HPC and HPDA Projects in DLR Aeronautics and Space Research

Dr.-Ing. Achim Basermann

German Aerospace Center (DLR), Cologne

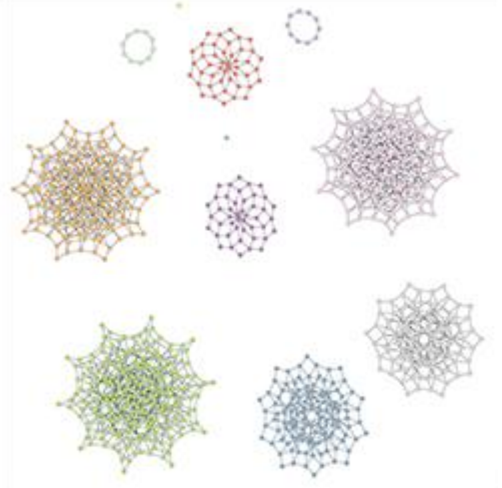
Simulation and Software Technology

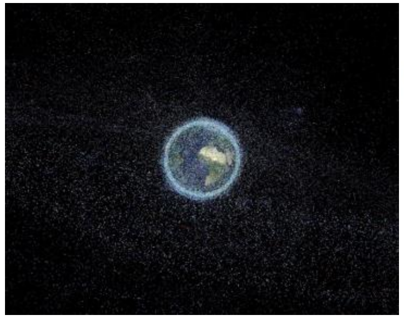
Head of Department „High-Performance Computing“

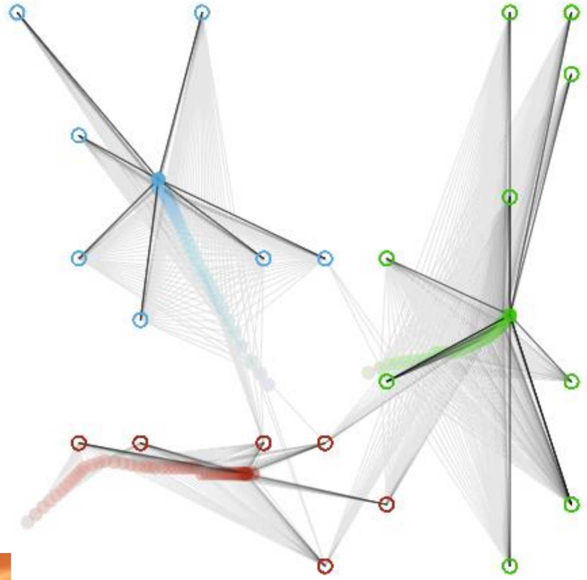
DLR

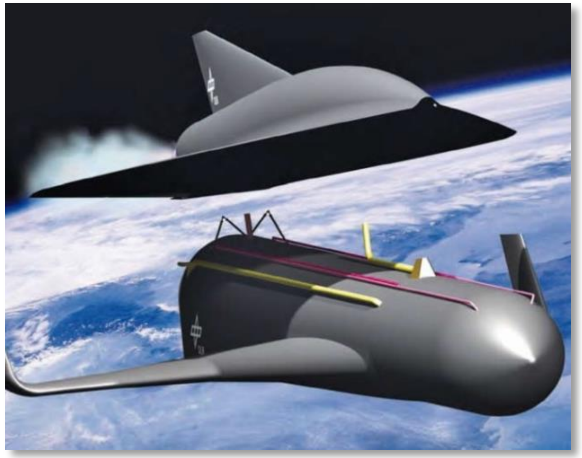
Survey

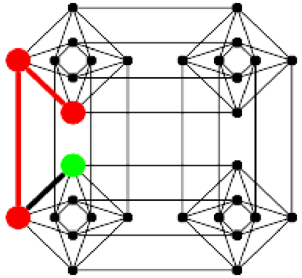
- **Our Department SC-HPC at DLR**
- **Exascale Computing and Performance Engineering**
- **Big Data & High Performance Machine Learning**
  - Space Debris Management
  - Rocket Engine Combustion Analysis
- **Multi-Disciplinary Optimization**
- **Quantencomputing**











DLR

German Aerospace Center

- **Research Institution**
  - Research areas: aeronautics; space research and technology; transport; energy; digitalization; defence and security
  - national and international cooperations

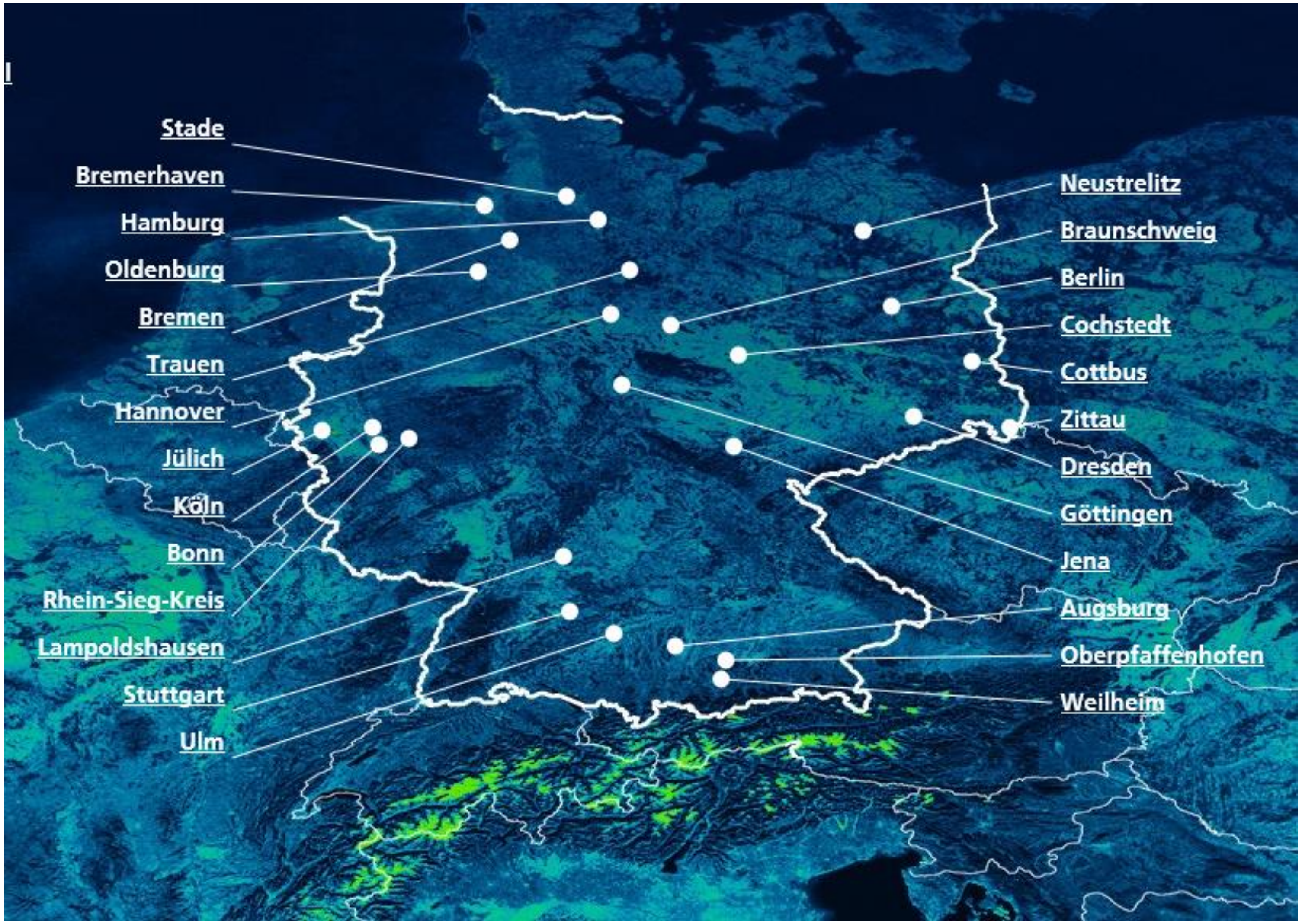
- **Space Agency**

- **Project Management Agency**

DLR Locations and Employees

Approx. 8600 employees across
47 institutes and facilities at 27 sites.

Offices in Brussels, Paris,
Tokyo and Washington.

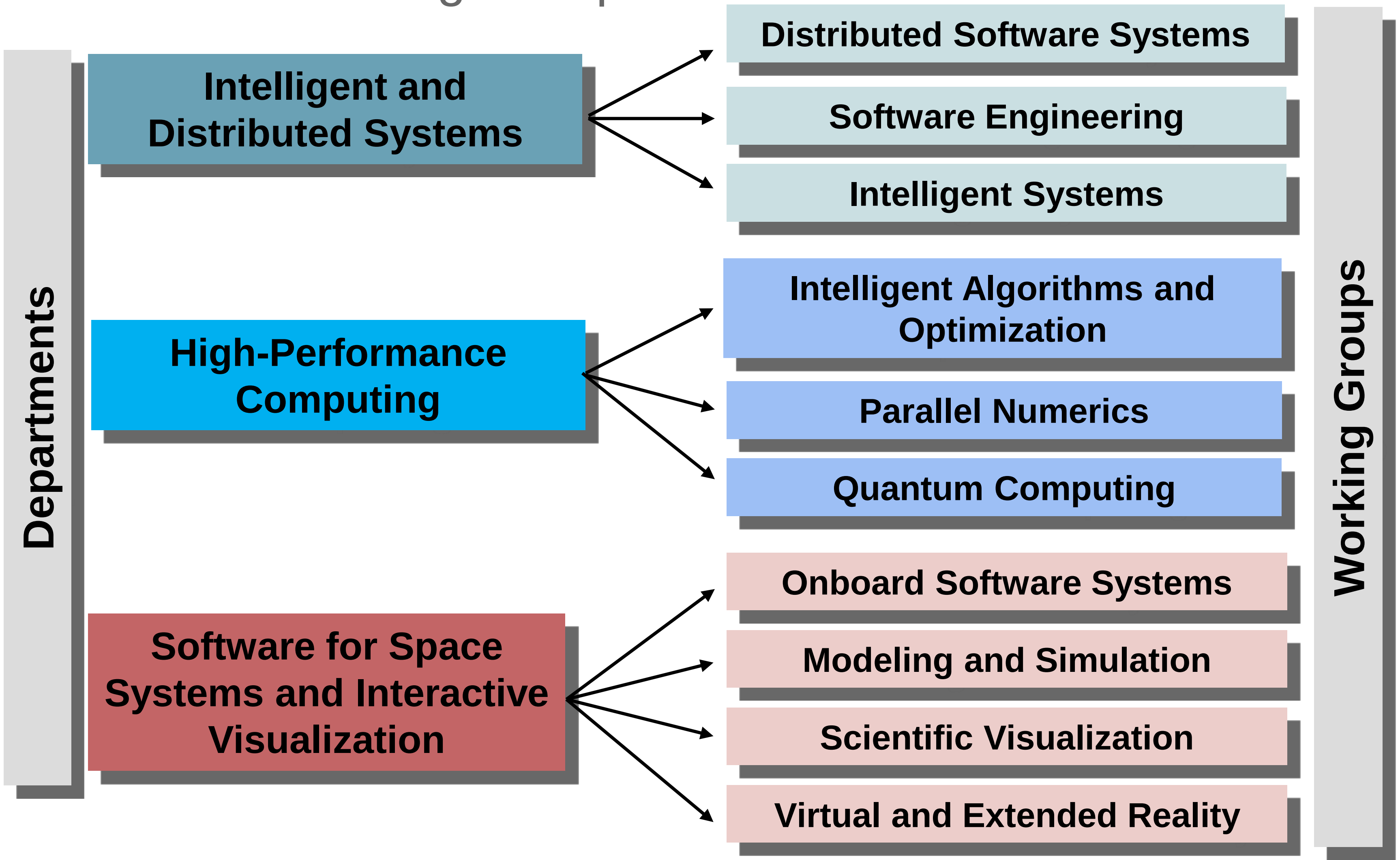


DLR Simulation and Software Technology

- stands for **innovative software engineering**,
- develops **challenging individual software solutions** for DLR, and
- is partner in **scientific projects** in the area of simulation and software technology.

DLR Institute Simulation and Software Technology

Scientific Themes and Working Groups



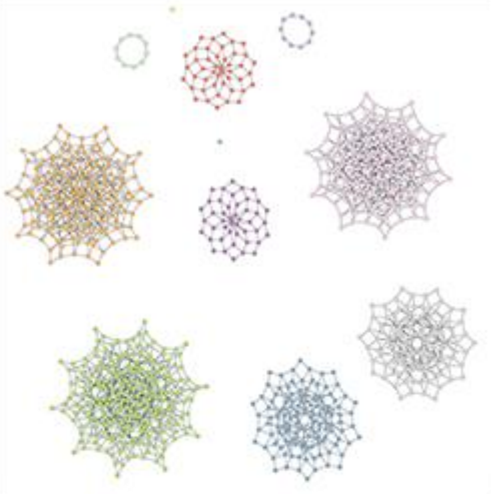
High Performance Computing
Teams

Department
High Performance Computing
Head: Dr. Achim Basermann
Deputy: Dr. Margrit Klitz

Intelligent Algorithms & Optimiziation
Dr. Martin Siggel

Parallel Numerics
Dr. Jonas Thies

Quantum Computing
Dr. Tobias Stollenwerk



Exascale computing and Performance Engineering

ESSEX goes Oakforest-PACS

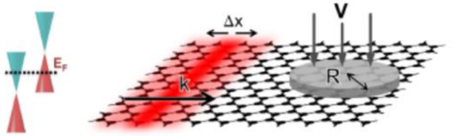
Graphvisualisierung der möglichen Zustandsänderungen des Heisenberg Spinkettenmodells

DLR

Motivation: Requirements for Exascale Computing

DFG Project ESSEX

Quantum physics/information applications



Large,
Sparse

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

and beyond….

$$\boldsymbol{H\,x = \lambda\,x}$$

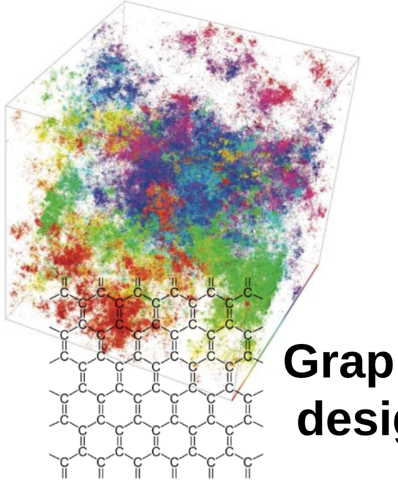
"Few" (1,…,100s) of eigenpairs

"**Bulk**" (100s,…,1000s) eigenpairs

$$\underbrace{\{\lambda_1, \lambda_2, \ldots, \ldots, \ldots, \ldots, \lambda_k, \ldots, \ldots, \ldots, \ldots, \lambda_{n-1}, \lambda_n\}}$$

