Maxeler University program: The idea

What can we do for the academic groups?

- ✓ Provide dataflow HPC hardware and software free or at strongly reduced cost
- ✓ Share our expertise in dataflow implementation of computational algorithms
- ✓ Help in securing research funding for projects involving dataflow computing

How can we profit from the interaction with academic groups?

- ✓ We would like to see major, non-incremental scientific results being achieved with dataflow technology – we consider this as the best possible advertising
- ✓ We would like to expand the use of dataflow systems to entirely new areas where their commercial potential is not at all clear
- ✓ We would like to create an expertise base in dataflow system programming, especially in the key scientific centres in the world

“The exciting thing about this program is that it covers a wide spectrum of application areas in high performance computing and brings together centres of excellence in HPC using FPGA in USA, Europe, Japan and China into a powerful community”
(Ram Subramanian, Worldwide Manager of the Xilinx University Program)

Maxeler University Program Members

Korea University
Stanford University
Universität Hamburg — Der Forschung | Der Lehre | Der Bildung
FAU Friedrich-Alexander Universität Erlangen-Nürnberg
Max-Planck-Gesellschaft
Manchester Metropolitan University
Nanyang Technological University
Universität Paderborn
香港中文大學 The Chinese University of Hong Kong
Universidade de Lisboa
KIT Karlsruhe Institute of Technology
Politecnico di Milano
The University of Tokyo
Nagasaki University 長崎大学
Heriot Watt University
Berkeley University of California
复旦大学
Goethe Universität Frankfurt am Main
University of Windsor — thinking forward
Chalmers
University of Kragujevac
Technion Israel Institute of Technology
NUS National University of Singapore
University of Oxford
LMU Ludwig-Maximilians-Universität München
The Hong Kong Polytechnic University 香港理工大學
University of Belgrade
Technische Universität Kaiserslautern
東北大学 Tohoku University
UIC University of Illinois at Chicago
JAIST Japan Advanced Institute of Science and Technology
Ss. Cyril & Methodius University of Skopje, Macedonia
UBC
清華大學 Tsinghua University
The University of Manchester — Manchester Business School
UiO University of Oslo
Technical University of Crete
Imperial College London
The University of Hong Kong
UCL
UBC
TU Delft — Delft University of Technology
UCLA
AGH University of Science and Technology
조선대학교 Chosun University
Northeastern University

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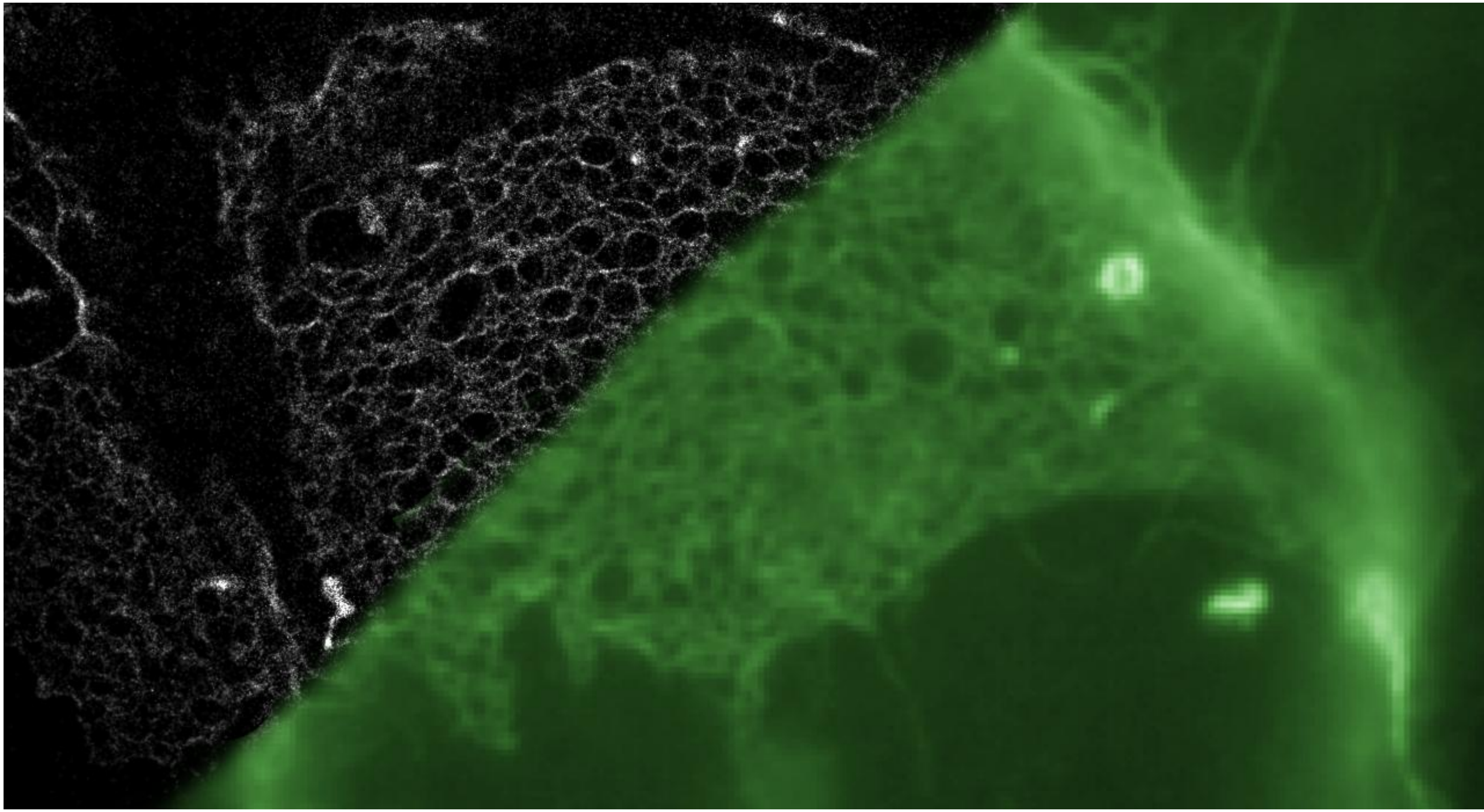
Maxeler University Program Members

