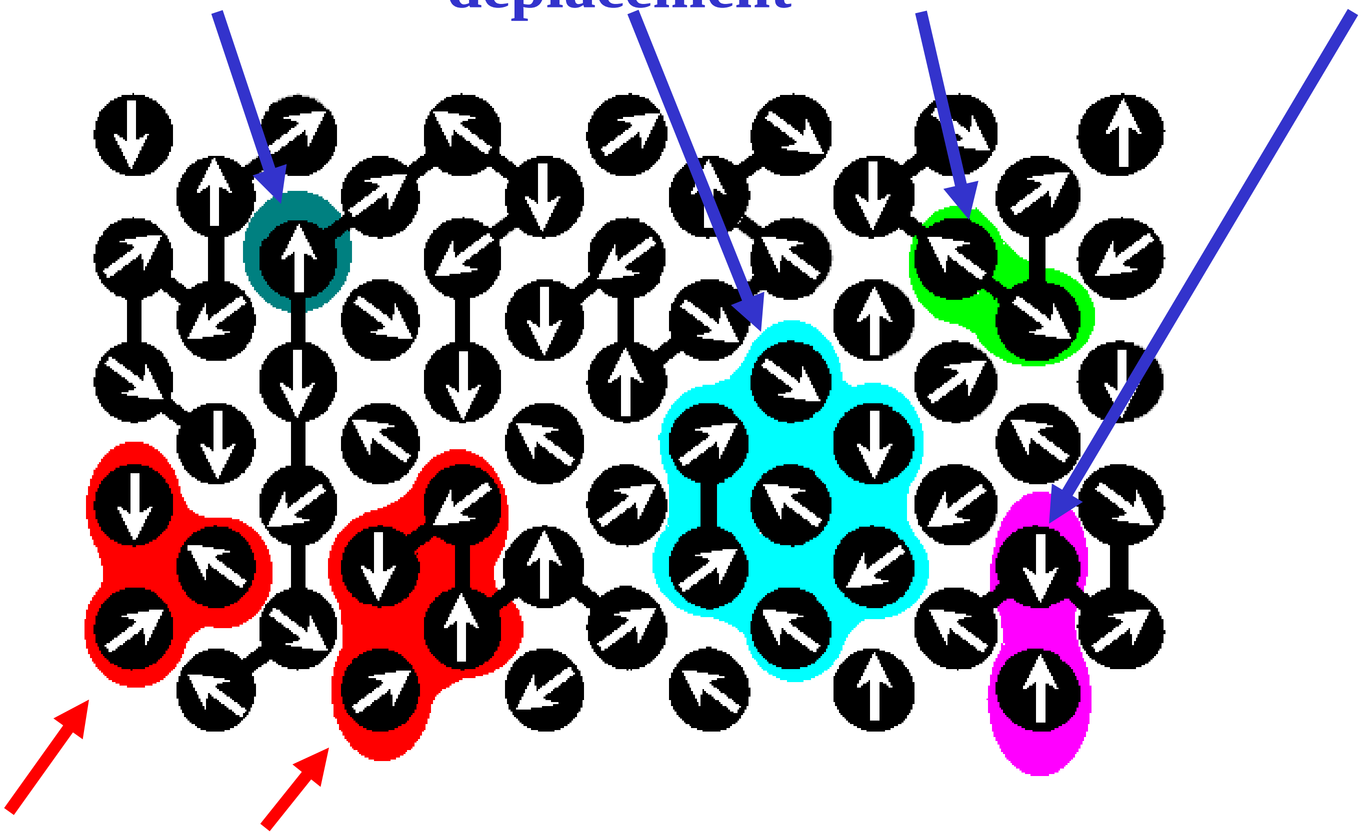
Step two

Looking for loops of cooperative movements

The particles may be chemically bounded

Attempt of movements, which will not cause the particles' deplacement



Cooperative movements

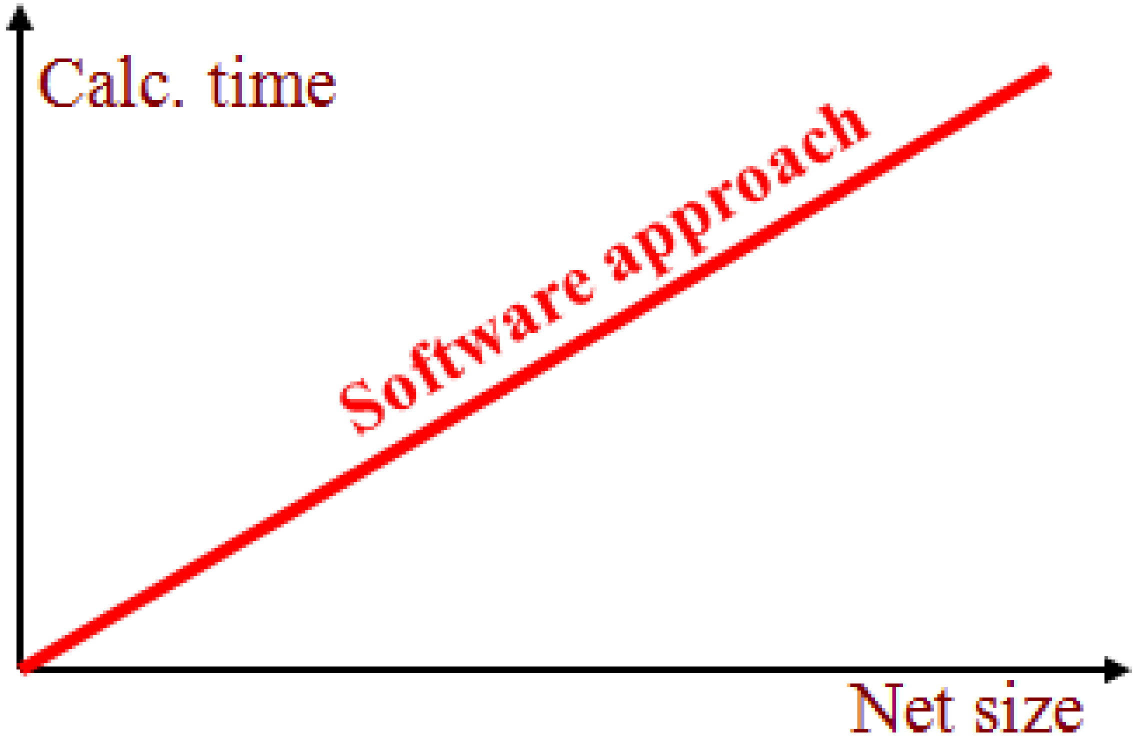
2

Step three

The deplacement of the coopertive loop's elements by one net position in the randomized direction (translation)

Software (sequential) implementation of DLL algorithm is

TIME CONSUMING !!!