Good approximation to full spectrum (e.g. Density of States)

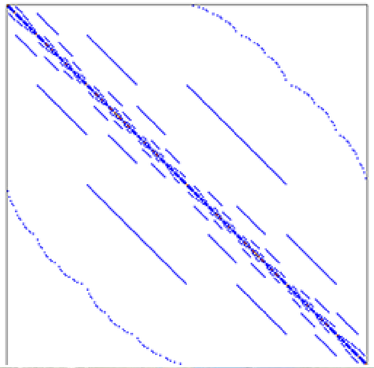
→ Sparse eigenvalue solvers of broad applicability



Graphen design

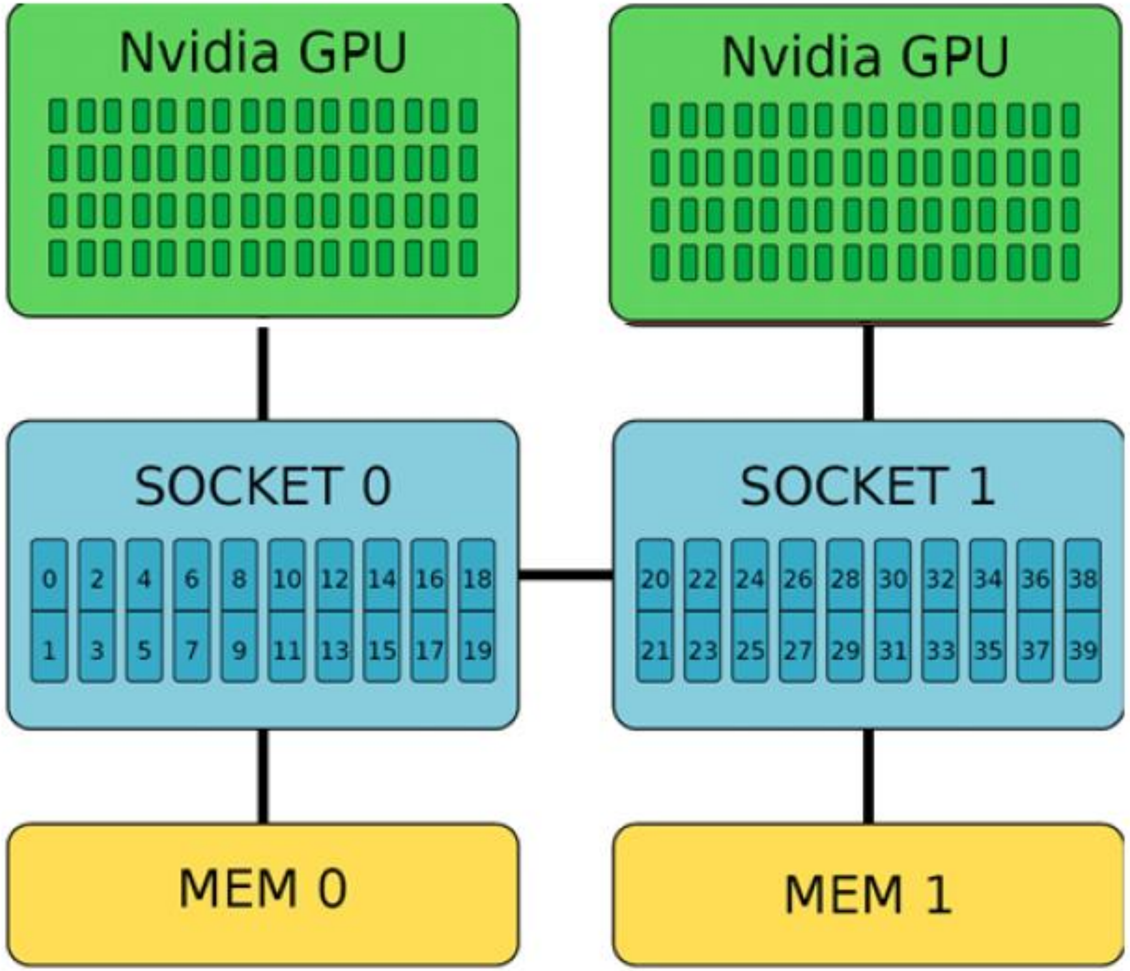
University of Tokyo
University of Tsukuba

Sparse matrix



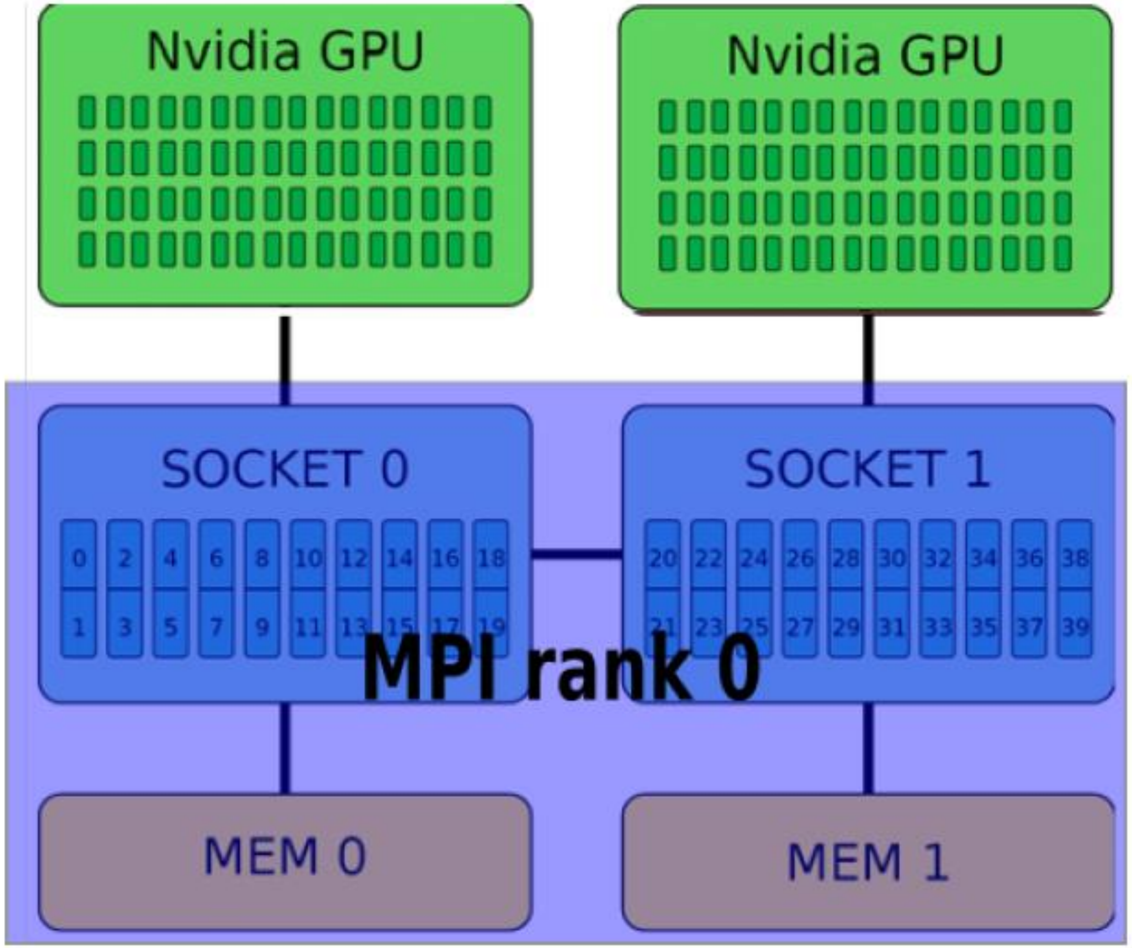
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs



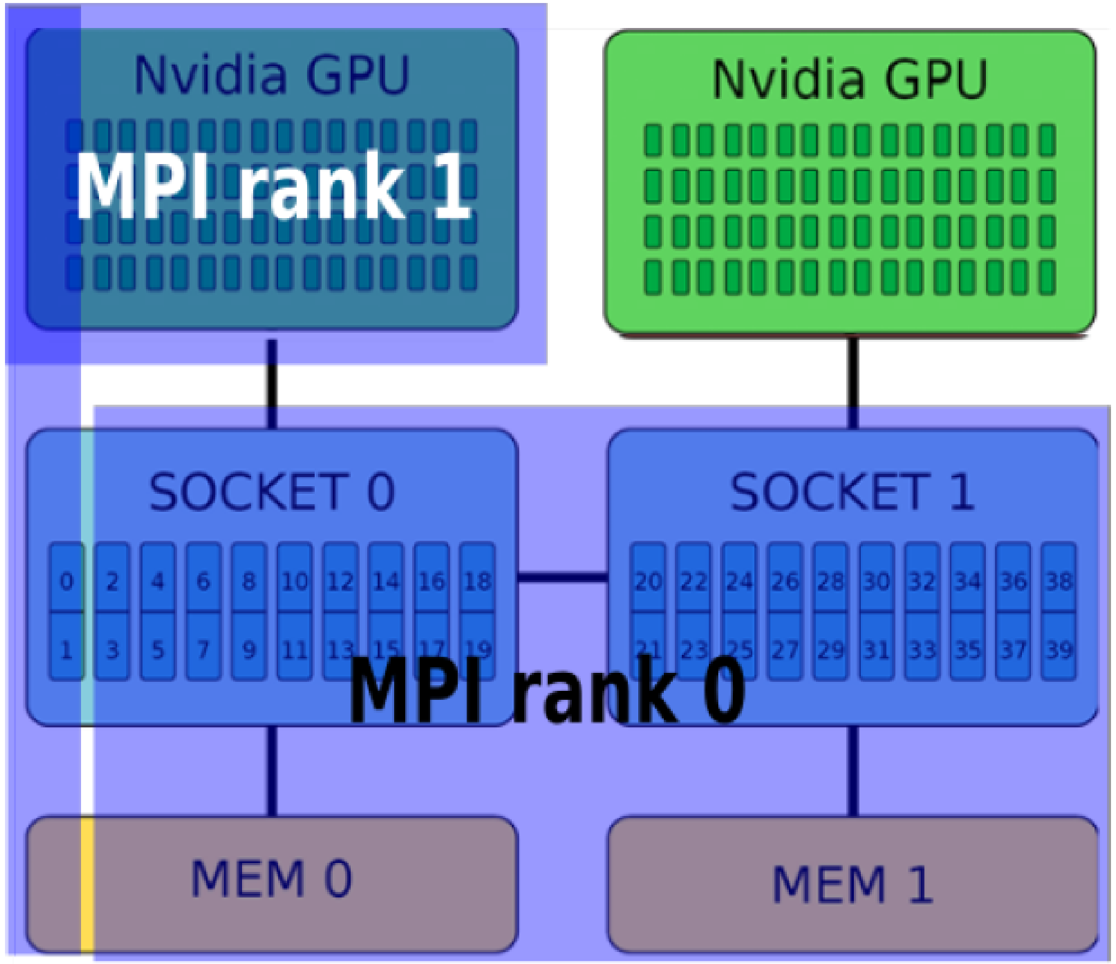
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU



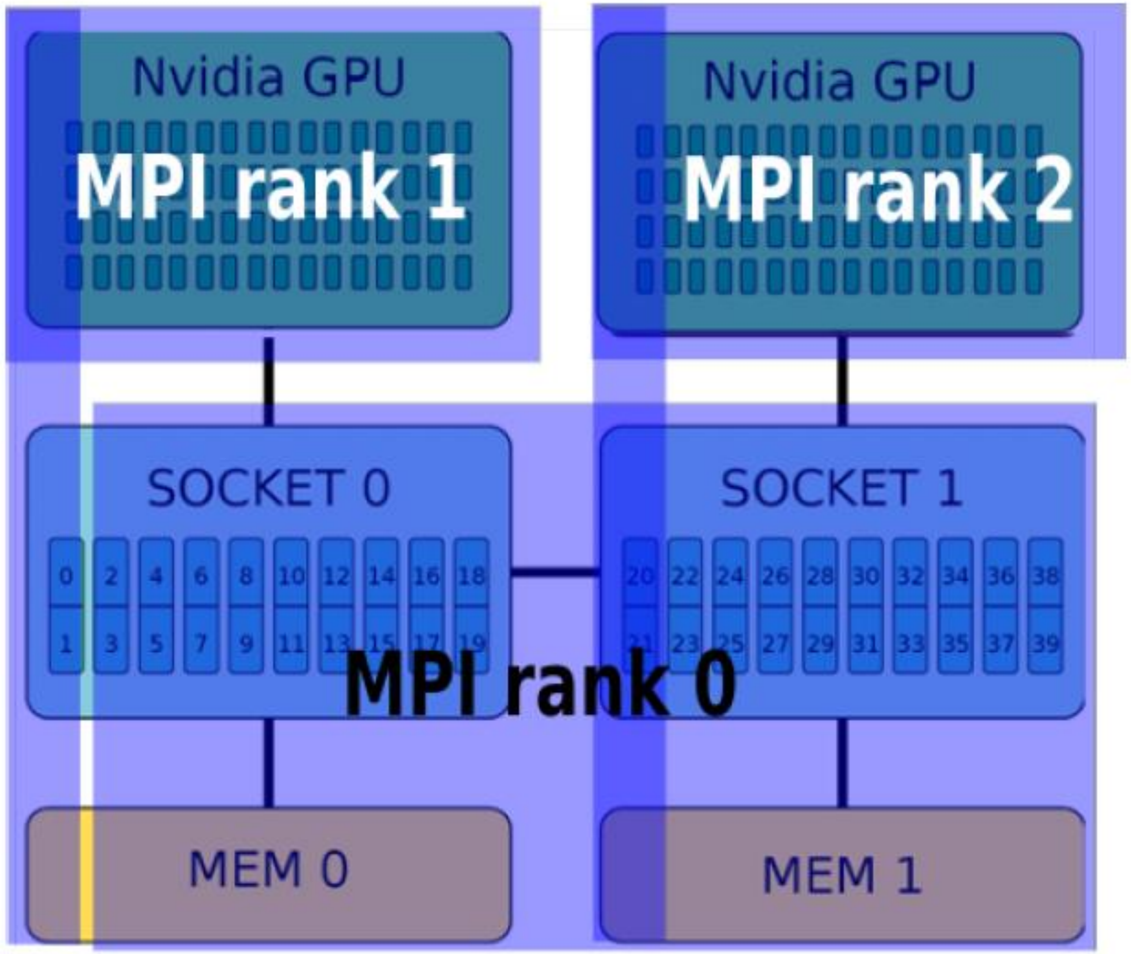
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU



The ESSEX Software Infrastructure: MPI + X with GHOST

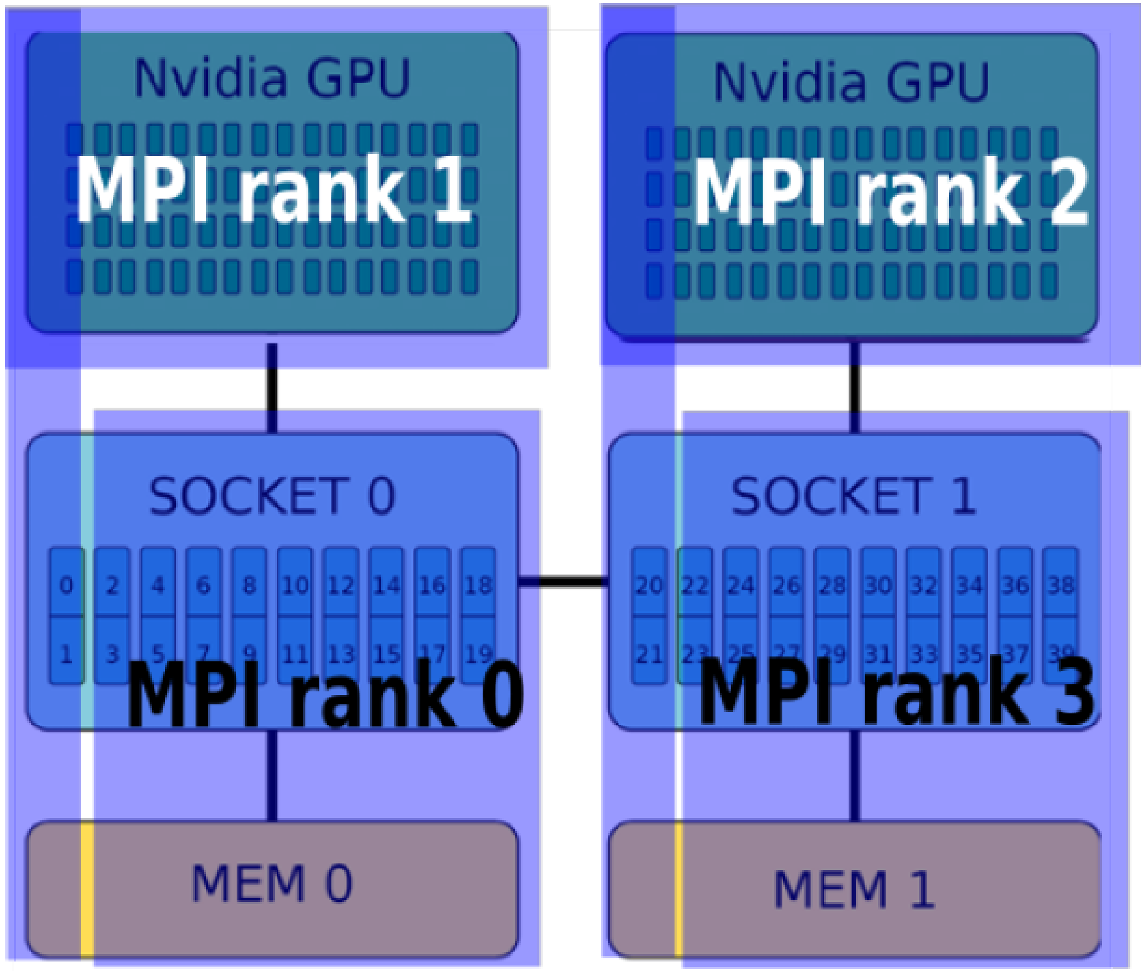
- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU
- -np 3: use CPU and both GPUs



The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU
- -np 3: use CPU and both GPUs
- -np 4: use one process per socket and one for each GPU

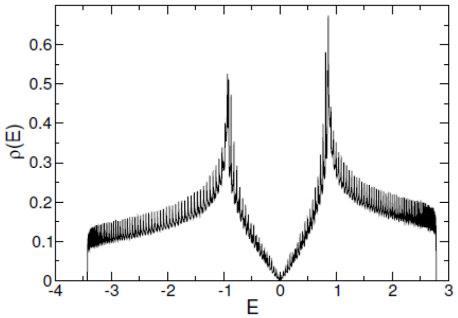
Option: distribute problem according to memory bandwidth measured

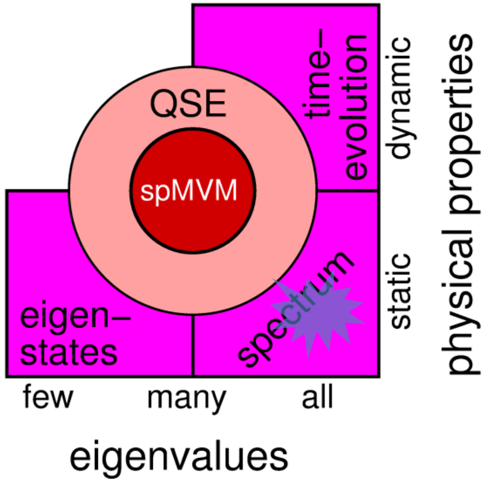


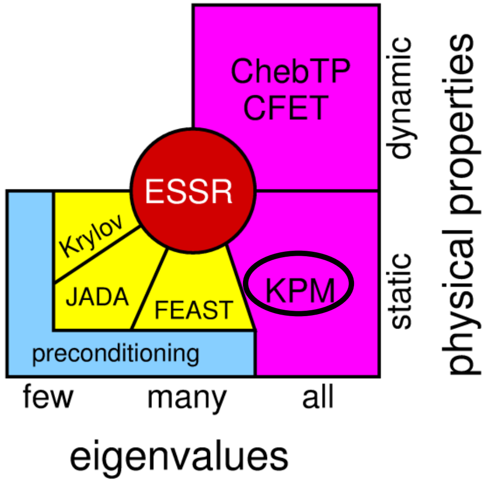
Application, Algorithm and Performance: Kernel Polynomial Method (KPM) – A Holistic View

- Compute **approximation to the complete eigenvalue spectrum** of large sparse matrix A (with $X = I$)

$$X(\omega) = \frac{1}{N}\mathrm{tr}[\delta(\omega - H)X] = \frac{1}{N}\sum_{n=1}^{N}\delta(\omega - E_n)\langle\psi_n, X\psi_n\rangle$$







The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

Basic algorithm – Compute Cheyshev polynomials/moments:

Building blocks:
(Sparse) linear algebra library

Application:
Loop over random initial states

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\mathrm{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\mathrm{swap}(|w\rangle, |v\rangle)$
    $|u\rangle \leftarrow H|v\rangle$ ▷ spmv() Sparse matrix vector multiply
    $|u\rangle \leftarrow |u\rangle - b|v\rangle$ ▷ axpy() Scaled vector addition
    $|w\rangle \leftarrow -|w\rangle$ ▷ scal() Vector scale
    $|w\rangle \leftarrow |w\rangle + 2a|u\rangle$ ▷ axpy() Scaled vector addition
    $\eta_{2m} \leftarrow \langle v|v\rangle$ ▷ nrm2() Vector norm
    $\eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ dot() Dot Product
  end for
end for

Algorithm:
Loop over moments

The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

Basic algorithm – Compute Cheyshev polynomials/moments:

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
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  for $m = 1$ to $M/2$ **do**
    $\text{swap}(|w\rangle, |v\rangle)$
    $|u\rangle \leftarrow H|v\rangle$ ▷ spmv()
    $|u\rangle \leftarrow |u\rangle - b|v\rangle$ ▷ axpy()
    $|w\rangle \leftarrow -|w\rangle$ ▷ scal()
    $|w\rangle \leftarrow |w\rangle + 2a|u\rangle$ ▷ axpy()
    $\eta_{2m} \leftarrow \langle v|v\rangle$ ▷ nrm2()
    $\eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ dot()
  end for
end for

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\text{swap}(|w\rangle, |v\rangle)$
    $|w\rangle = 2a(H - b\mathbb{1})|v\rangle - |w\rangle$ &
    $\eta_{2m} = \langle v|v\rangle$ &
    $\eta_{2m+1} = \langle w|v\rangle$ ▷ aug_spmv()
  end for

Augmented Sparse Matrix Vector Multiply

The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

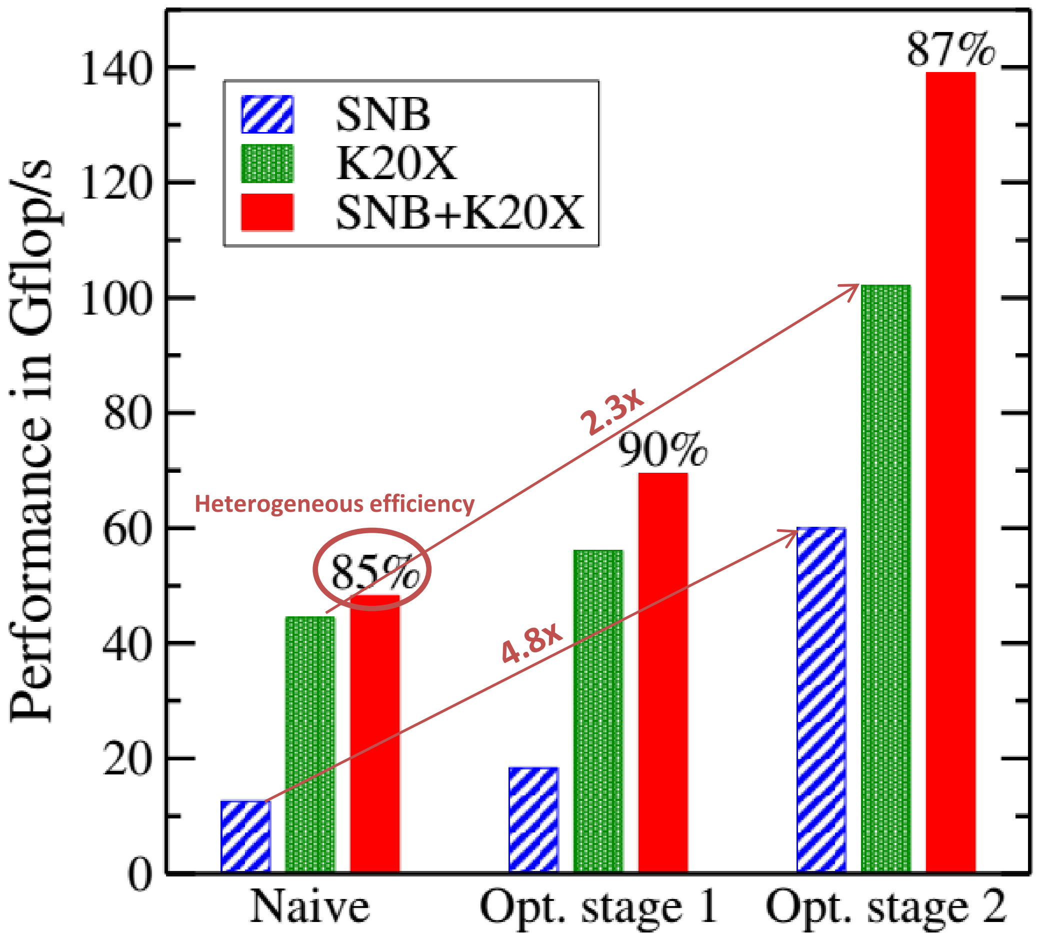
Basic algorithm – Compute Cheyshev polynomials/moments:

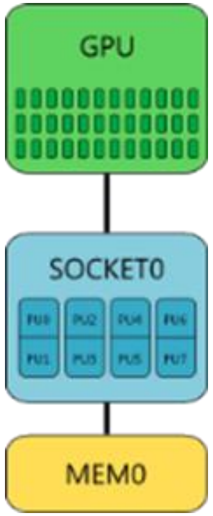
for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\mathrm{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\mathrm{swap}(|w\rangle, |v\rangle)$
    $|w\rangle = 2a(H - b\mathbb{1})|v\rangle - |w\rangle$ &
      $\eta_{2m} = \langle v|v\rangle$ &
      $\eta_{2m+1} = \langle w|v\rangle$ ▷ aug_spmv()
  end for

$|V\rangle := |v\rangle_{0..R-1}$ ▷ Assemble vector blocks
$|W\rangle := |w\rangle_{0..R-1}$
$|V\rangle \leftarrow |\mathrm{rand}()\rangle$
Initialization steps and computation of μ_0, μ_1
for $m = 1$ to $M/2$ **do**
  $\mathrm{swap}(|W\rangle, |V\rangle)$
  $|W\rangle = 2a(H - b\mathbb{1})|V\rangle - |W\rangle$ &
    $\eta_{2m}[:] = \langle V|V\rangle$ &
    $\eta_{2m+1}[:] = \langle W|V\rangle$ ▷ aug_spmmv()
end for