Maxeler University Program Members

- Tsinghua University
- University of Tokyo
- Technion-Israel Institute of Technology
- University of Oslo
- University of Hamburg
- Nanyang Technological University
- National University of Singapore
- Korea University
- Japan Advanced Institute of Science and Technology
- University of Kaiserslautern
- Universität Erlangen-Nürnberg
- Manchester Metropolitan University
- Politecnico di Milano
- Hunan University
- Stanford University
- Universität Paderborn
- Universität Hamburg
- Goethe-Universität Frankfurt am Main
- Tohoku University
- University of Lisbon
- Chalmers University of Technology
- Northeastern University
- University of Edinburgh
- Heriot-Watt University
- Delft University of Technology
- University of Oxford
- Hong Kong University
- University of Illinois at Chicago
- The Chinese University of Hong Kong
- Max-Planck-Institut für molekulare Genetik
- Karlsruhe Institute of Technology
- Nagasaki University
- University of California Berkeley
- University of British Columbia
- Imperial College London
- University of Brlgrade
- University of Novi Sad
- Kragujevac University
- AGH University of Science and Technology
- University of Windsor, Ontario
- Manchester Business School
- Fudan University
- Hong Kong Polytechnic University
- Univ. Sts Cyril and Methodius
- TU Crete
- UCL
- UCLA
- UBC-EOS
- Chosun University
- Ludwig-Maximilians Universität München

MAX-UP: The scope of subjects

- **Financial modelling**
- **Quantum chemistry**
- **Bio-chemical engineering**
- **Geophysics**
- **Atmospheric physics**
- **Strong-field laser physics**
- **Virtual reality and computer gaming**



KIRCHHOFF-
INSTITUTE
FOR PHYSICS

Localization microscopy enhances the resolution of fluorescence light microscopy (shown in green) by about an order of magnitude. Single fluorescent molecules act as switchable markers. Their detected signals can be fitted with a two-dimensional Gaussian distribution and thus located with sub-pixel resolution. Using MaxCompiler we achieved a hardware acceleration of 225 in signal detection and fitting.

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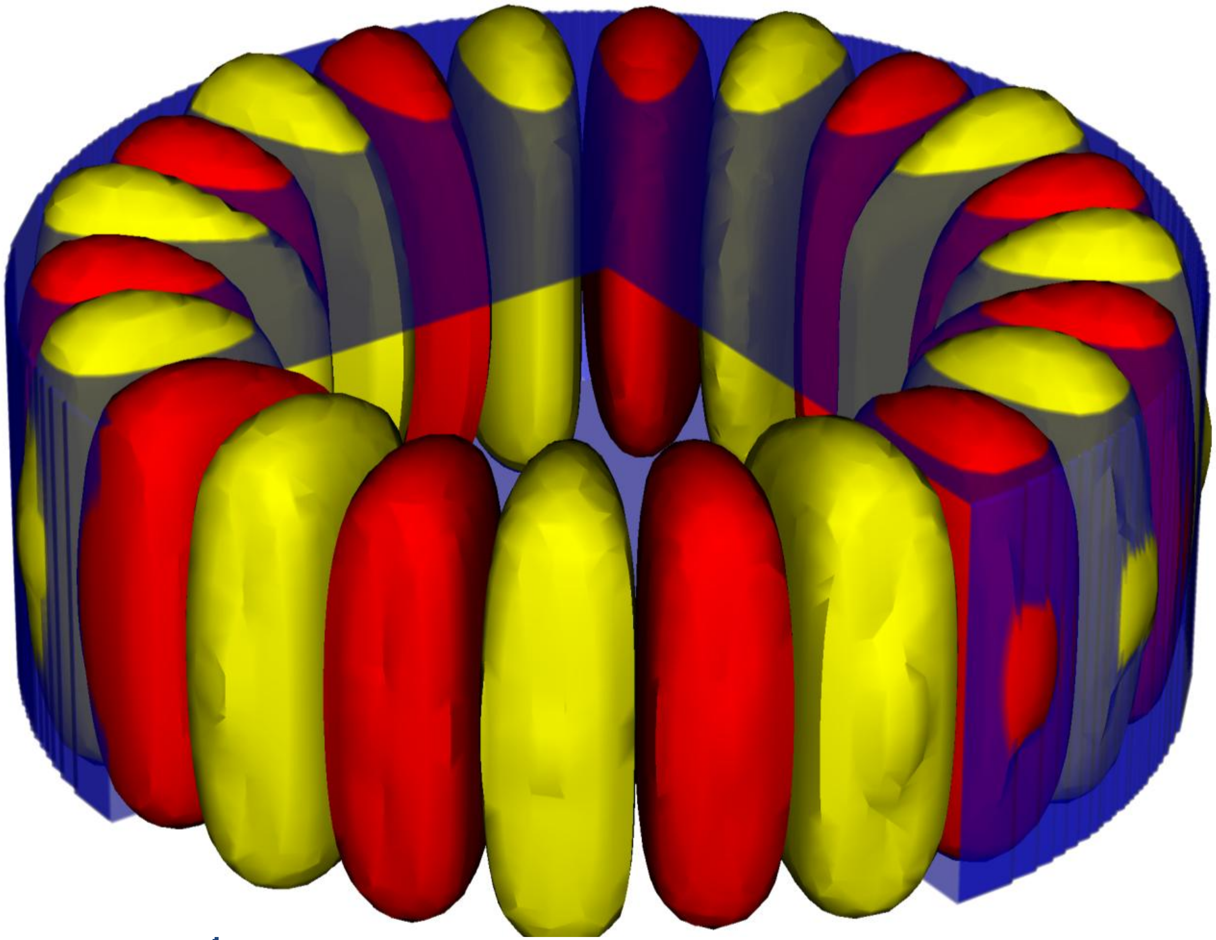