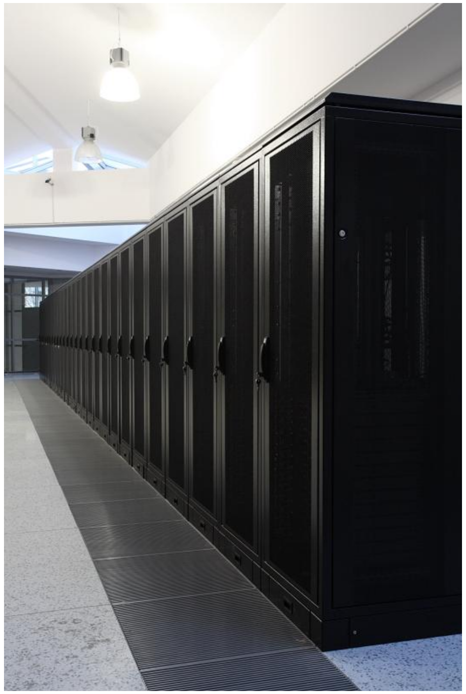
Supercomputers

Roadrunner (Los Alamos)
122 400 cores
1026 TFLOPS

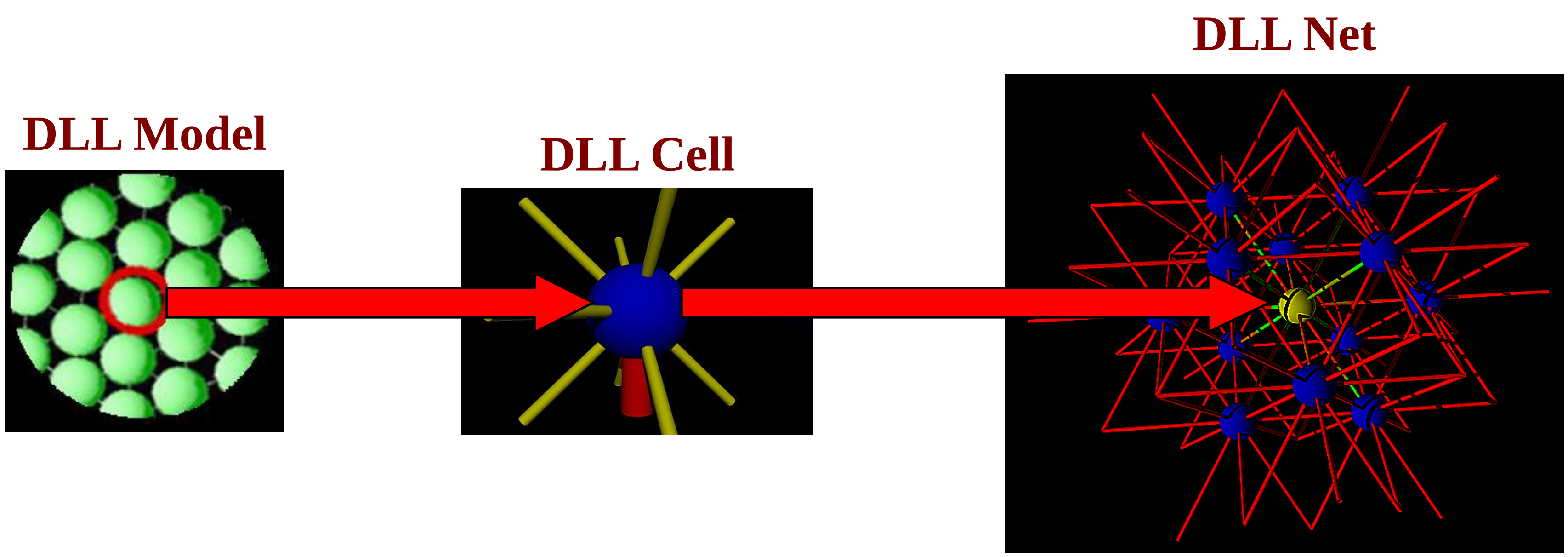
Galera (Gdańsk)
5 376 cores
50 TFLOPS

7 000 000 PLN
7 tons

16th in Europe
45th in the World



Due to **MANY INTERCONNECTIONS** general purpose clusters do not solve the problem...



Supercomputer DLL
J. Jung i P. Polanowski, 2002

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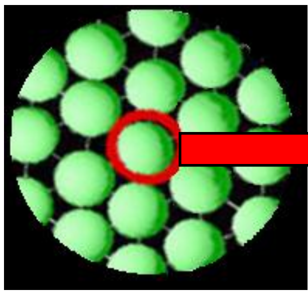
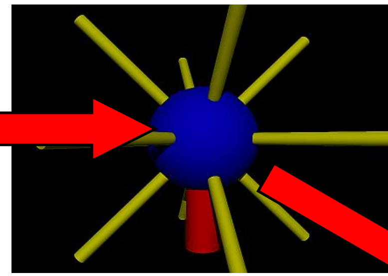
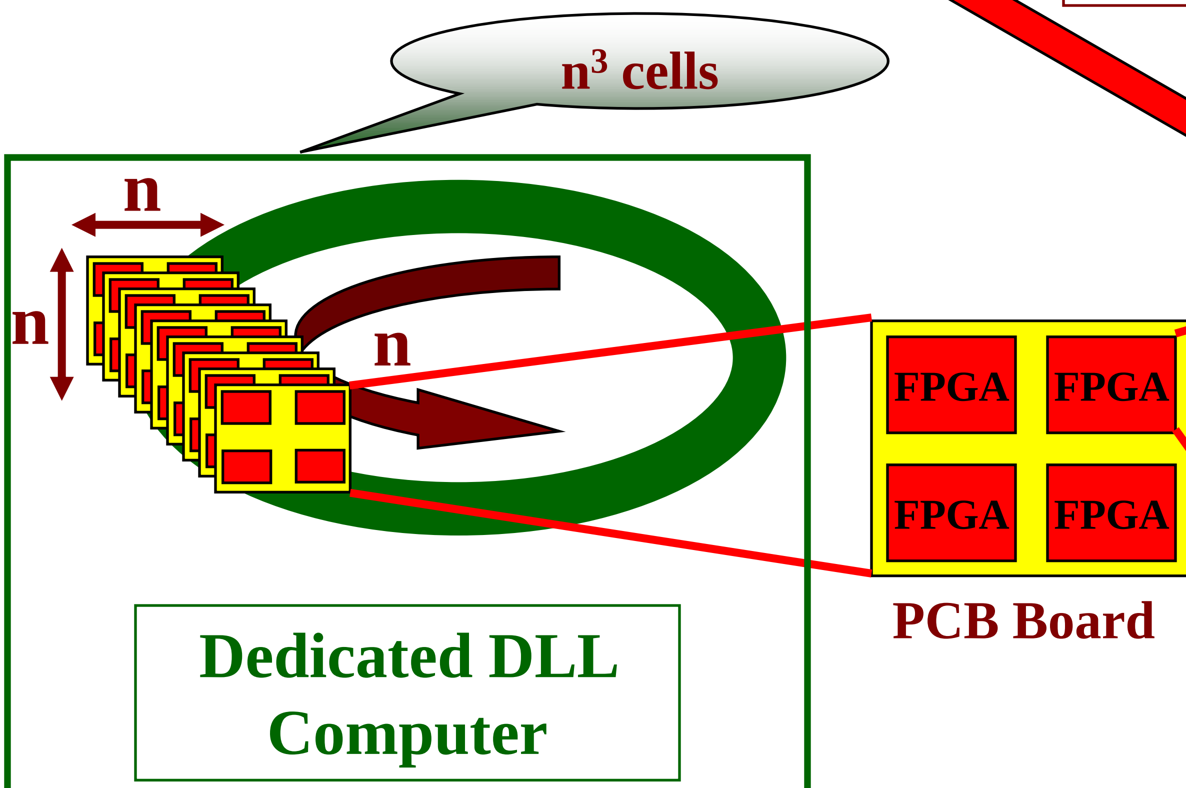
DLL Model