Augmented Sparse Matrix
Multiple Vector Multiply

KPM: Heterogenous Node Performance



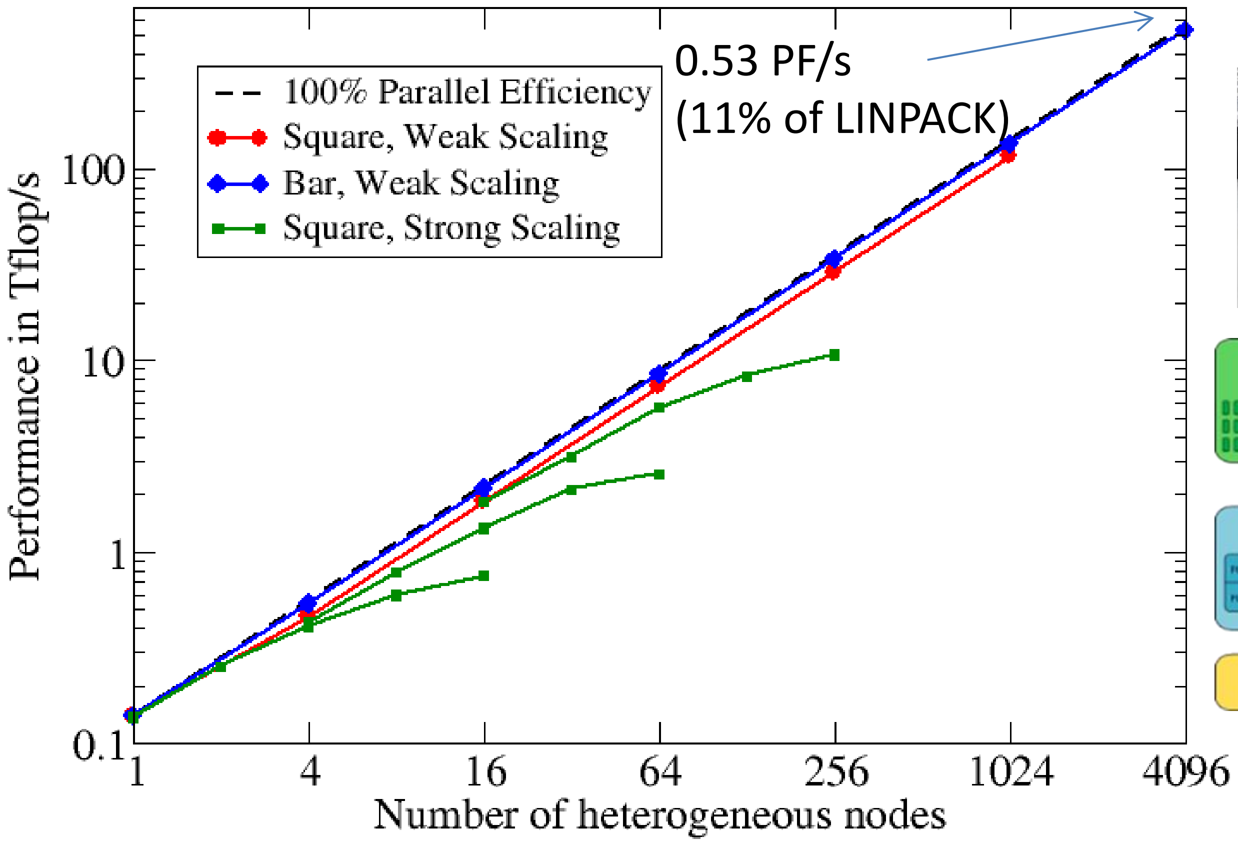


NVIDIDA K20X

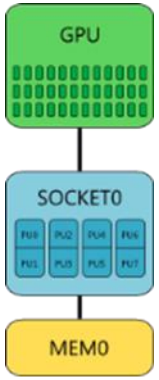
Intel
Xeon E5-2670 (SNB)

- Topological Insulator Application
- Double complex computations
- Data parallel static workload distribution

KPM: Large Scale Heterogenous Node Performance



CRAY XC30 – PizDaint*



- 5272 nodes
- Peak: 7.8 PF/s
- LINPACK: 6.3 PF/s
- Largest system in Europe

Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems
M. Kreutzer, A. Pieper, G. Hager, A. Alvermann, G. Wellein and H. Fehske, IEEE IPDPS 2015

*Thanks to CSCS/T. Schulthess for granting access and compute time

Scalability on Oakforest-PACS

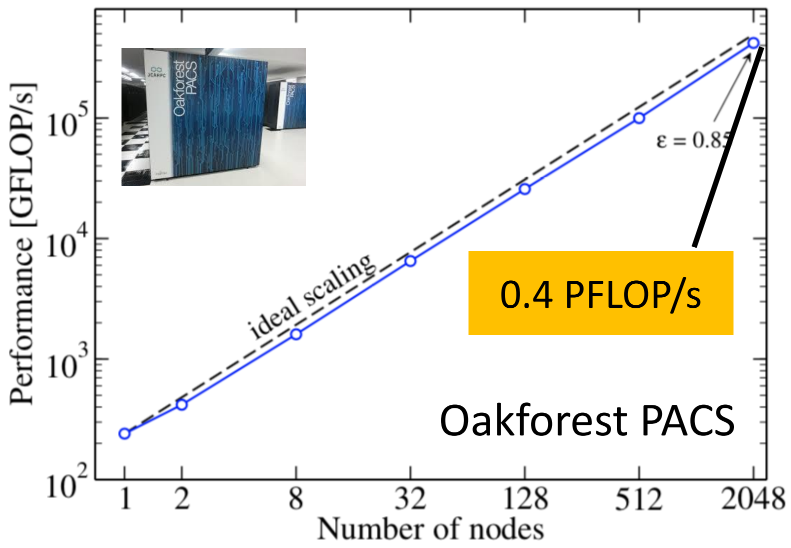
seit 6 / 2018 auf Platz Nummer 12 der TOP 500 The List.

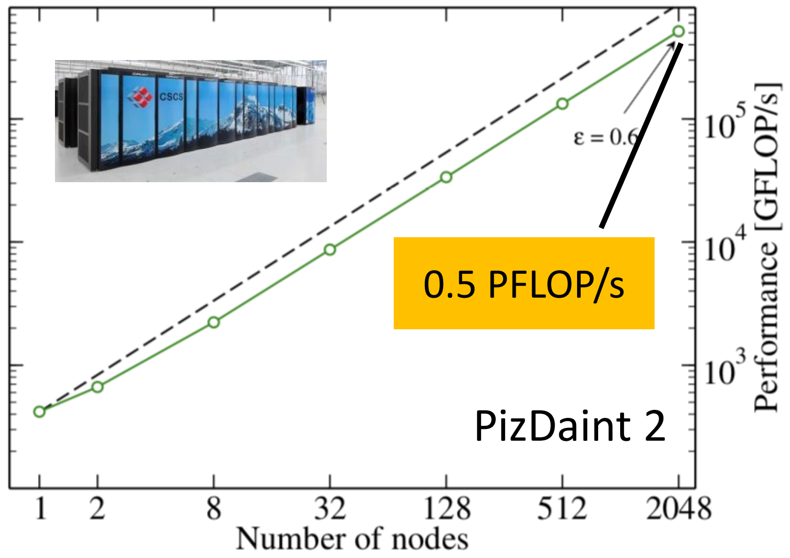
Cores: Memory: Processor: Interconnect:	556,104 919,296 GB Intel Xeon Phi 7250 68C 1.4GHz (KNL) Intel Omni-Path
Linpack Performance (Rmax) Theoretical Peak (Rpeak)	13.554 PFlop/s 24.913 PFlop/s
Nmax HPCG [TFlop/s]	9,938,880 385.479

Impression of the Oakforest-PACS supercomputer at the Japanese joint center for advanced HPC (JCAHPC).

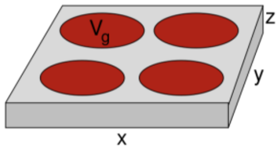
Large scale performance – weak scaling

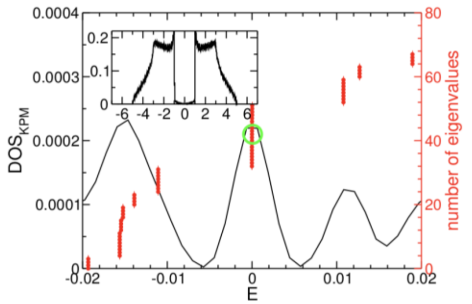
Computing 100 inner eigenvalues on matrices up to $n = 4 \times 10^9$

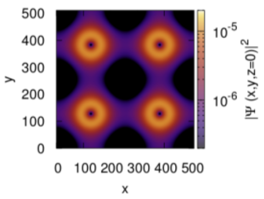




Typical Application[1]:
Topological Insulator







[1] Pieper, A., et al. Journal of Computational Physics 325, 226–243 (2016)

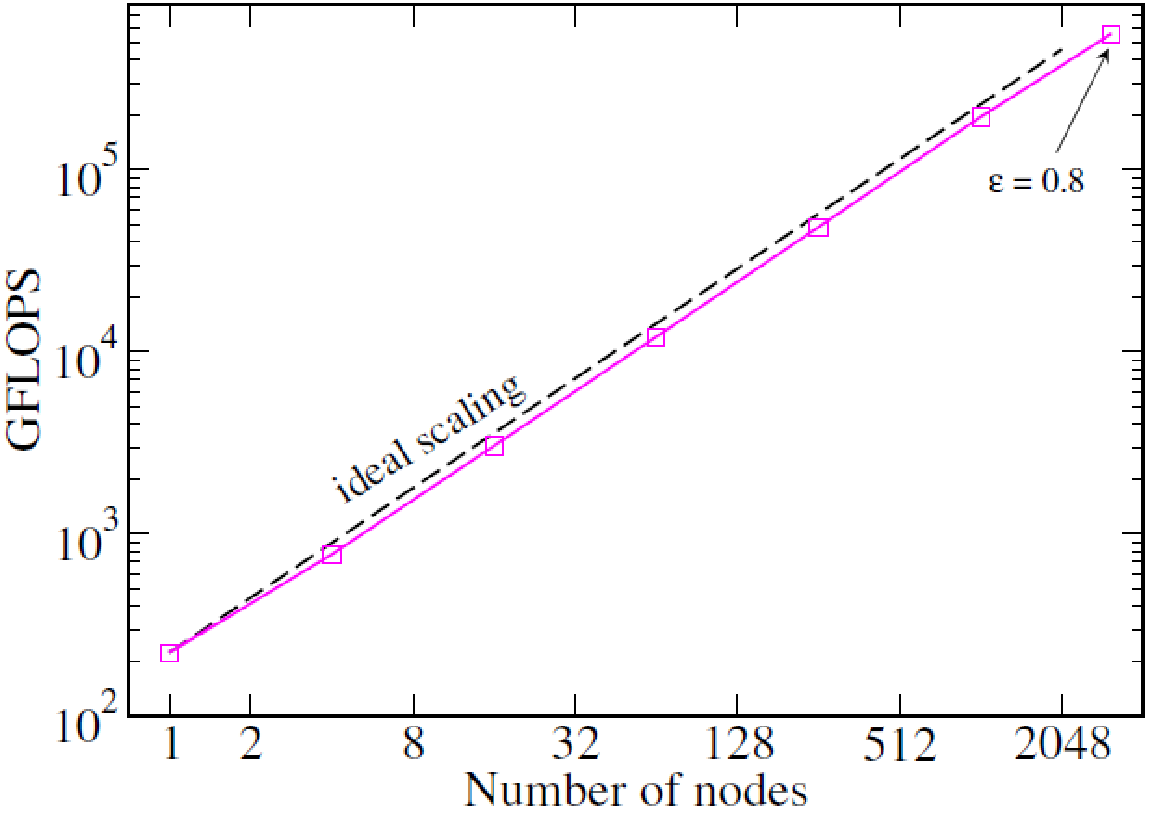
Large scale performance – weak scaling

Computing 100 inner eigenvalues on matrices up to $n = 4 \times 10^9$

SUPERMUC (SNG)
Leibniz Supercomputing Centre (LRZ) in Garching

6480 CPU-only dual-socket nodes with Intel Skylake-SP

311,040 compute cores



Weak scaling of BEAST-P on SNG for problems of size 2^{21} (1 node) to 1.53×2^{32} (3136 nodes, about half of the full machine)

How to ensure the quality of the ESSEX software: Basics

- **Git** for distributed software developement
  - **Merge-request workflo**w for code review; changes only in branches
  - Visualization of git repository development

```
[==========] Running 1 test from 1 test case.
[----------] Global test environment set-up.
[----------] 1 test from AddTest
[ RUN      ] AddTest.TwoAndTwo
test2.cc:6: Failure
      Expected: Add(2, 2)
      Which is: 4
To be equal to: 5
[  FAILED  ] AddTest.TwoAndTwo (0 ms)
[----------] 1 test from AddTest (0 ms total)

[----------] Global test environment tear-down
[==========] 1 test from 1 test case ran. (1 ms total)
[  PASSED  ] 0 tests.
[  FAILED  ] 1 test, listed below:
[  FAILED  ] AddTest.TwoAndTwo

 1 FAILED TEST
```

- Own MPI extension for **Google Test**

- Realization of **continuous-integratio**n with Jenkins server

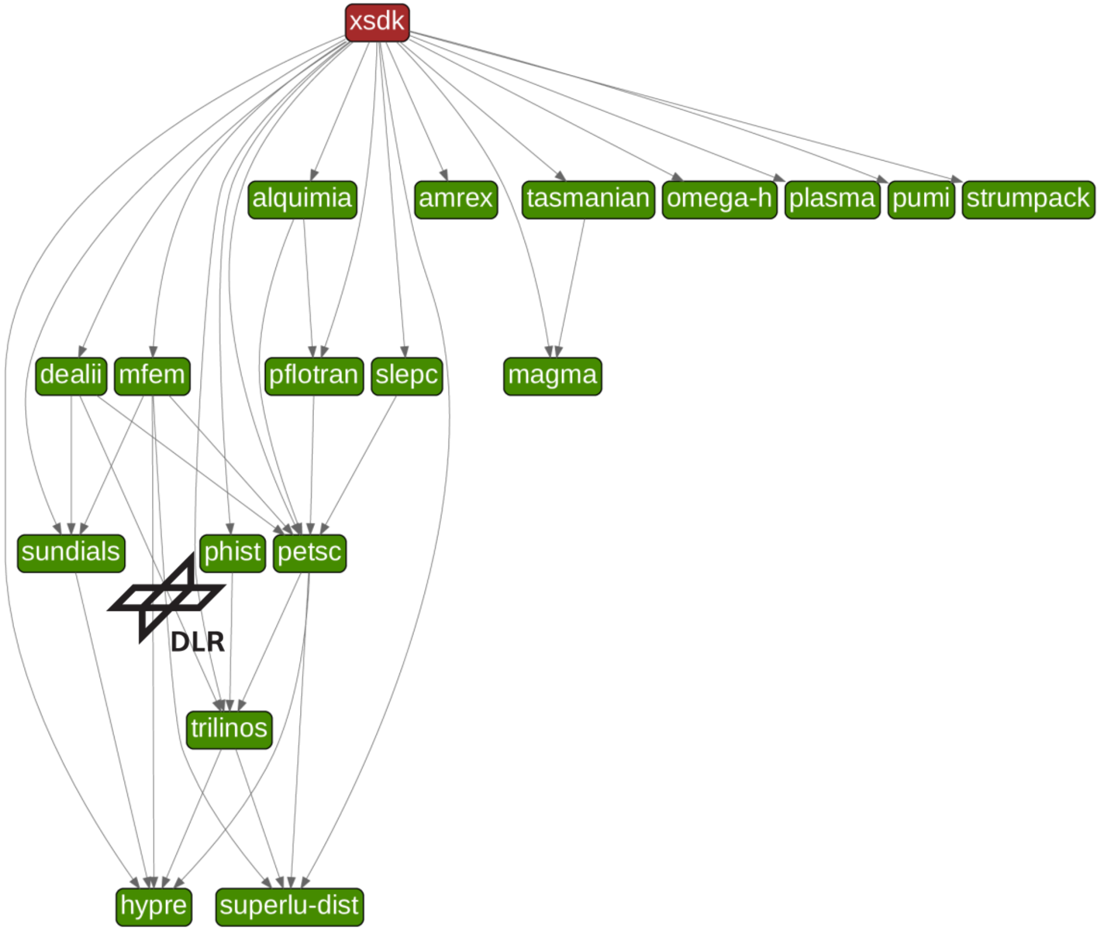
Towards common standards and community software for extreme-scale computing