Acceleration of simulations of computational nanophotonics using Maxeler MaxGenFD Finite Difference Compiler for dataflow

UNIVERSITÄT PADERBORN

Die Universität der Informationsgesellschaft

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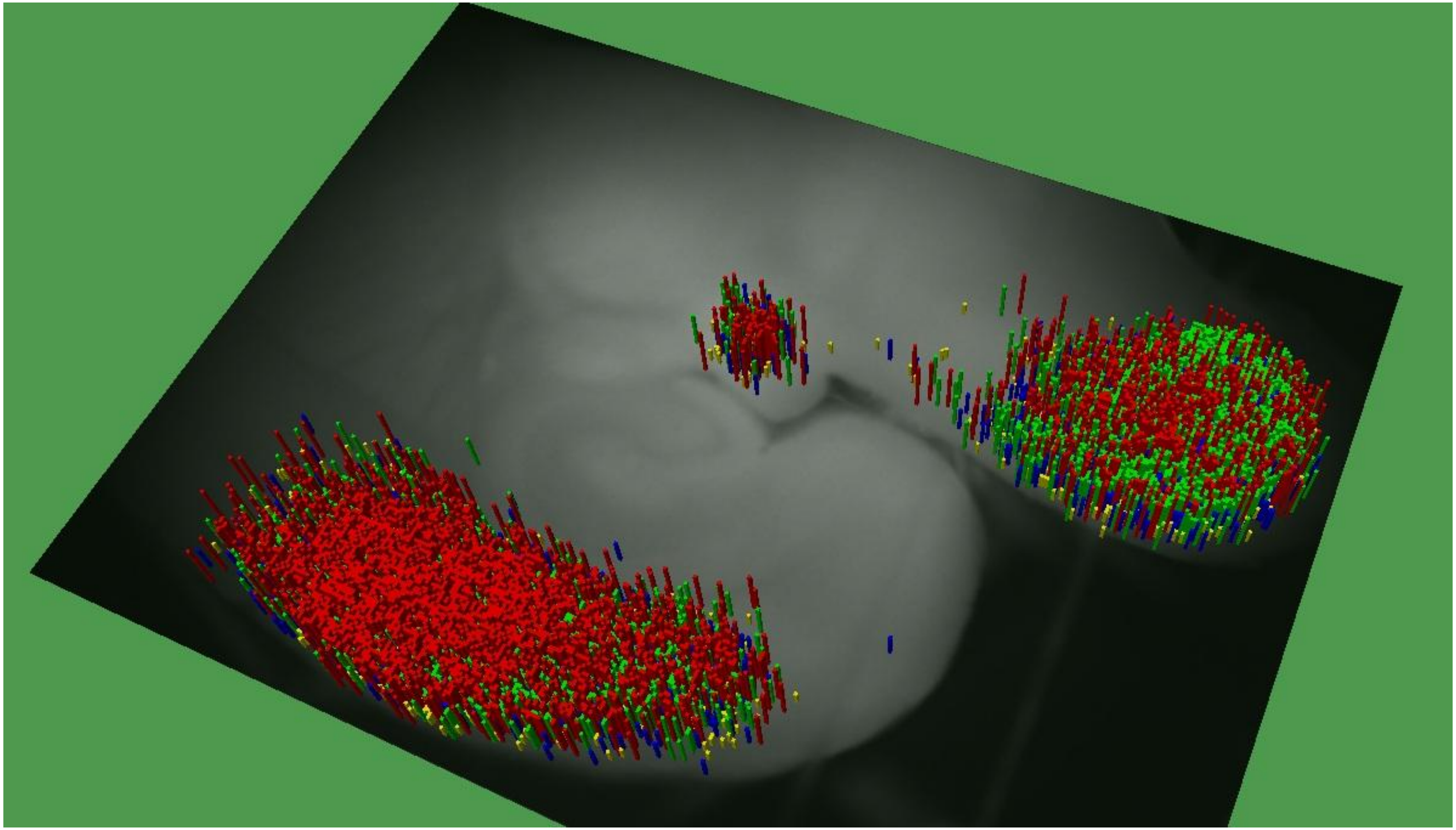