DLL Cell

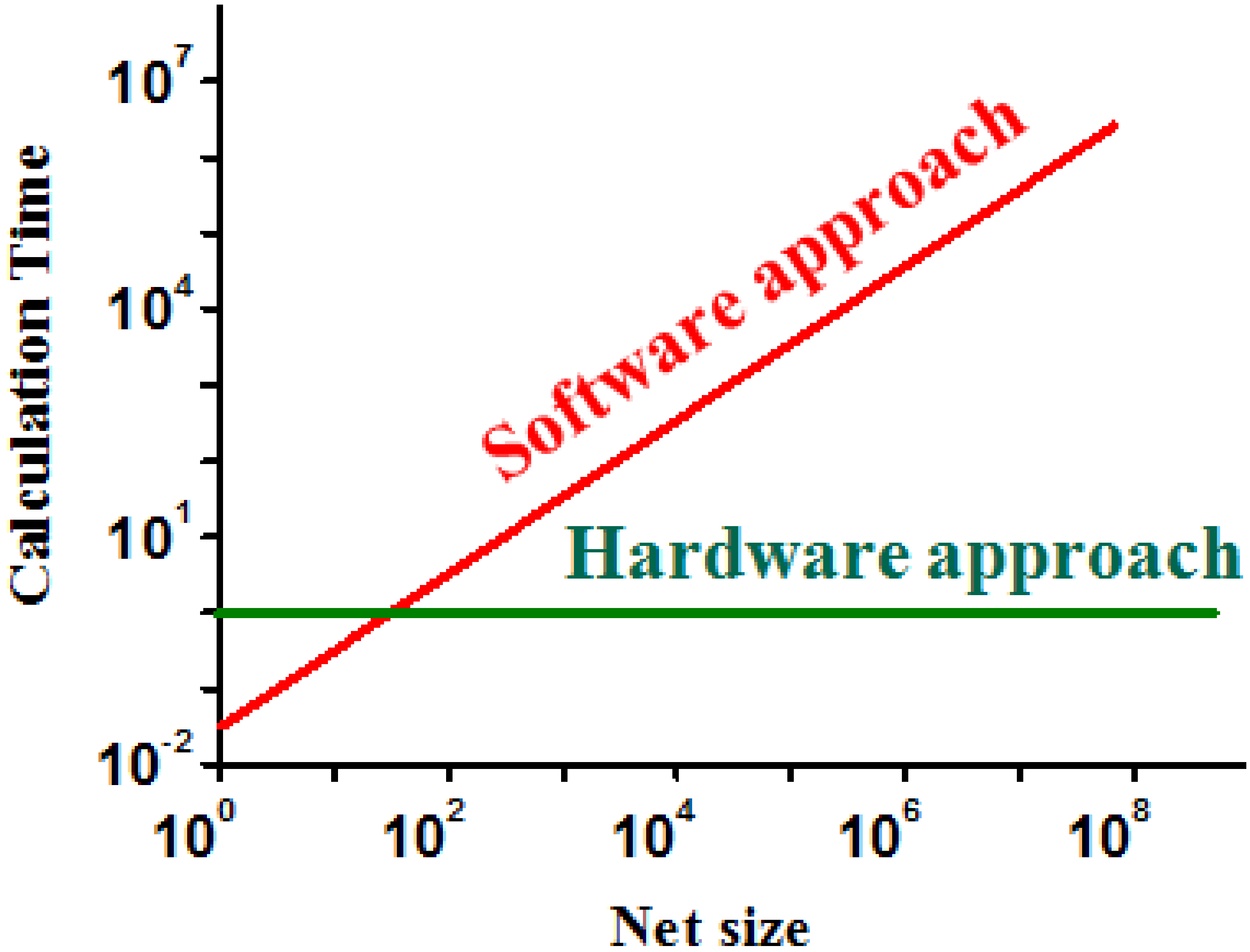


Each cell implemented **SEPARATELY !!!**
All cells work in **PARALLEL !!!**



FPGA

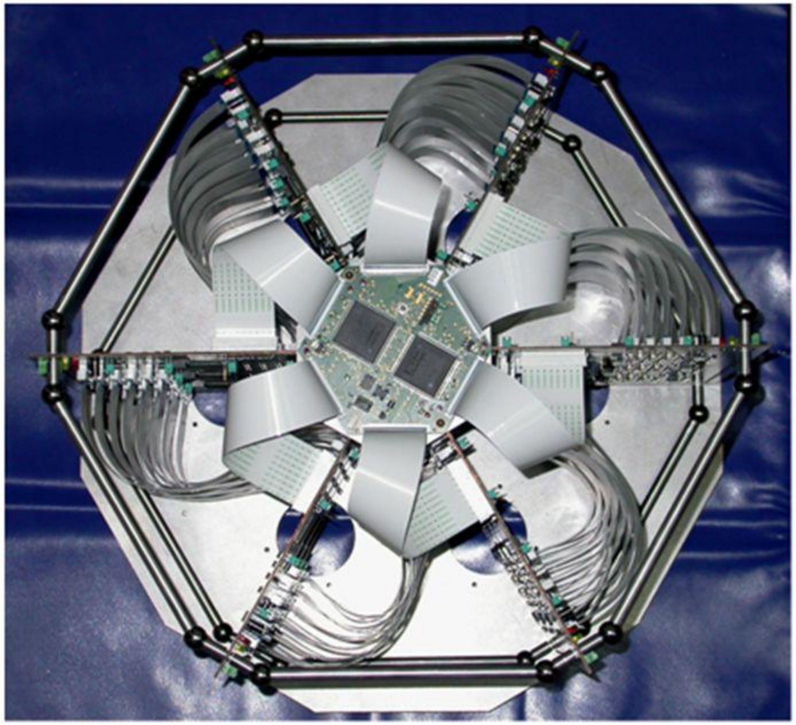
Main calculations are based on data exchanged only among **ADJACENT CELLS !!!**