As we approach the Exa-scale, requirements on robustness, portability, scalability and interoperability of scientific software are rapidly increasing

xSDK: Extreme-scale Scientific Software Development Kit

- Joint open-source effort of DOE labs and other international teams (https://xsdk.info/)
- DLR contributes a hybrid-parallel library for solving sparse eigenvalue problems on heterogenous supercomputers
- (https://bitbucket.org/essex/phist/)

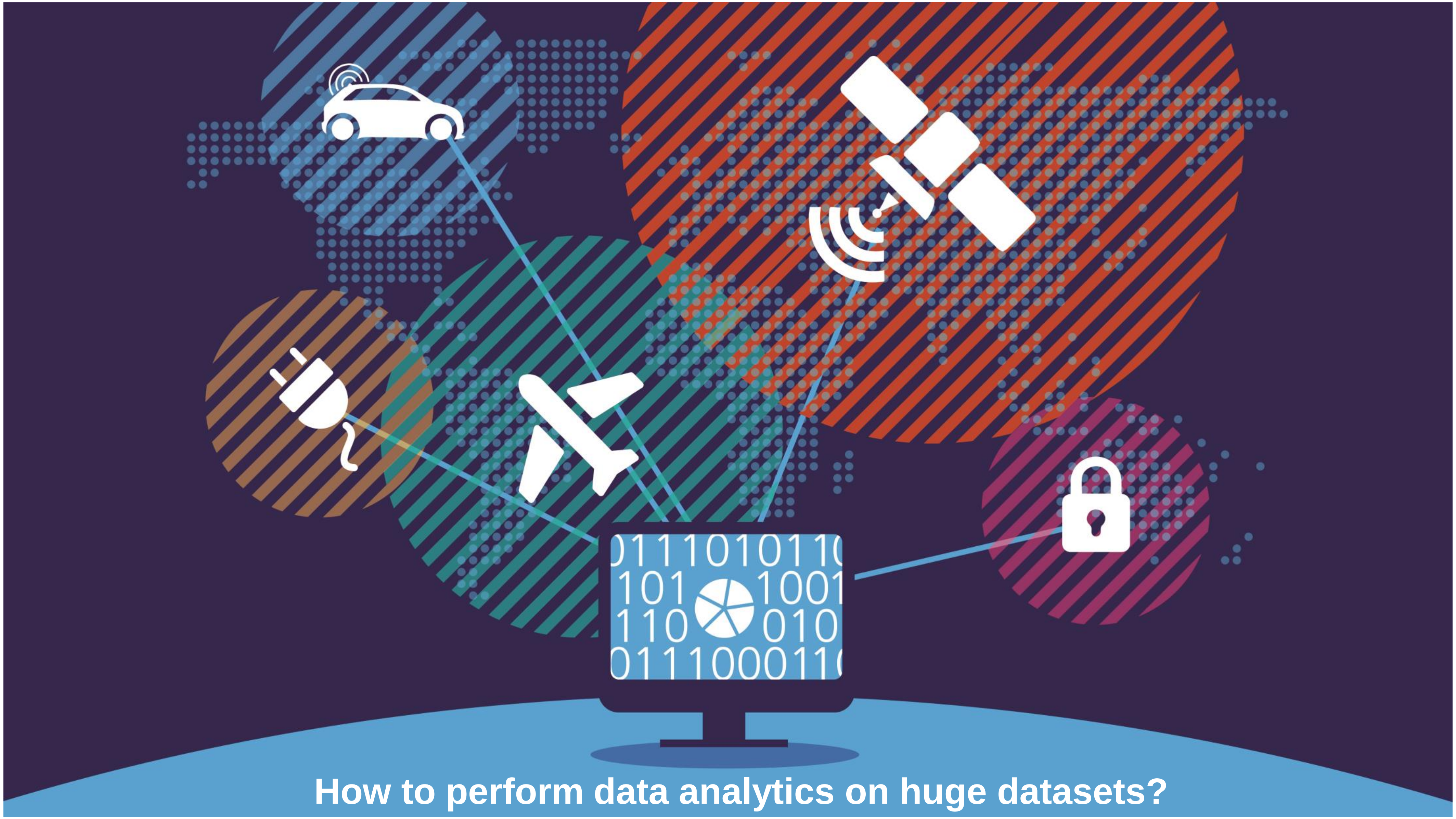
Towards common standards and community software for extreme-scale computing



Big Data & High Performance Machine Learning

DLR

Big Data @ DLR


0111010110
101 1001
110 010
0111000110
How to perform data analytics on huge datasets?

Example 1: Space Debris Management

Picture from
http://kidsnews.hu/2018/03/az-urszemetrol/

Knowledge for Tomorrow

The space debris problem

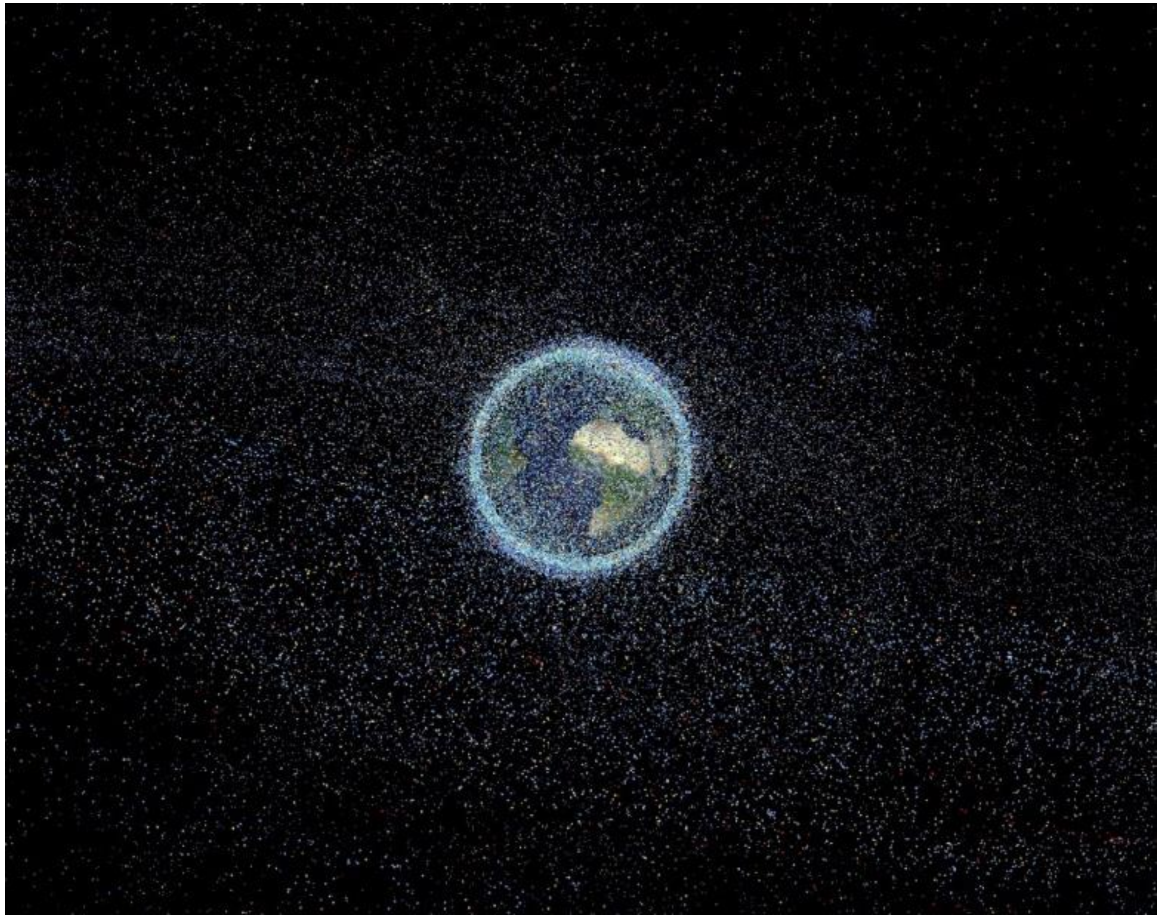
Space Debris

All non-active, non-cooperating orbital objects like

- Old or defect satellites
- Lost Tools
- Debris of all kind (e.g. from satellite collisions)

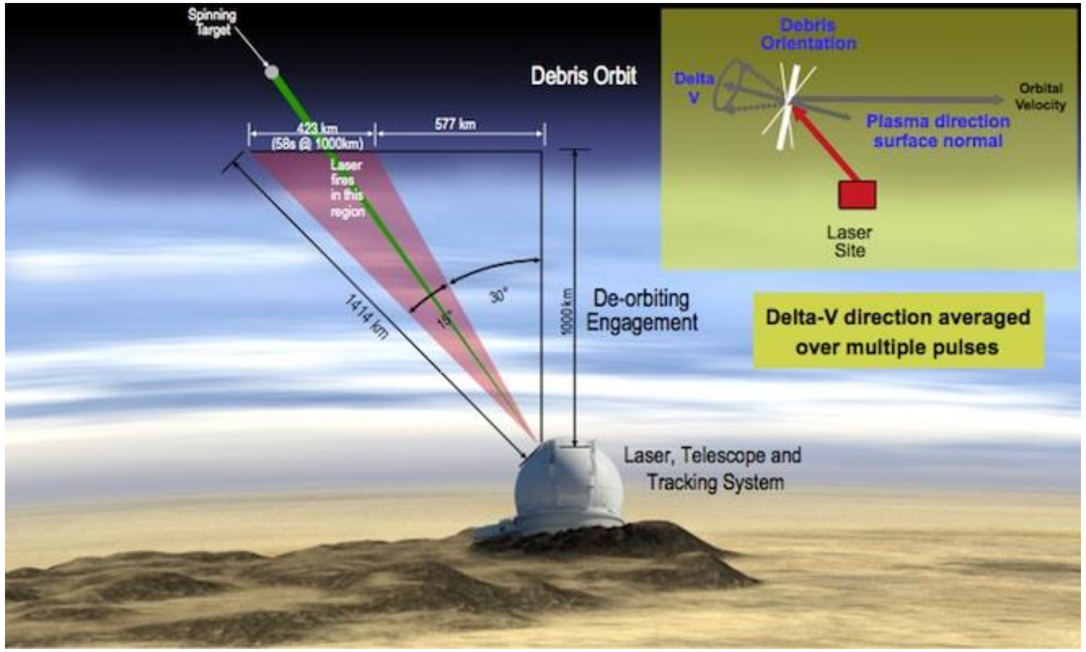
- Impose danger already from 1 cm size
- ~1 000 000 objects, around 18.000 tracked in database

Simulated collision of projectile with 7 km/s on aluminum plate. Picture: ESA.



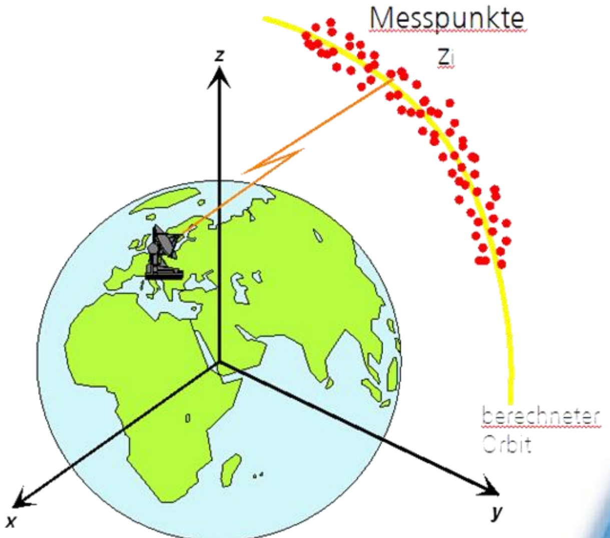
Our solution: Software BACARDI

- Database of all orbits from known space objects (Group „Space Situational Awareness")
- Methods being used:
  - Orbit determination of 1.000.000 objects
  - Propagation
  - Object identification
  - Collision prediction for mission support
- „Bacardi Viewer" allows a 3D visualization of objects from the BACARDI database



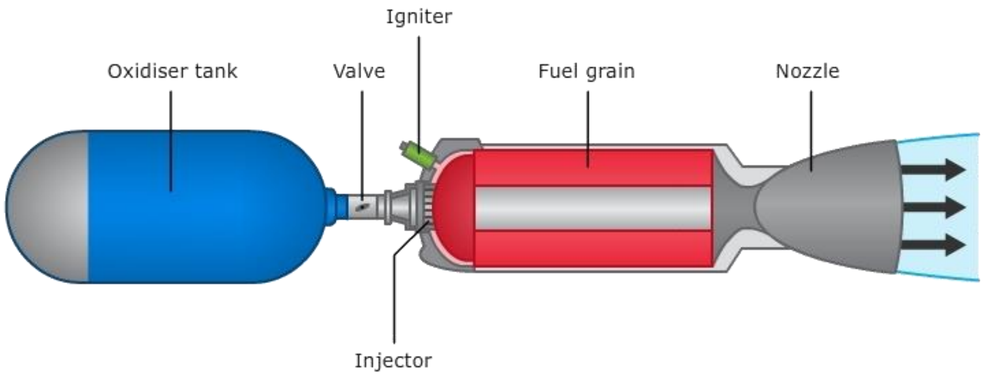
Tracking of space debris with lasers

Image source: https://www.wired.com/2011/10/space-junk-laser/



Example 2:
Rocket engine combustion analysis

- **Goal**: Cost reduction of rocket engines, be competitive with e.g. Space-X



Hybrid rocket engine

- Pressurized fluid oxidizer
- Solid fuel
- A valve controls, how much oxidizer gets into the combustion chamber

- Advantages
  - Cheap
  - Controllable

Example 2:
Rocket engine combustion analysis

- **Goal**: Cost reduction of rocket engines, be competitive with e.g. Space-X

Hybrid rocket engine

- Pressurized fluid oxidizer
- Solid fuel
- A valve controls, how much oxidizer gets into the combustion chamber

- Advantages
  - Cheap
  - Controllable

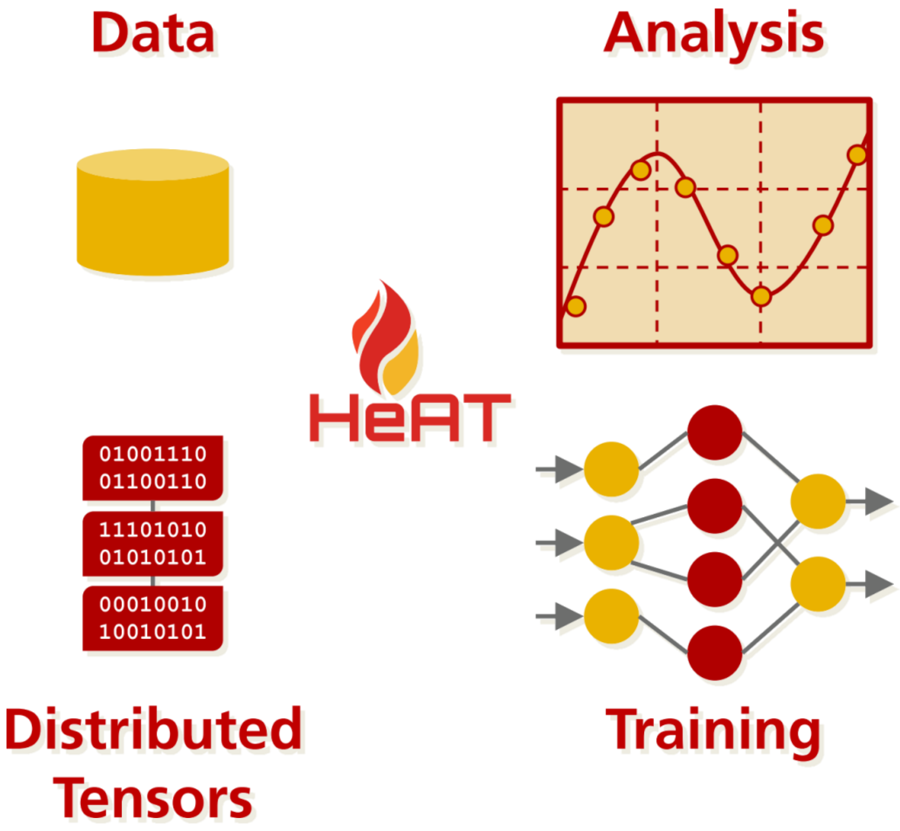
Question: Can we detect problems / inefficiencies during combustion?