UIC University of Illinois at Chicago

Brain network analysis
Dynamic community analysis on corpus callosum to identify functional regions. By accelerating the linear correlation calculation, Maxeler dataflow engines can build brain networks on-the-fly while the lab experiment is running.

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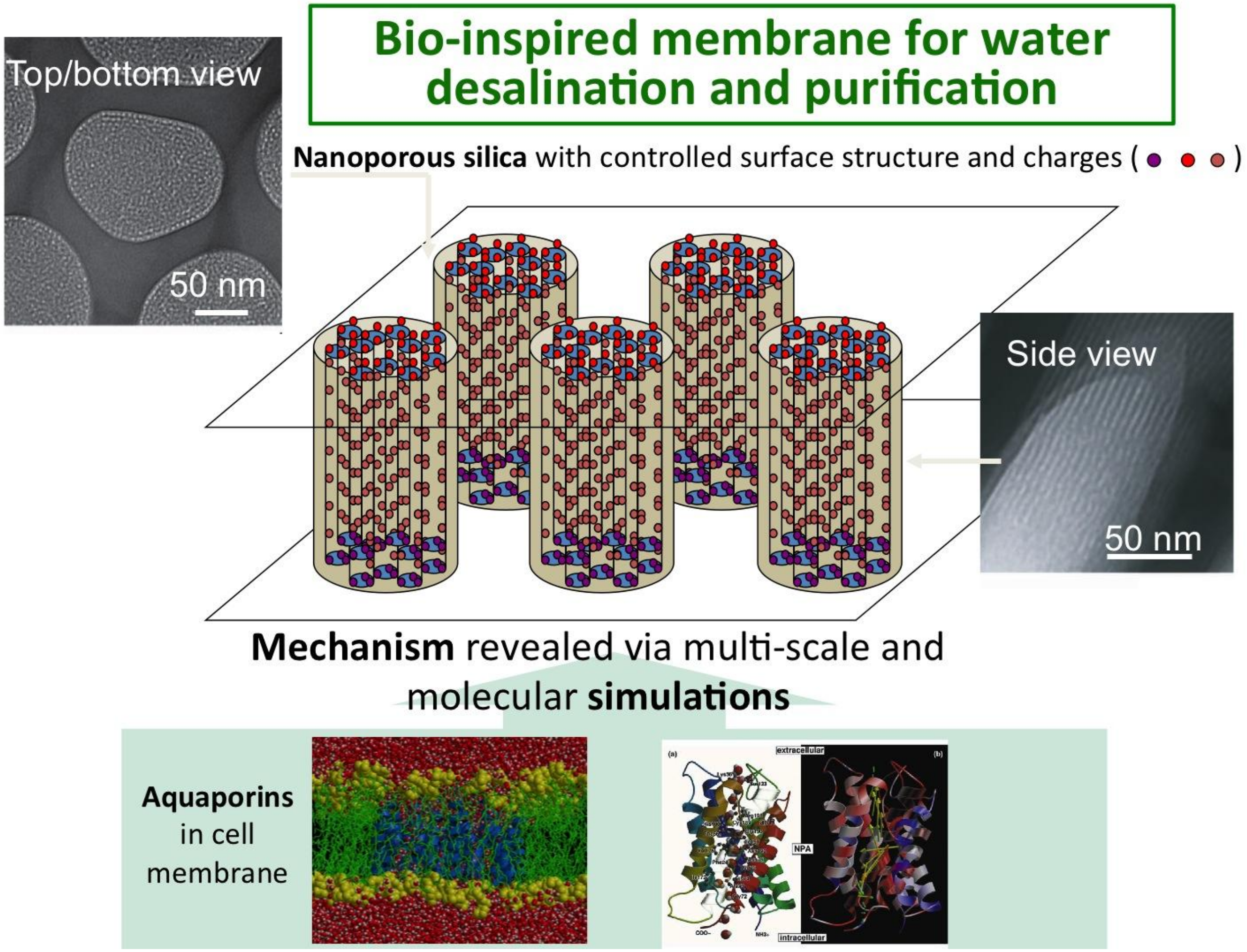

Simulation-Aided Design and Synthesis of Bio inspired Membranes for Water Desalination and Purification

CAVE automatic virtual environment

This project will investigate the use of dataflow architectures in creation of *high-end immersive virtual reality*. The goal is to build a proof of concept simulator with *extremely low latency*.