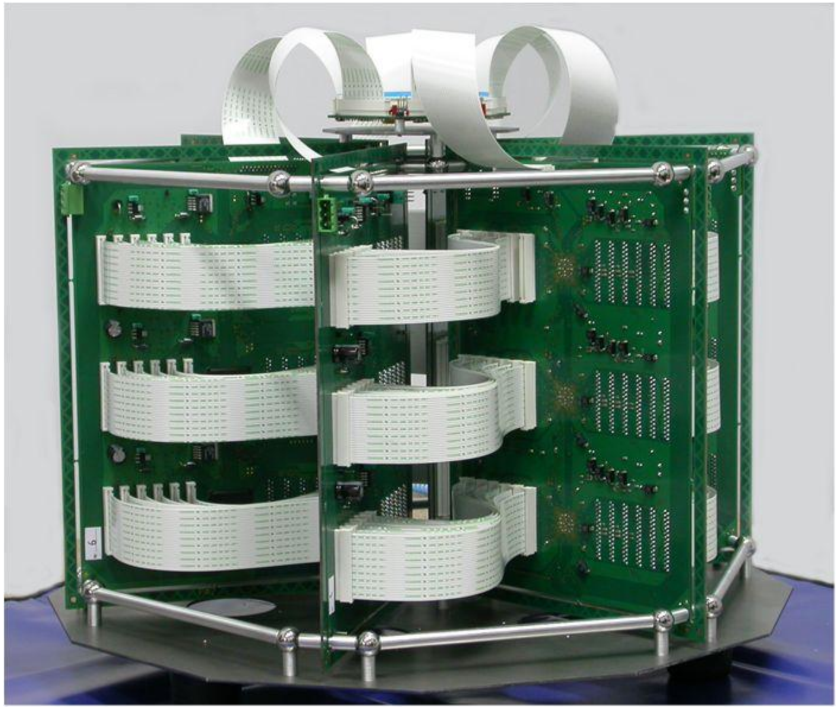


First approach
2005-2008

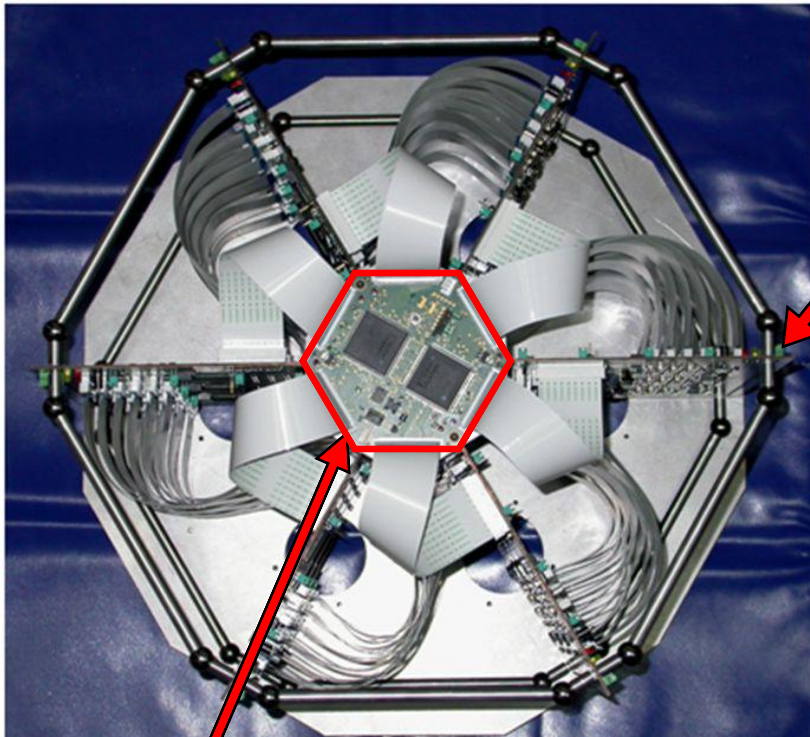
μSuperkomputer DLL:

- Net size: 6x6x6 (**216 cells)**
- 8 FPGA devices (XC3S4000)