Challenge: High speed camera produces huge data sets

Our solution: Software HeAT!

- HeAT = Helmholtz Analytics Toolkit
- Python framework for **parallel**, **distributed** data analytics and machine learning
- Developed within the Helmholtz Analytics Framework Project since 2018
- AIM: Bridge data analytics and **high-performance computing**
- Open Source licensed, MIT

helmholtz-analytics/heat



How we started HeAT:
The Helmholtz Analytics Framework (HAF) Project

HELMHOLTZ
Analytics Framework

- Joint project of all 6 Helmholtz centers

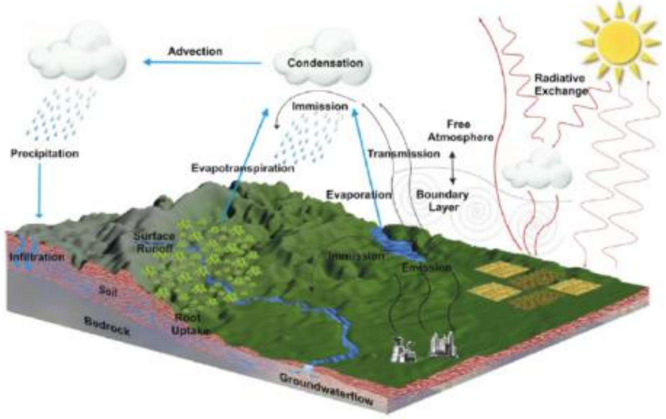
DLR · JÜLICH Forschungszentrum · KIT Karlsruher Institut für Technologie · dkfz. DEUTSCHES KREBSFORSCHUNGSZENTRUM IN DER HELMHOLTZ-GEMEINSCHAFT · DESY · HelmholtzZentrum münchen German Research Center for Environmental Health

- Goal: foster data analytics methods and tools within Helmholtz federation.

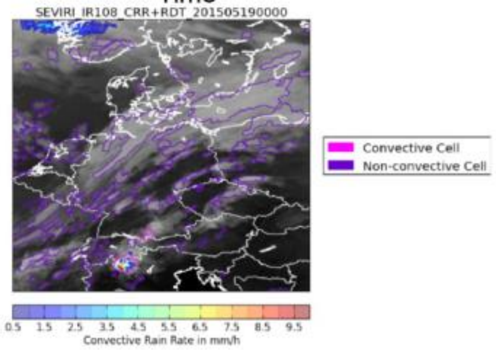
- Scope:
  - Development of domain-specific data analysis techniques
  - Co-design between domain scientists and information experts

Motivation: HAF applications

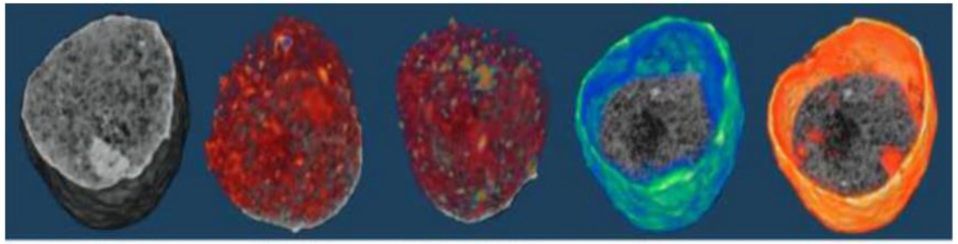
Earth System Modelling



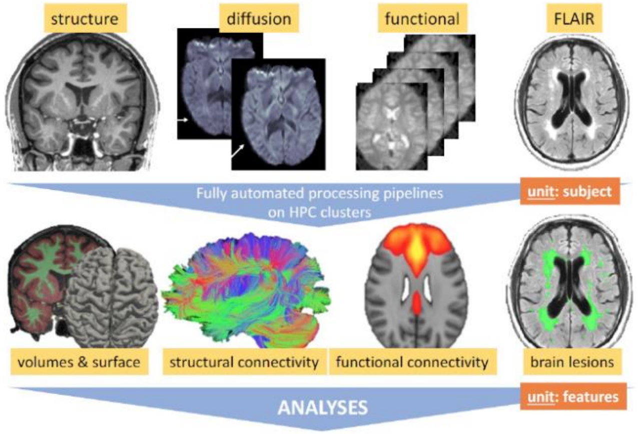
SEVIRI Satellite Images – Near Real Time



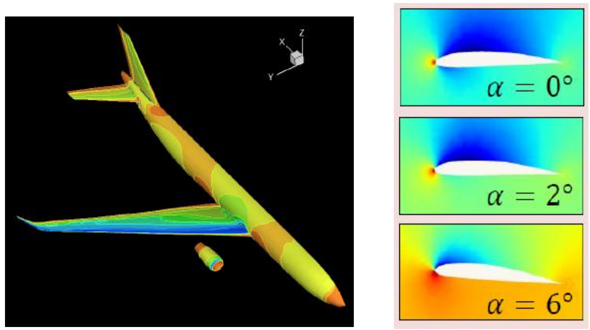
Research with Photons



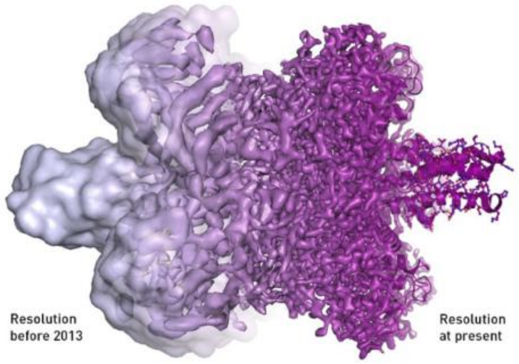
Neuroscience



Aeronautics and Aerodynamics

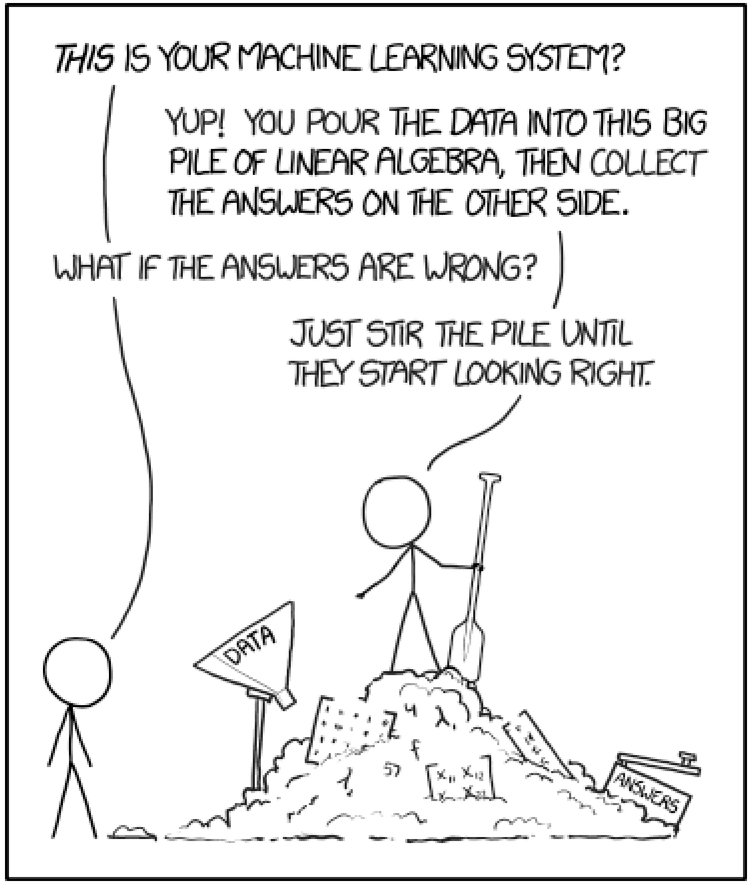


Structural Biology



HelmholtzZentrum münchen
German Research Center for Environmental Health

Greatest Common Denominator?



https://xkcd.com/1838/

Machine Learning

=

Data

+

Numerical Linear Algebra

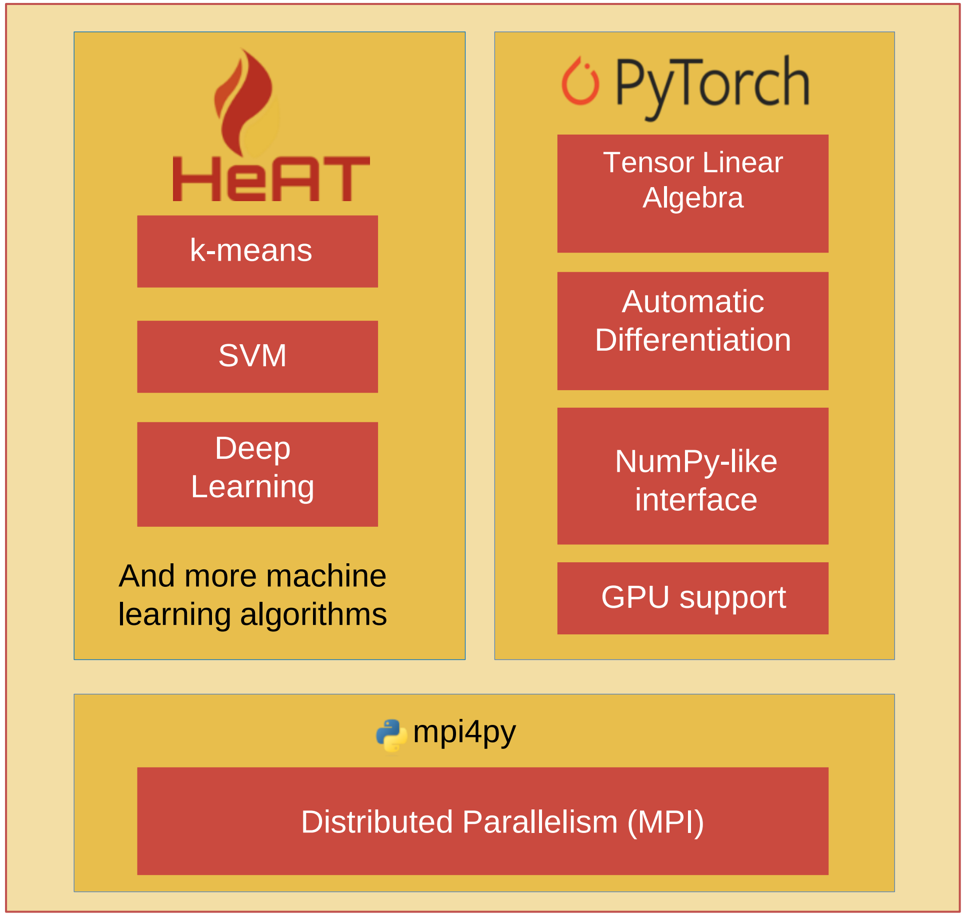
Scope

Facilitating applications of HAF in their work

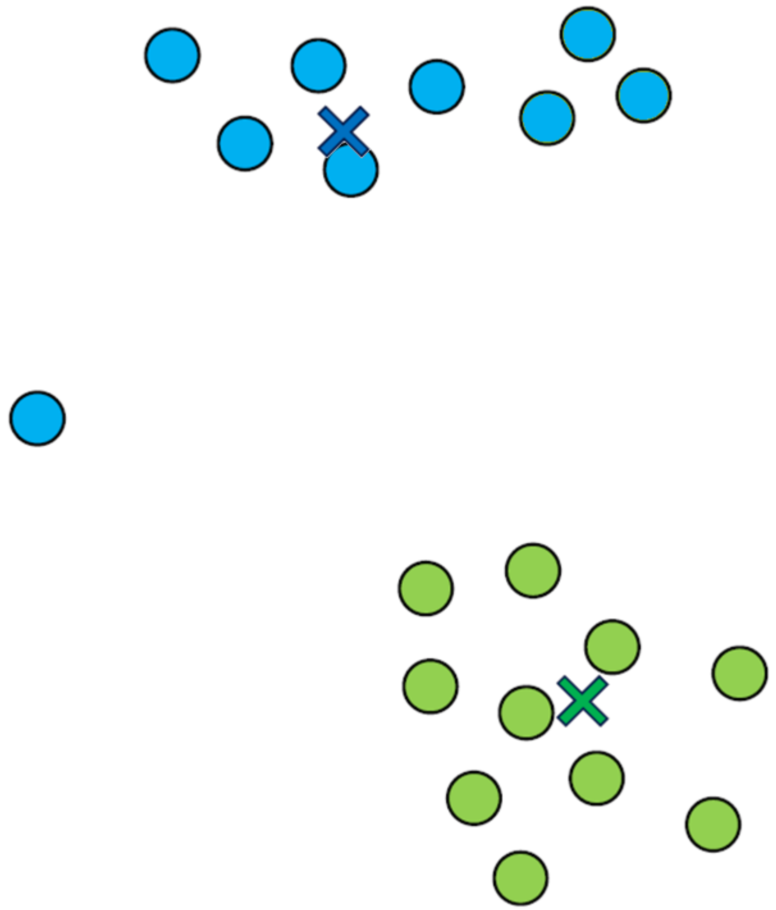
Bringing HPC and Machine Learning / Data Analytics closer together