UCL

A MAX-UP project example

W Vigor, A Thom*, M Bearpark, Chemistry, Imperial College; R Bruce, Maxeler
*now at Cambridge

Imperial College London

Astrochemistry

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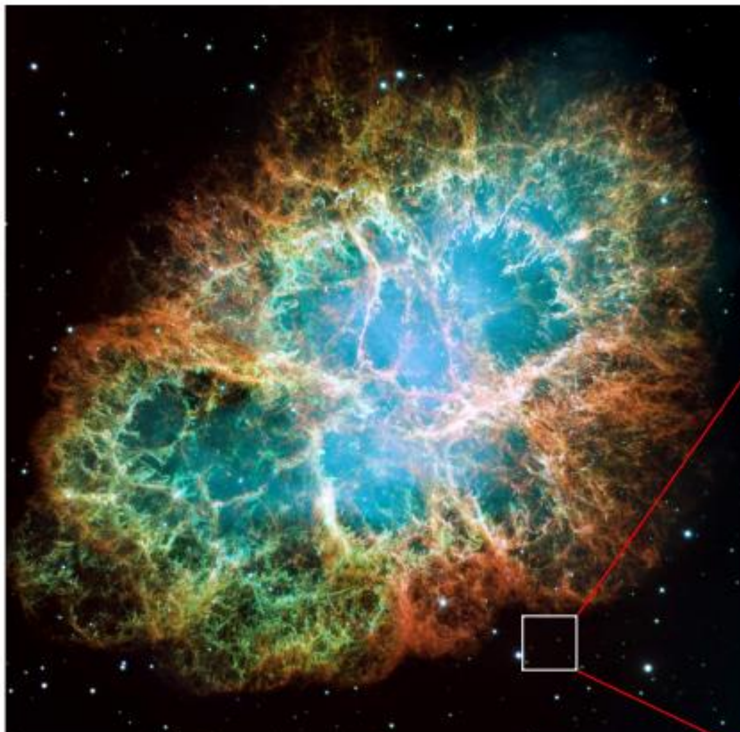
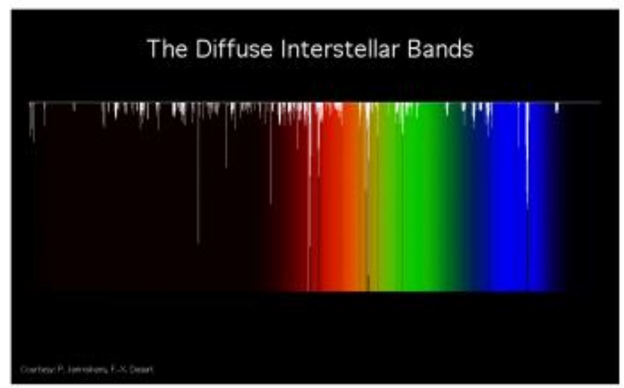
MAXIMUM PERFORMANCE COMPUTING



coronene: $C_{24}H_{12}$



http://www.nasa.gov/

P. Jenniskens and F.-X. Desert, *Astronomy and Astrophysics Supp. Ser.* **106**, 39–78 (1994)

Imperial College London

Chemistry

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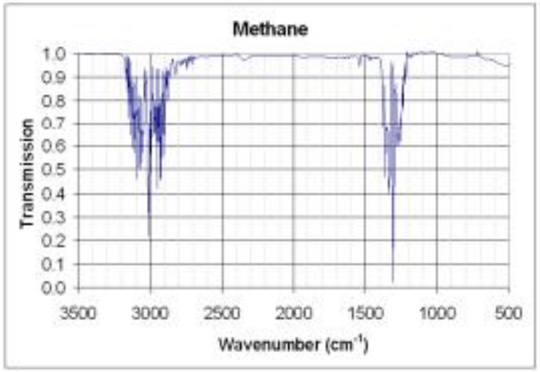
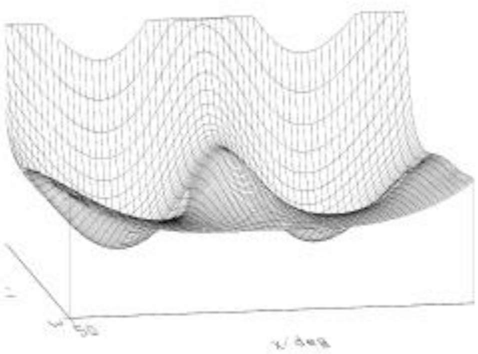
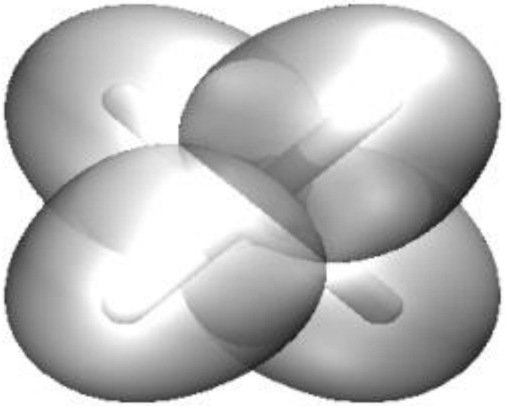
MAXIMUM PERFORMANCE COMPUTING