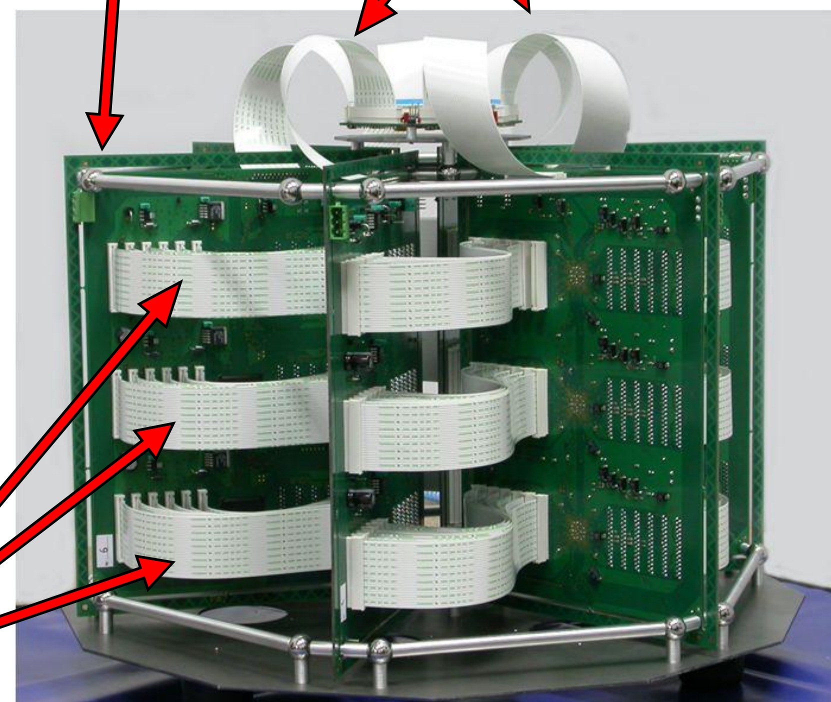


µSupercomputer DLL



PCB boards implementing network of DLL cells

Global Connections

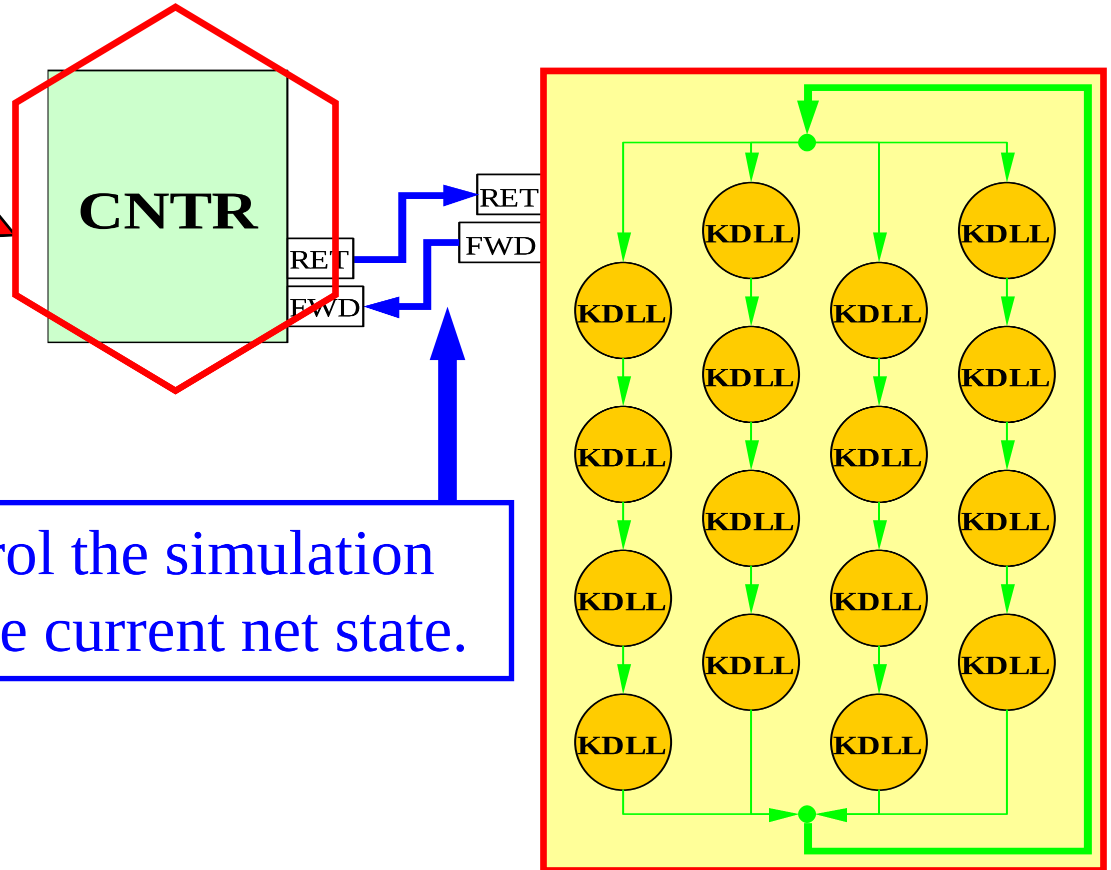


Control System

Local Interconnections

μSupercomputer DLL

Control System



Global connections control the simulation process and determine the current net state.

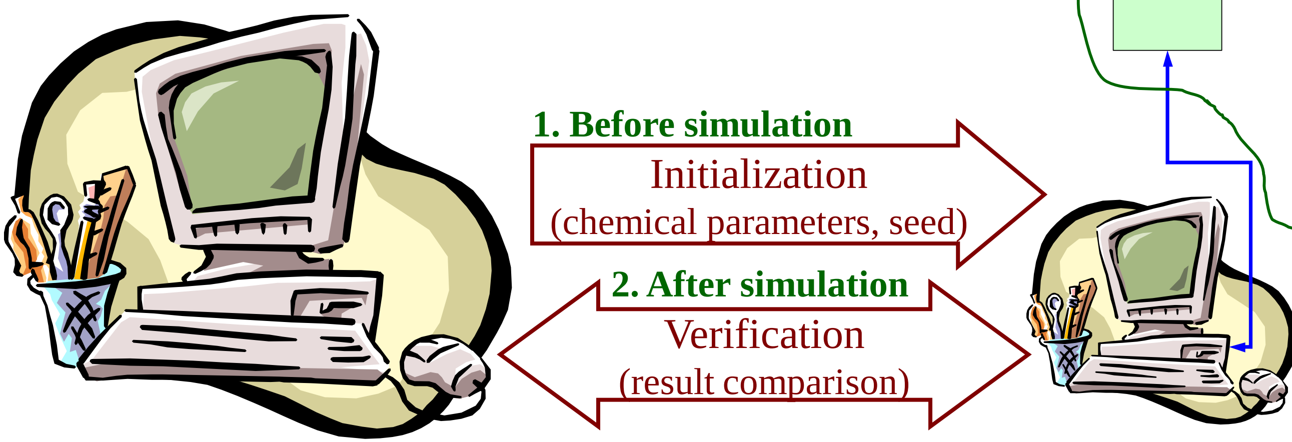
PCB boards implementing network of DLL cells

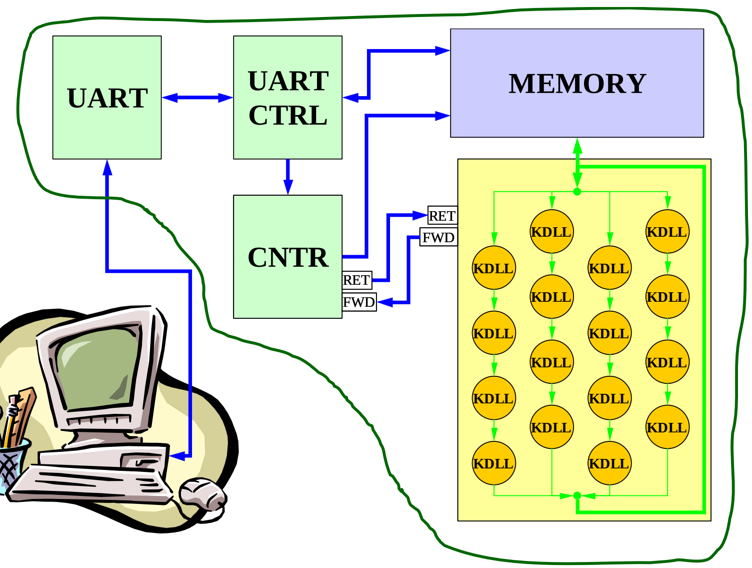
µSupercomputer DLL Verification 1:1

10 000 000 cycles

Software implementation of DLL algorithm. Standard **rand()** function replaced with dedicated **pseudorandom generator**.