Ease of use

Design



Data analysis with K-means clustering

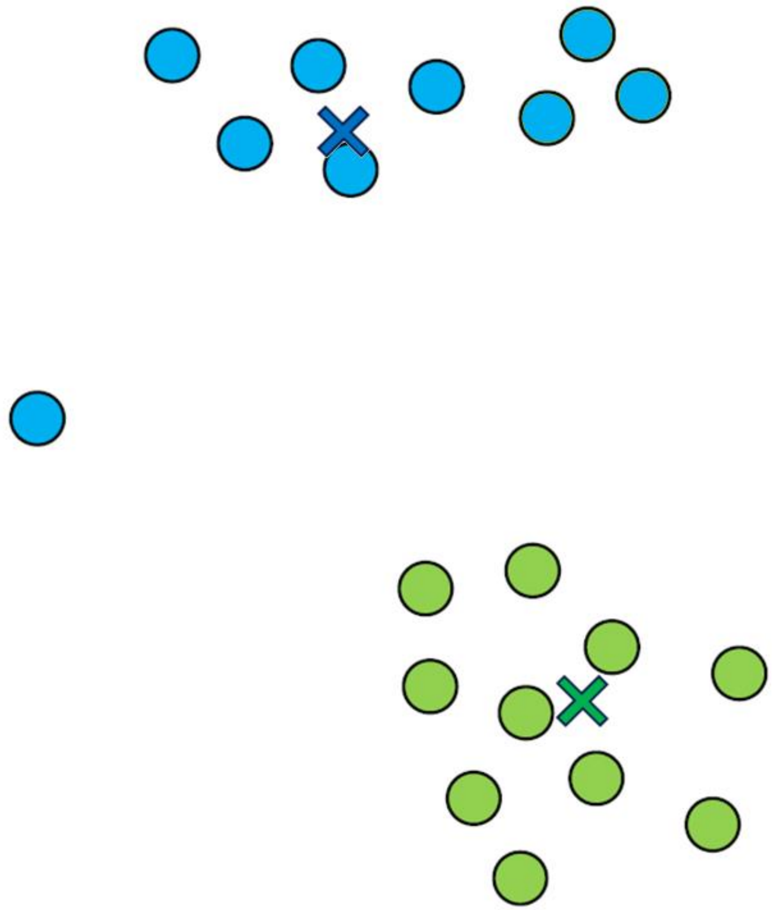


Idea: Separate dataset into k distinct clusters

1. Start with random cluster centroids (crosses)
2. Compute distance of every point to all centroids
3. Assign point to **closest centroid**
4. Update centroid positions at cluster center

Data analysis with K-means clustering

Numpy vs. HeAT



NumPy

```
>>> for i in range(self.n_clusters):
>>>     new_centroids[:, :, i:i+1] = ((data*selection).sum(axis=0, keepdims=True) /
                                      selction.sum(axis=0).clip(1.0, sys.maxsize))
```

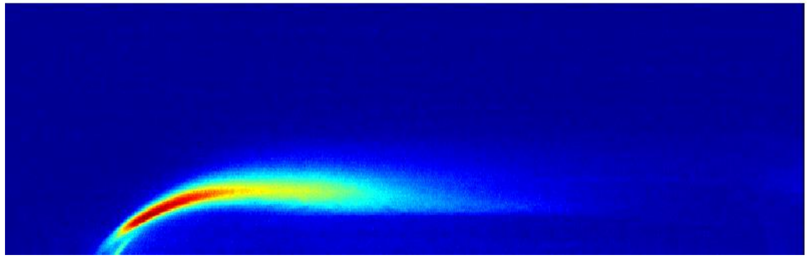
HeAT

```
>>> for i in range(self.n_clusters):
>>>     new_centroids[:, :, i:i+1] = ((data*selection).sum(axis=0) /
                                      selction.sum(axis=0).clip(1.0, sys.maxsize))
```

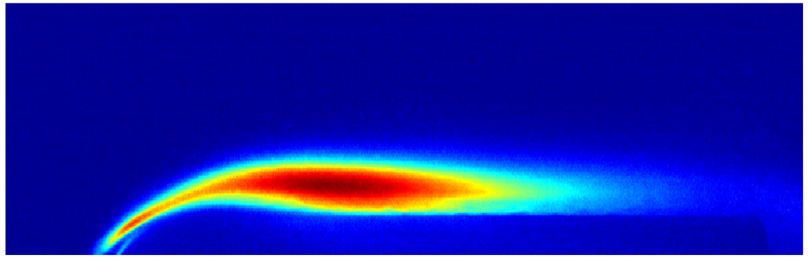
HeAT hides parallelism, looks like sequential NumPy code.

Combustion clustering results:
Resulting Clusters, k = 7

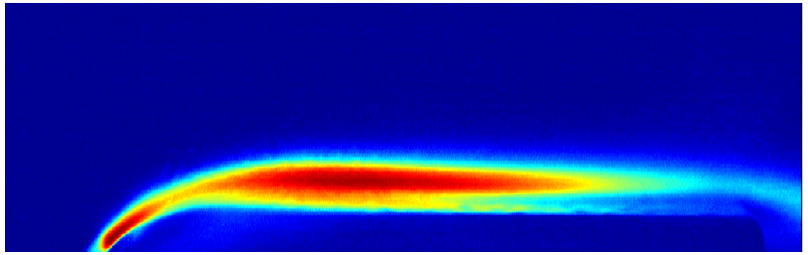
Centroid 0



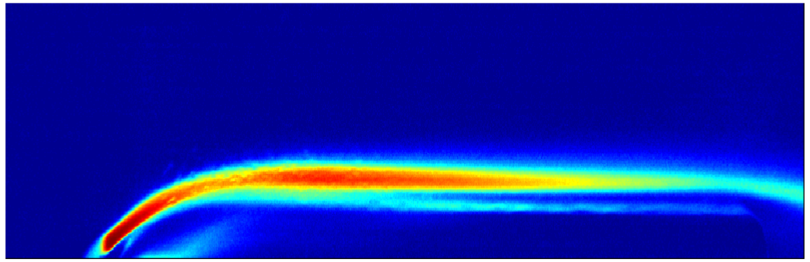
Centroid 1



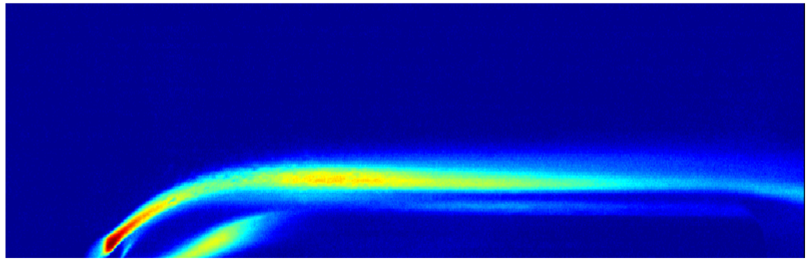
Centroid 2



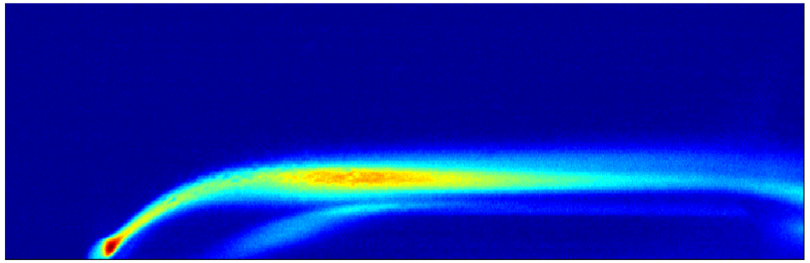
Centroid 3



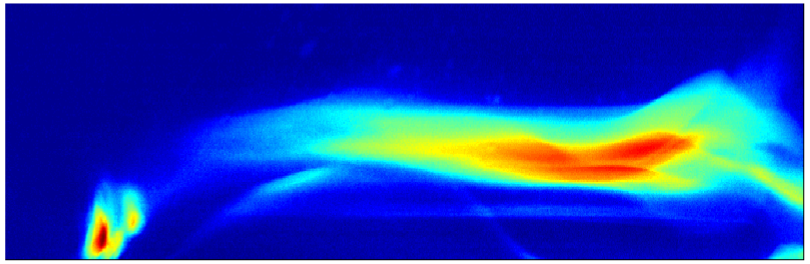
Centroid 4



Centroid 5

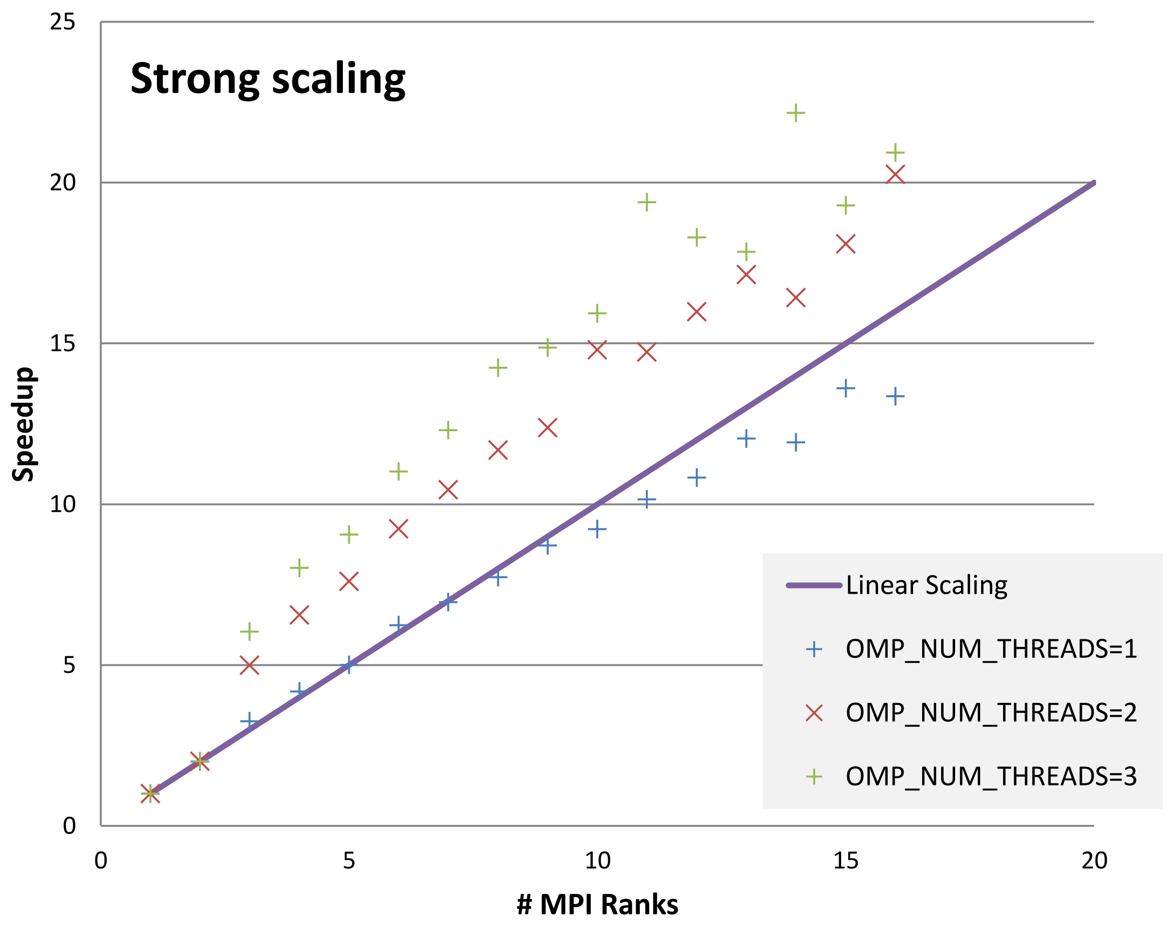


Centroid 6



Computational Performance

- Hybrid shared memory + distributed memory setting
- Variation of 1 … 16 MPI total ranks (processing units)
- How does the computing time reduce with number of processing units?
- First results look promising, testing on larger systems + graphic cards necessary



SC-HPC Highlights in the DLR Project ATEK: Propulsion Technologies and Components for Carrier Systems

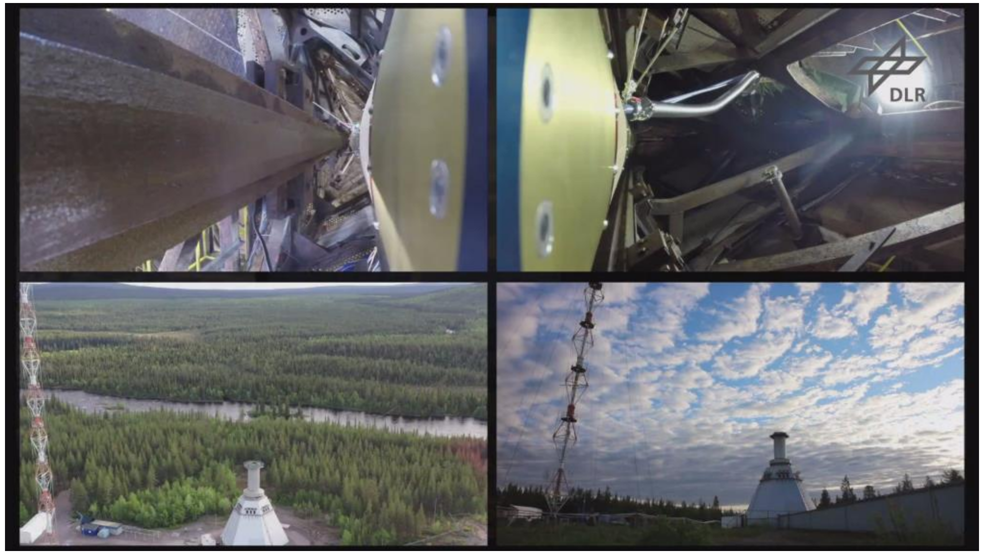
Contribution of HPC:

→ Data analysis (e.g. clustering) of 300k images from rocket engine combustion experiments.

→ Results validated with HeAT (Helmholtz Analytics Toolkit).