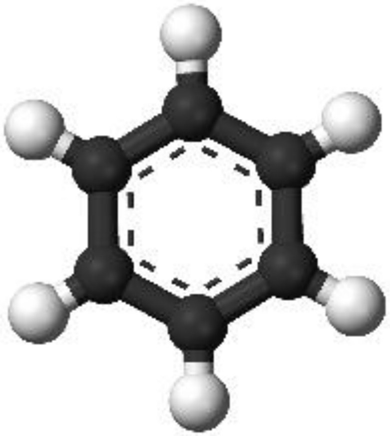




Vibrational spectrum $\Longleftarrow$ Energy surface $\Longleftarrow$ Electronic structure

R. Marquardt and M. Quack, *J. Phys. Chem. A* **108**, 3166–3181 (2004)

The Scaling Problem



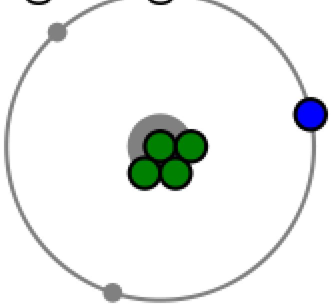
	CH_4	C_6H_6	$C_{24}H_{18}$
N	10	42	156
M	172	510	2500
N_d	10^9	10^{62}	10^{253}

FCI Quantum Monte Carlo

- Solutions to $\mathbf{H}\mathbf{c} = E\mathbf{c}$ also solve $e^{-\tau\mathbf{H}}\mathbf{c} = e^{-\tau E}\mathbf{c}$.
- Propagate $\frac{\partial \mathbf{c}}{\partial \tau} = -\mathbf{H}\mathbf{c}$.
- Lowest energy eigenvector $\mathbf{c}$ becomes dominant.

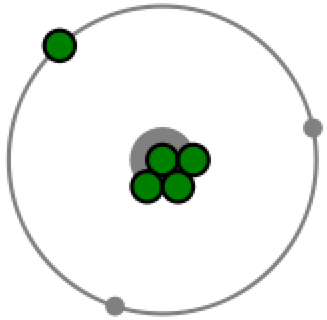
$$\frac{\partial c_{\mathbf{i}}}{\partial \tau} = -\sum_{\mathbf{j}} H_{\mathbf{ij}} c_{\mathbf{j}}.$$

- Represent $c_{\mathbf{i}}$ as populations of signed psips propagating through space.



Dynamics

$$\frac{\partial c_{\mathbf{i}}}{\partial \tau} = -[H_{\mathbf{ii}} - S]c_{\mathbf{i}} - \sum_{\mathbf{j}\to\mathbf{i}} H_{\mathbf{ij}} c_{\mathbf{j}}.$$

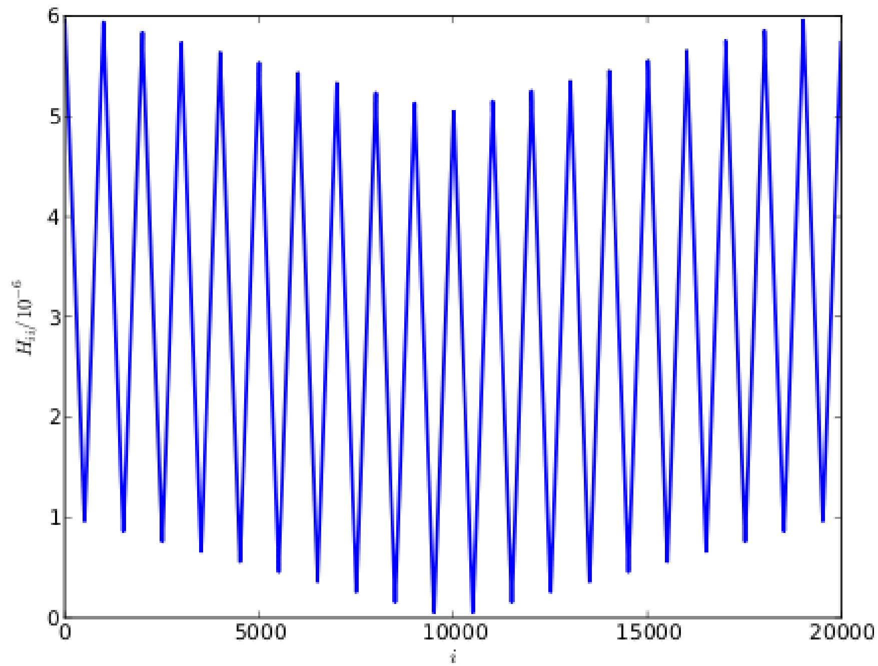


- Given a psip at $\mathbf{j}$, at time $\tau + \delta\tau$ spawn a new one at randomly chosen $\mathbf{i}$ based on $-\delta\tau H_{\mathbf{ij}}$. This samples $\sum_{\mathbf{j}}$.
- Psips at $\mathbf{i}$ die based on $\delta\tau(H_{\mathbf{ii}} - S)$.
- Start $S = \min H_{\mathbf{ii}}$. Once enough psips created change S in response to population. e.g. for growth, make S more negative, so more death.
- Opposite-signed psips at the same determinant annihilate.