µSupercomputer DLL with the same **pseudorandom generator.**

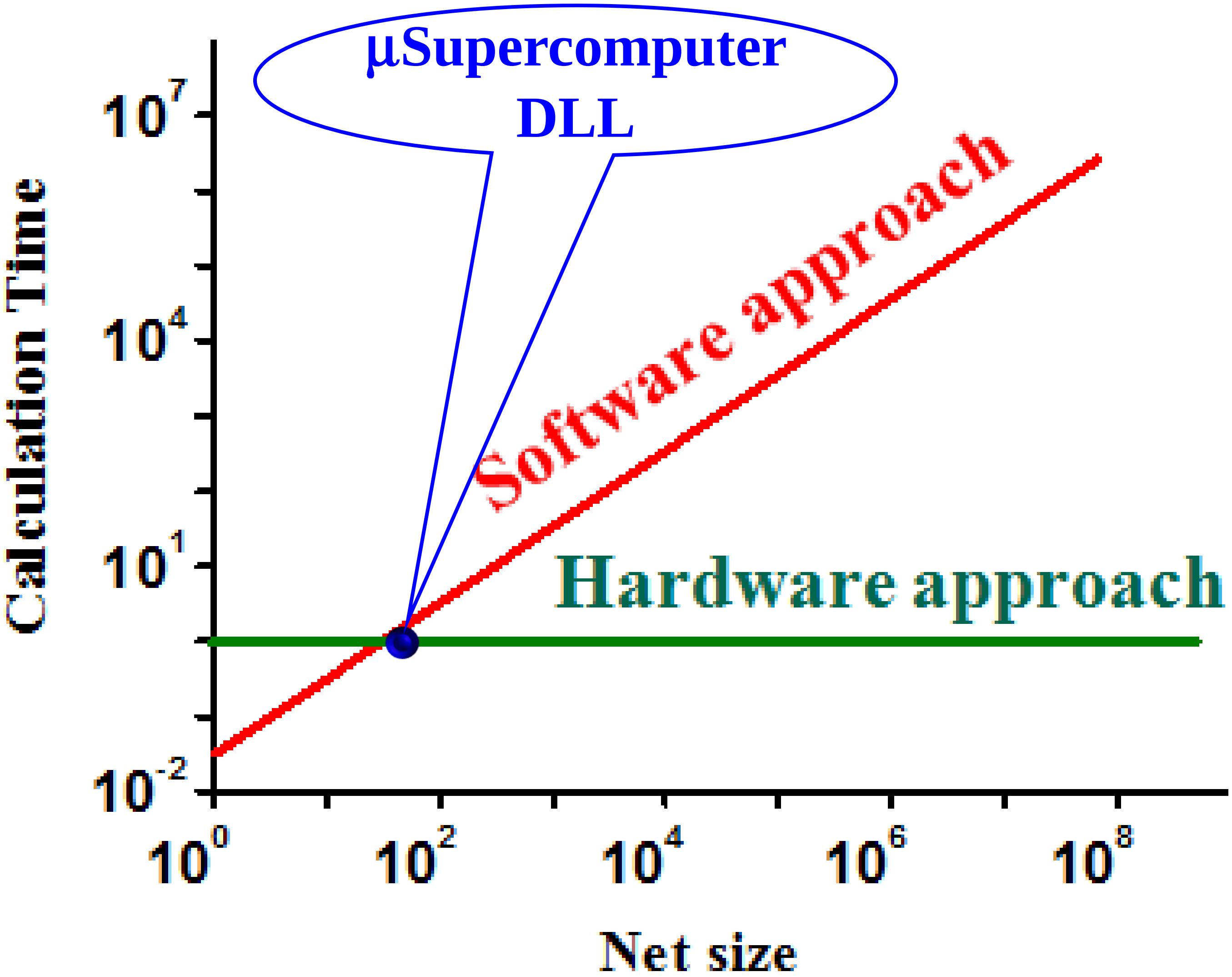




Clock freq.: 3.4 GHz → **136:1** → Clock freq.: 25 MHz

Calc. time: **101 s** → **-40%** → Calc. time: **65 s**

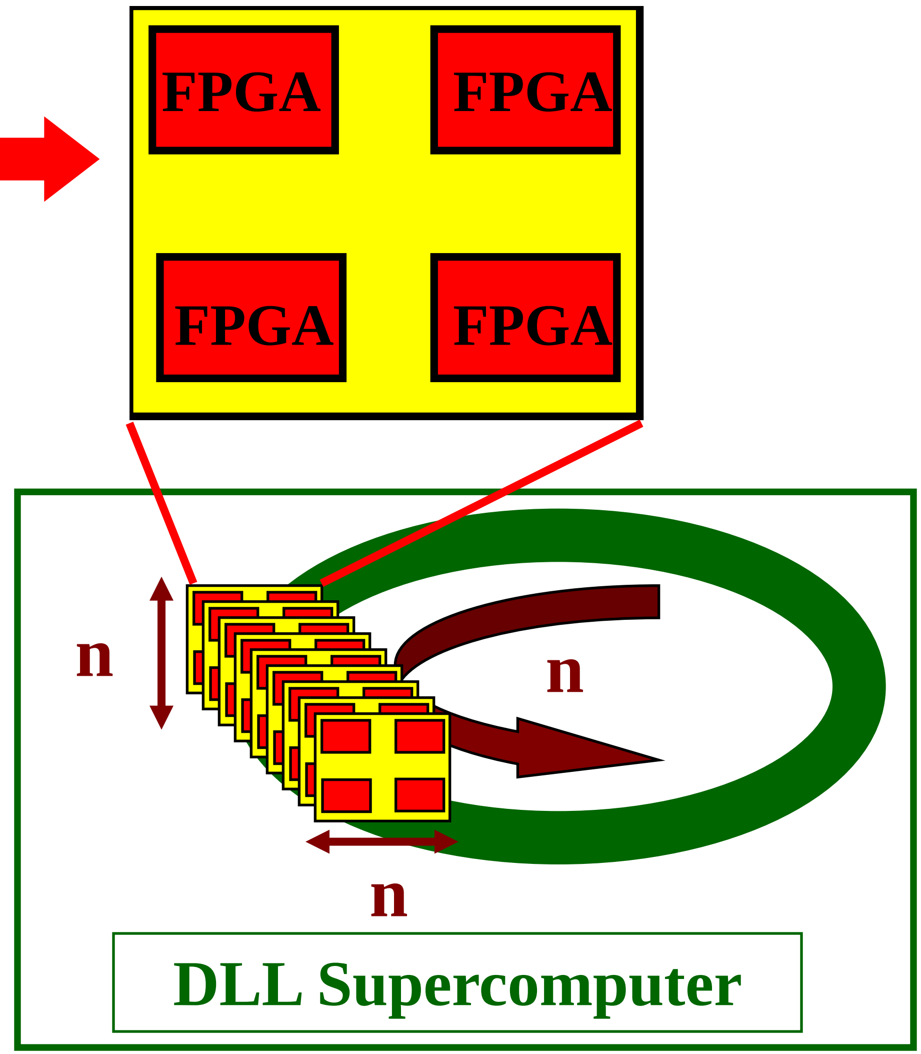
µSupercomputer DLL



Near future

2009-2012 – Grant sponsored by Polish Government

Elementary module of final Supercomputer

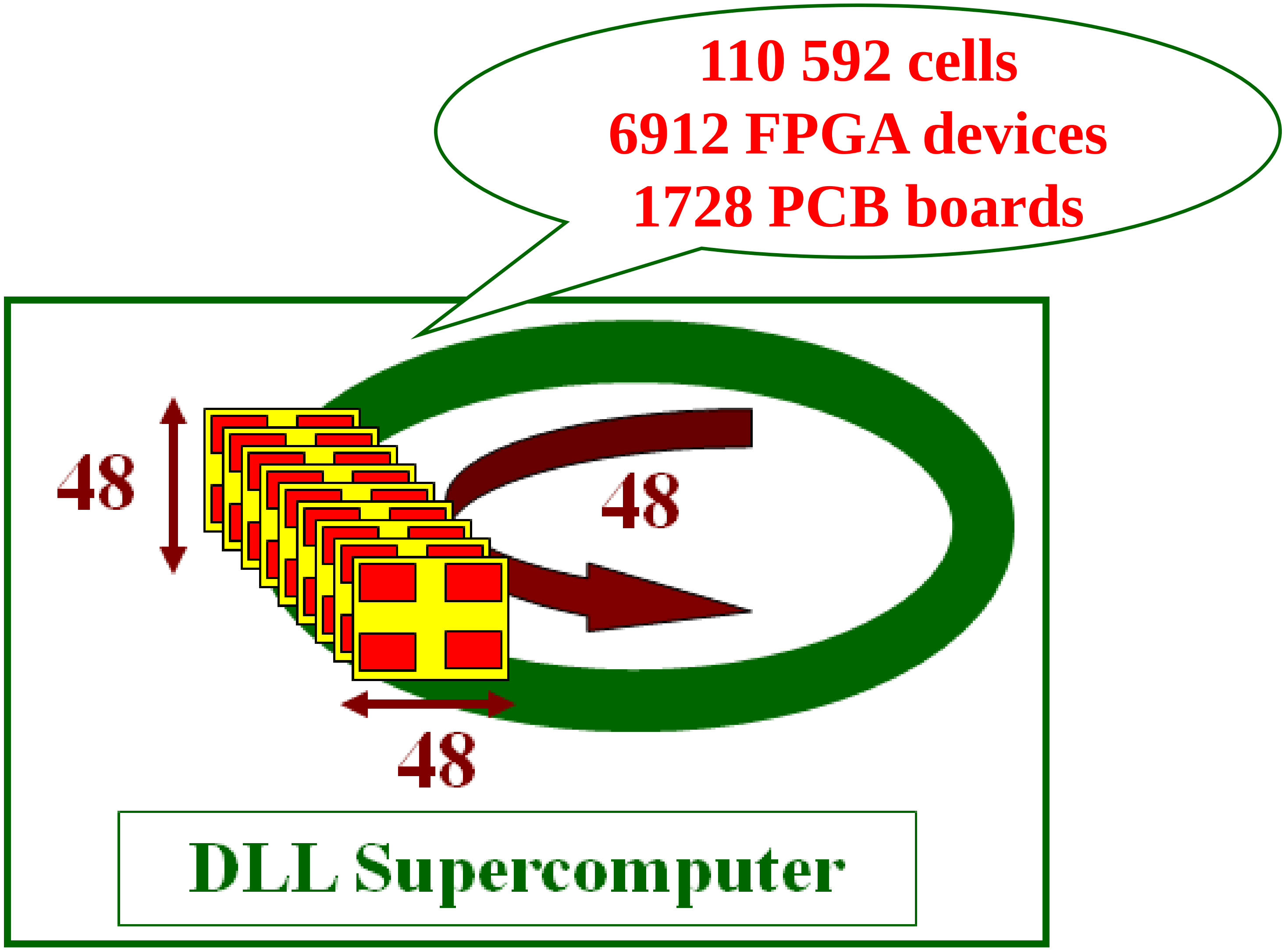


Main issues:

- Architecture, interface and mechanical structure
- Efficient data exchange protocols
- Power supply, configuration and synchronization
- Defect detection and elimination