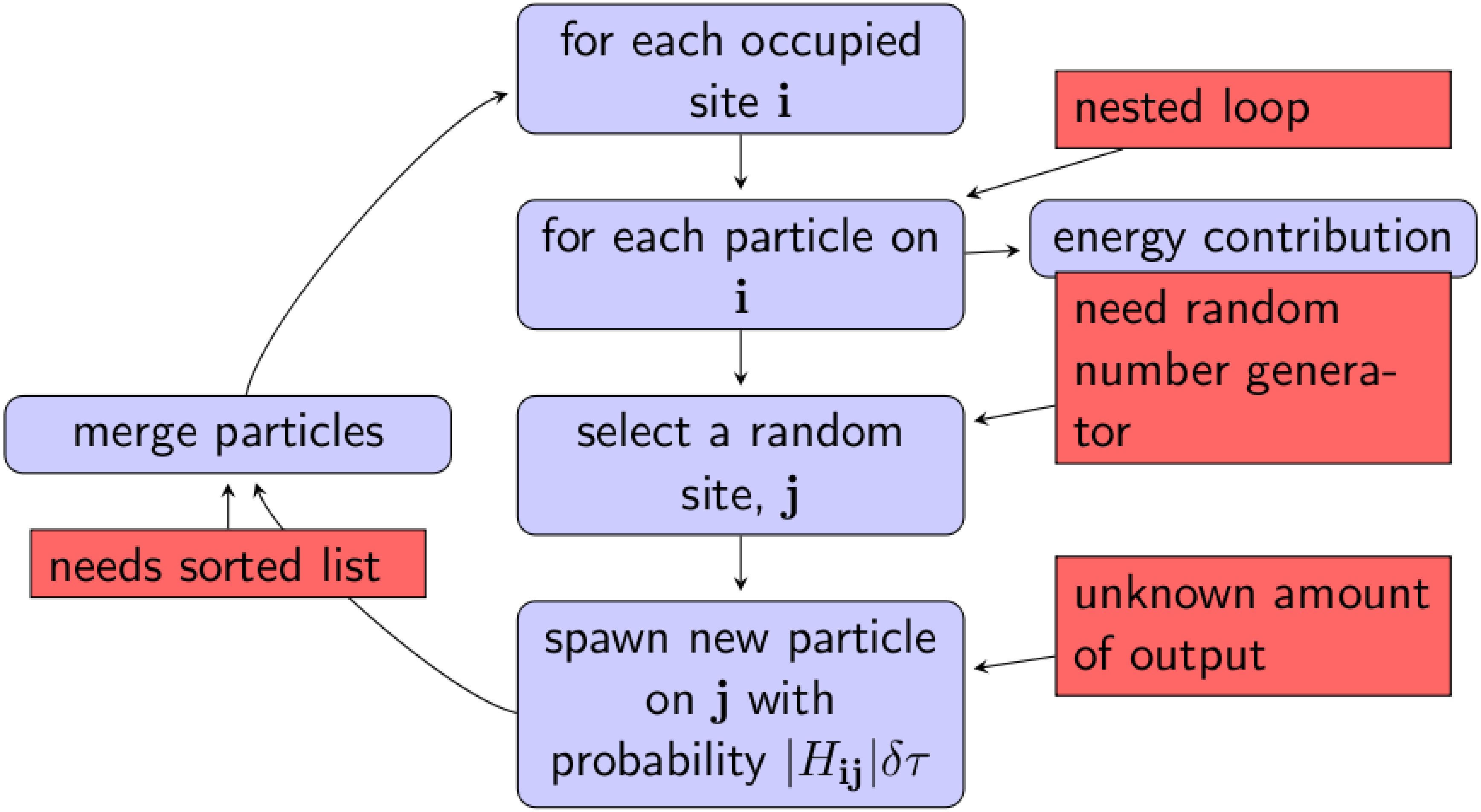
Toy System

- Real elements of $\mathbf{H}$ are very complicated.
- Sparse Toy matrix used for testing.