Plan for future

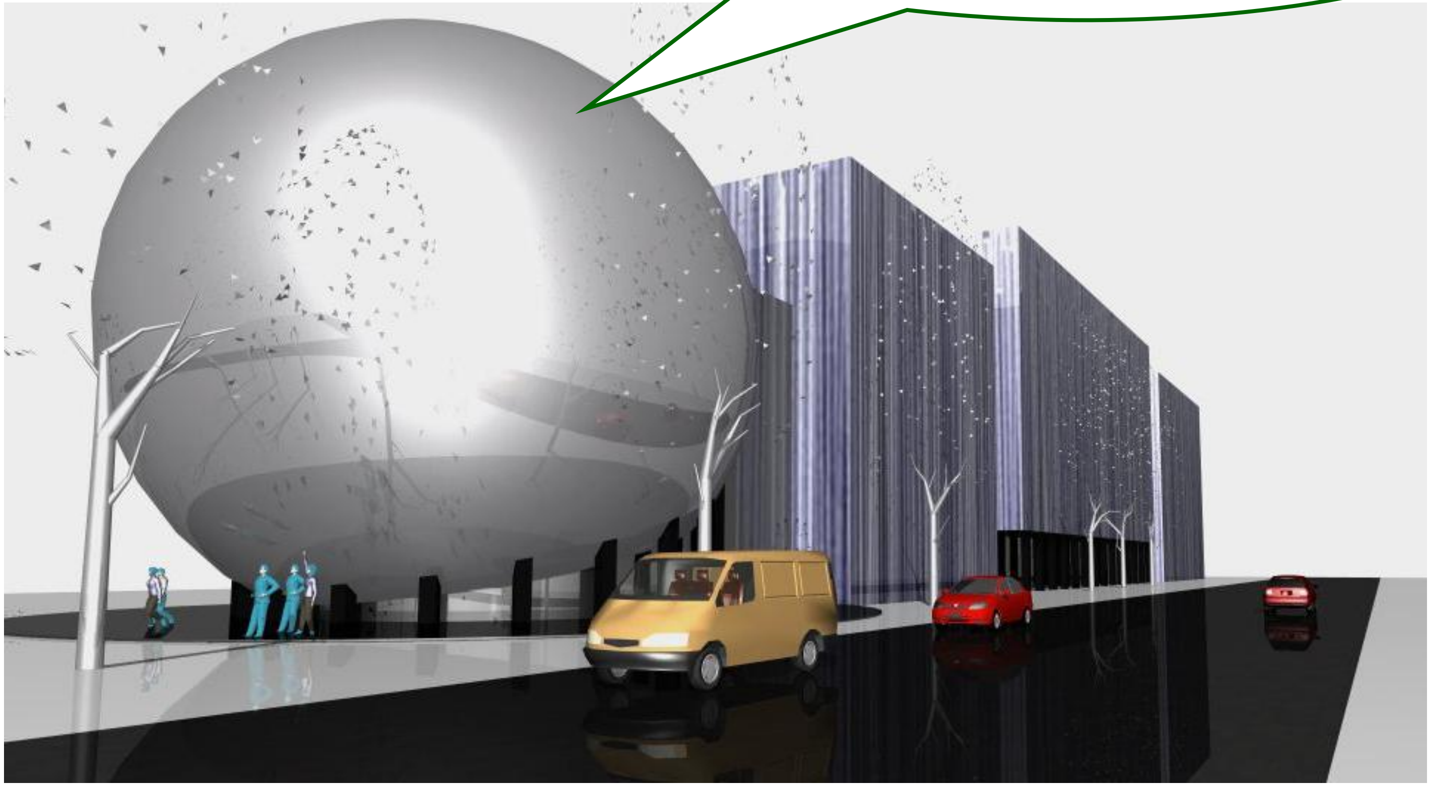
2010 – 2015 - European Centre of Bio- and Nanotechnology (ECBNT)



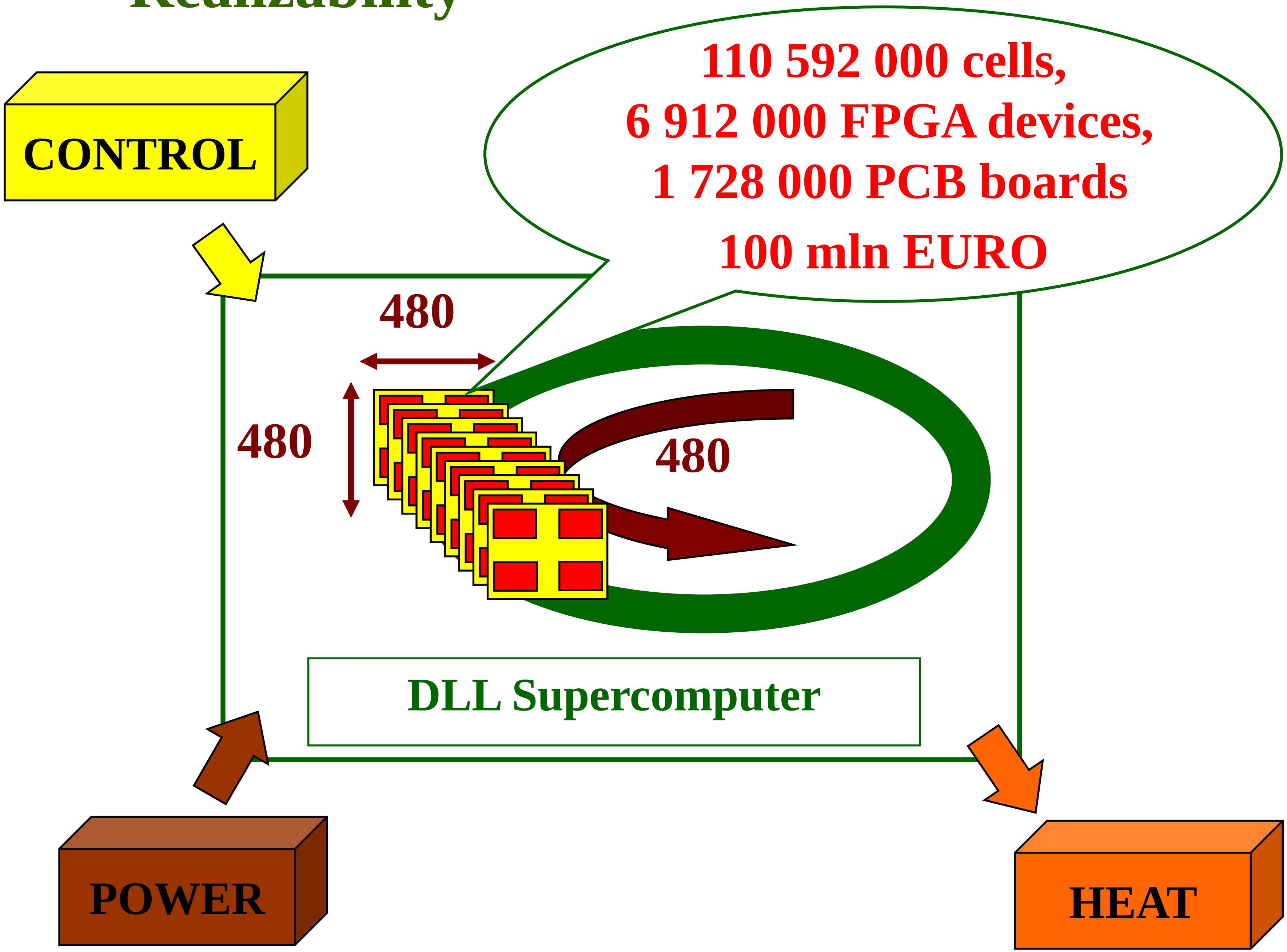
Plan for future

2010 – 2015 - European Centre of Bio- and Nanotechnology (ECBNT)

DLL Supercomputer
110 592 cells
4 mln EURO



Realizability



Thank you