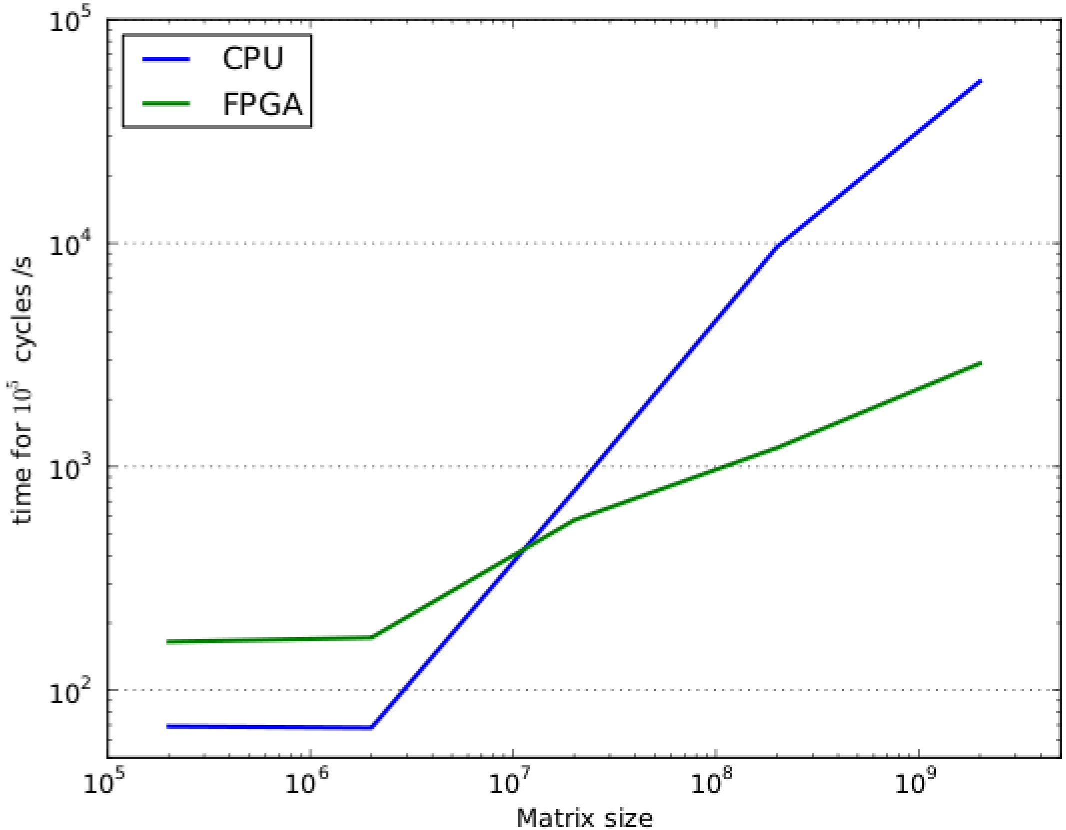
$$\mathbf{H} = \begin{pmatrix} H_{11} & a & 0 & 0 & \cdots & 0 \\ a & H_{22} & a & 0 & \cdots & 0 \\ 0 & a & H_{33} & a & & 0 \\ \vdots & & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & a & H_{p-1p-1} & a \\ 0 & 0 & \cdots & 0 & a & H_{pp} \end{pmatrix}$$



Problems


for each occupied site $\mathbf{i}$
nested loop
for each particle on $\mathbf{i}$
energy contribution
need random number generator
merge particles
select a random site, $\mathbf{j}$
needs sorted list
unknown amount of output
spawn new particle on $\mathbf{j}$ with probability $|H_{\mathbf{ij}}|\delta\tau$

Results

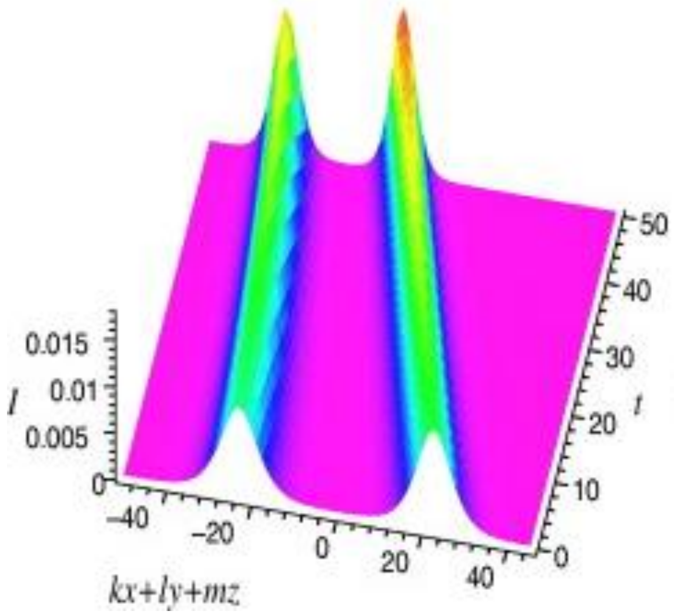

CPU
FPGA
time for 10^5 cycles /s
10^5
10^4
10^3
10^2
10^5
10^6
10^7
10^8
10^9
Matrix size

What next?

- 2D Hubbard model
- Real life FCI for molecules, such as polycyclic aromatic hydrocarbons (PAHs)

MAX-UP: The future

- Strengthening existing subjects: bio-informatics, quantum chemistry, … with new collaborations
- Bringing new subjects: chemical engineering, bio-engineering, …
- Strengthening the existing UK, German, US bases of MAX-UP
- Expansion to Eastern Europe, South America, Australia, …
- Research funding applications with MAX-UP members: iCASE PhD studentships (UK), ERC synergy grants, …



Acceleration of an algorithm based on the Gross Pitaevskii equation.

Execution time for two iterations:
CPU execution time: 50s
Dataflow execution time: 4.9s

Achieved speedup: 10.2x

Programmer:
Sasha Stojanovic
stojsasa@etf.bg.ac.rs

Advisor:
Veljko Milutinovic
vm@etf.bg.ac.rs

University of Belgrade

Note: Comparison is made between a single core CPU without using any of extensions available in today's modern processors and a single dataflow implementation on the oldest and smallest MAX 2 Maxeler card. Using modern CPUs equipped with several cores, each one with extensions for parallel processing of data, and modern Maxeler card with higher capacity, bandwidth to memory and host, and working frequency, will result in decreased execution times in both cases, but it is expected that the speedup will not change significantly.

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