→ Further work: - optimization of emission spectrum simulations

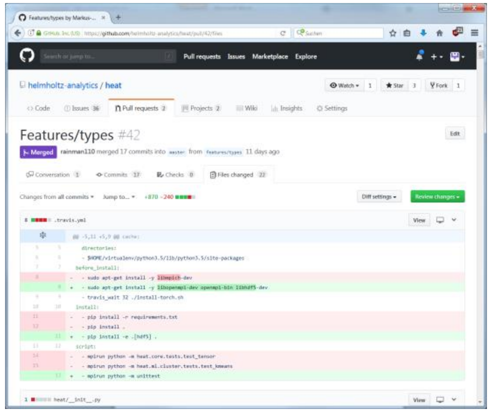
- data fusion in thermo-mechanical experiments



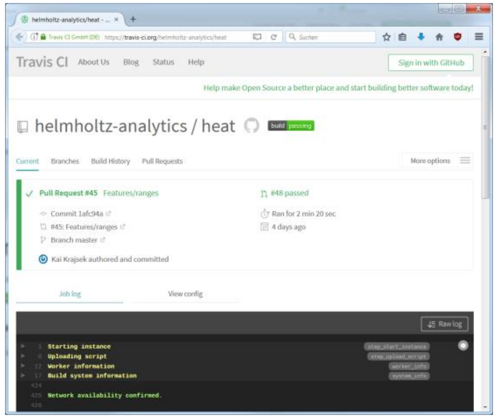
- ATEK research rocket was launched on June 13th 2019.
- The rocket reached an altitude of 239 km.
- It landed in a distance of 67 km from Esrange Space Center.
- All experiments were successful.

HeAT software: Transparent development process

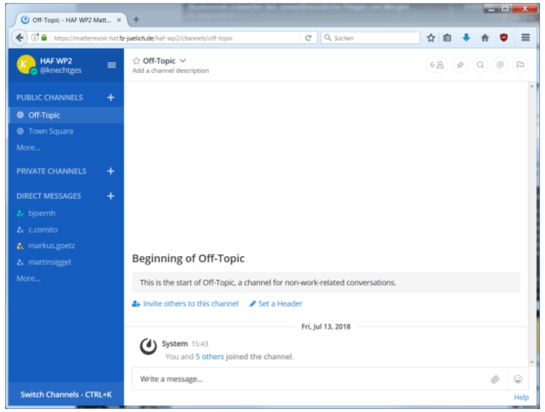
Github for code review,
issue tracking,
sprint planning



Travis for continuous integration



Mattermost for discussions

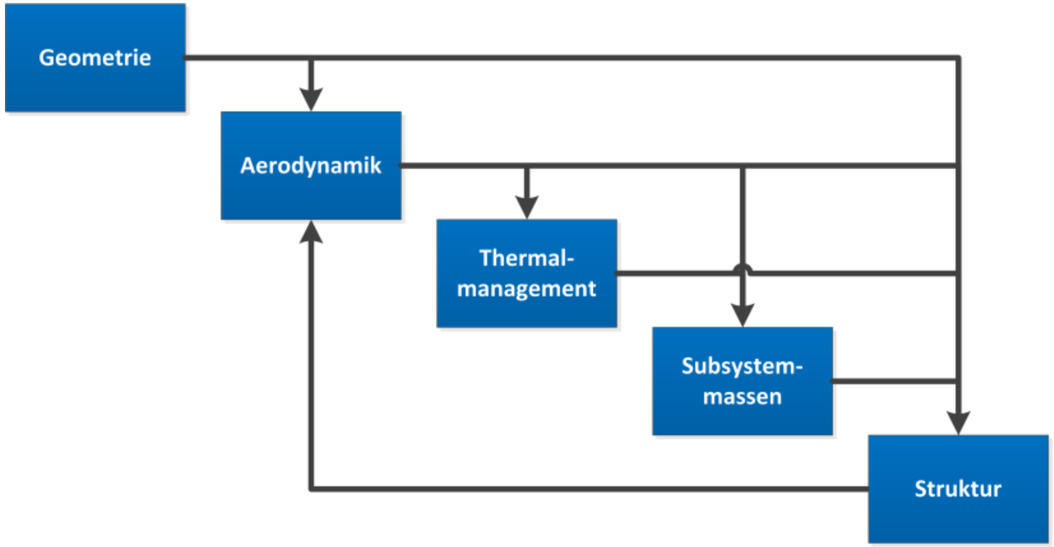


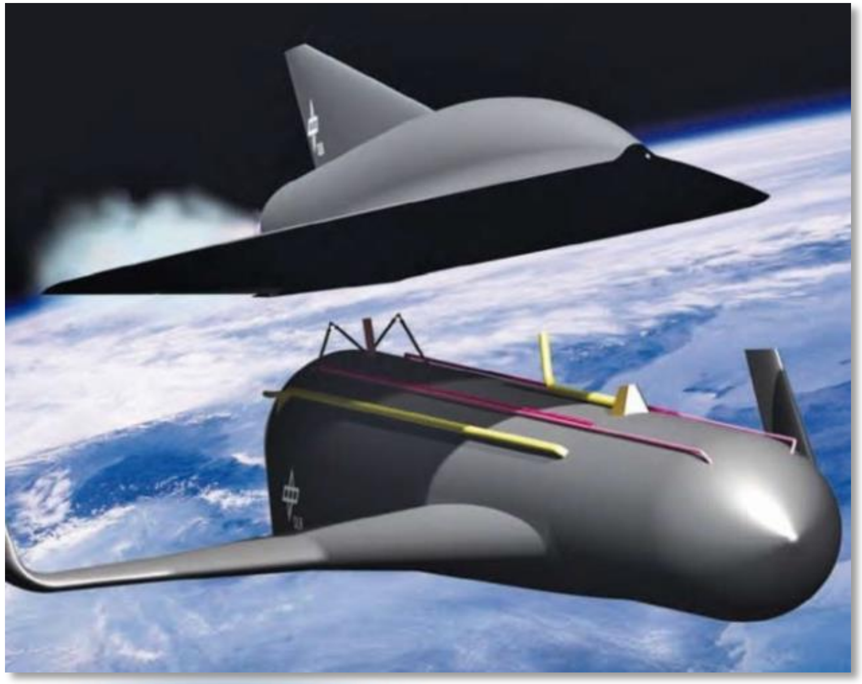
Scan me

Join us there!

https://github.com/
helmholtz-analytics

Multi-Disciplinary Optimization



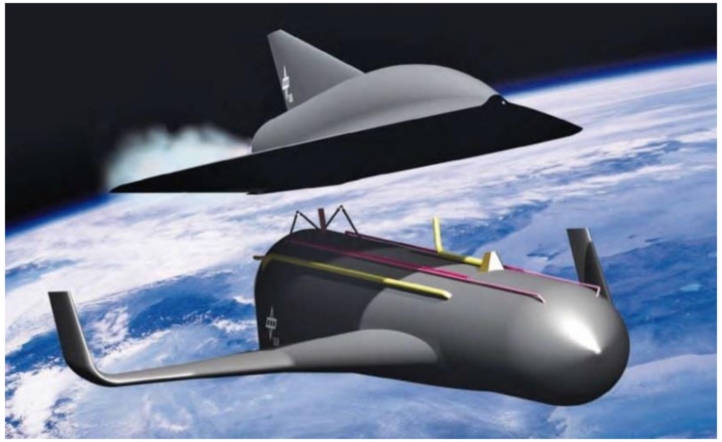


Analysis and Optimization of the Spaceliner Pre-Design

- Development of a hypersonic passenger spacecraft for long distance flights

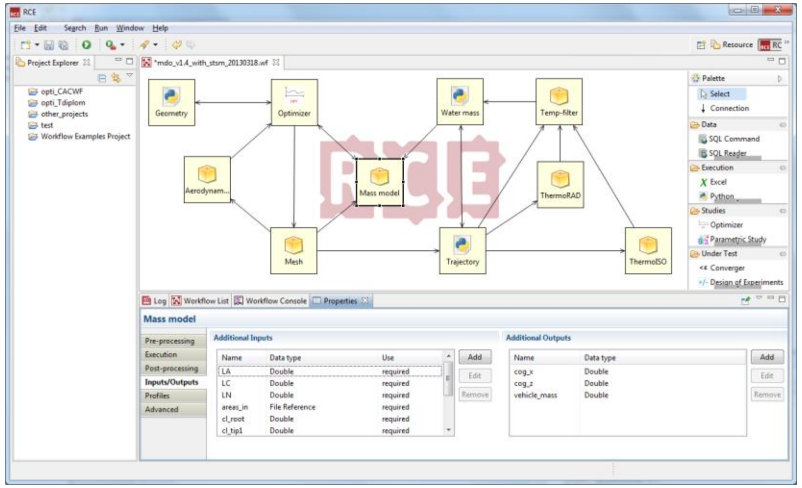
- Descent should be accomplished in gliding flight

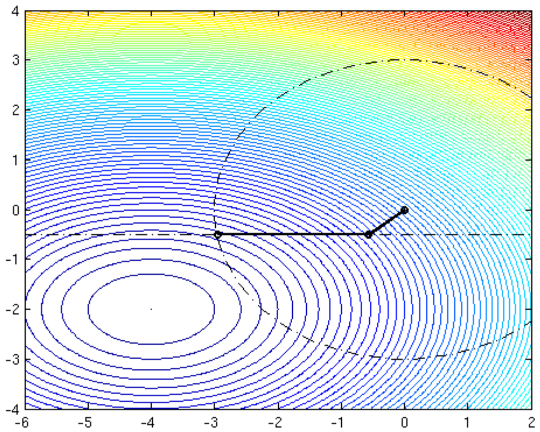
- **New research focus:** development of a hybrid structure with integrated thermal control units involving magnetohydrodynamic (MHD) effects with cooled magnets



Implementation of a Multidisciplinary Optimization Loop

- Implementation of the design as process graph in the software platform **RCE** (remote component environment) by coupling tools from different disciplines
- Problem: no derivatives available
- Up to now: use of derivative-free optimizers from toolbox **DAKOTA**
- **Our development:** new algorithm for nonlinear derivative-free constrained optimization
    - Derivative-free trust-region **SQP**-method





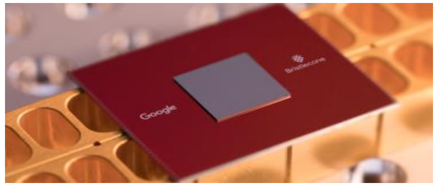
Quantencomputing

DLR

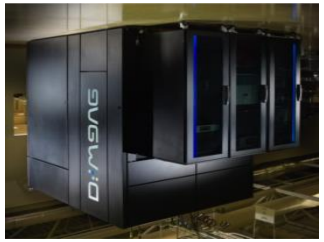
Quantum Computers for Solving Aerospace Problems

Challenges:

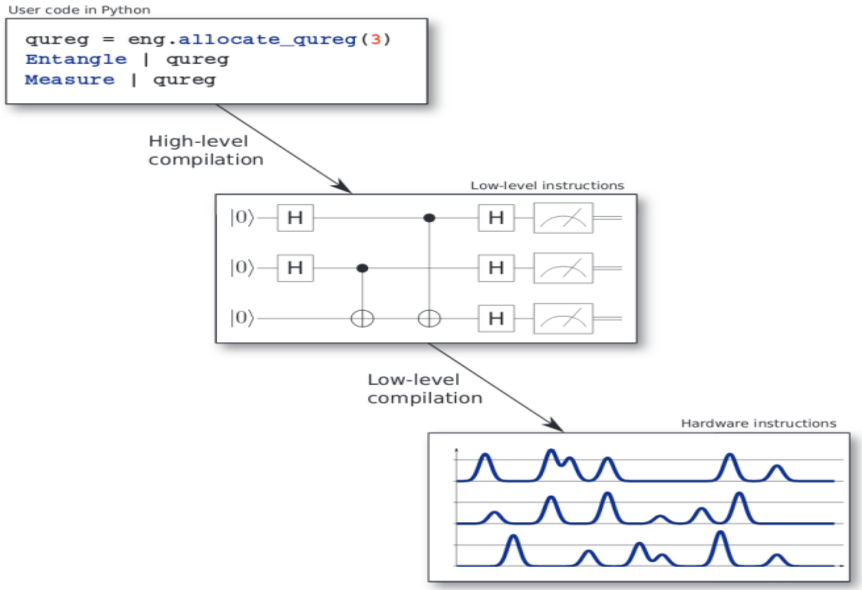
- Quantum computer interfaces are close to hardware
- Which quantum algorithms for which applications are superior to classical computing?



Google QC Chip



D-Wave Q. Annealer



Programming Quantum Computers
(arxiv:1612.08091)

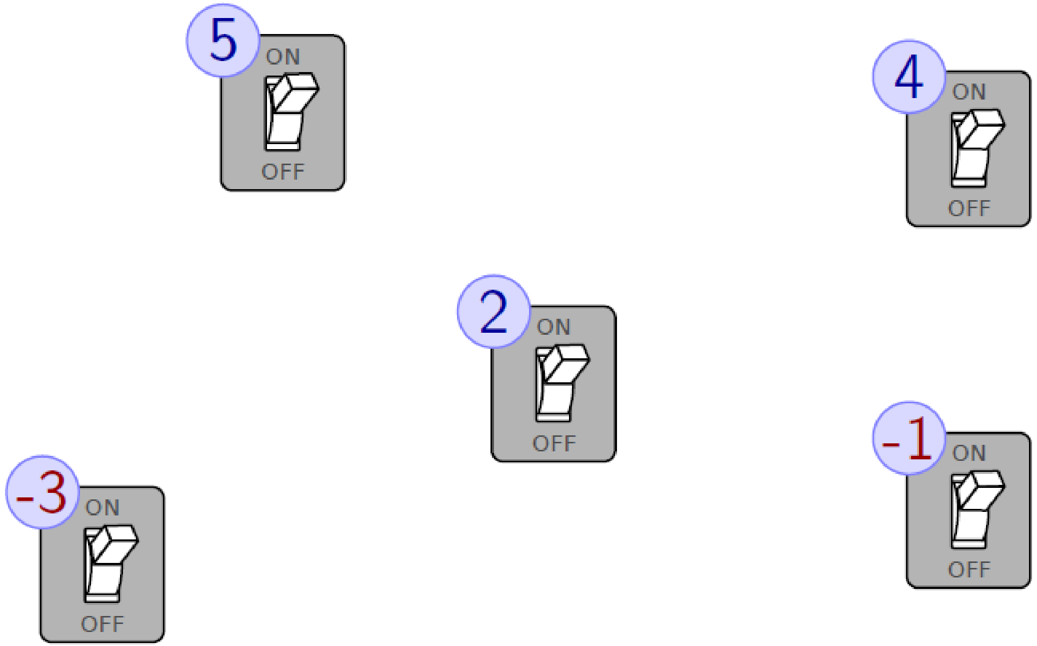
DLR QC Research:

- Investigate algorithms and applications for near-term QC devices
- Develop tools and algorithims to use QC-devices
- Perform experiments on early QC devices

Adiabatic Quantum Computer

- Optimizer for quadratic unconstrained binary problems (QUBO)

$$E = \sum_i H_i \, x_i \qquad \text{with } x_i \in \{0,1\}$$



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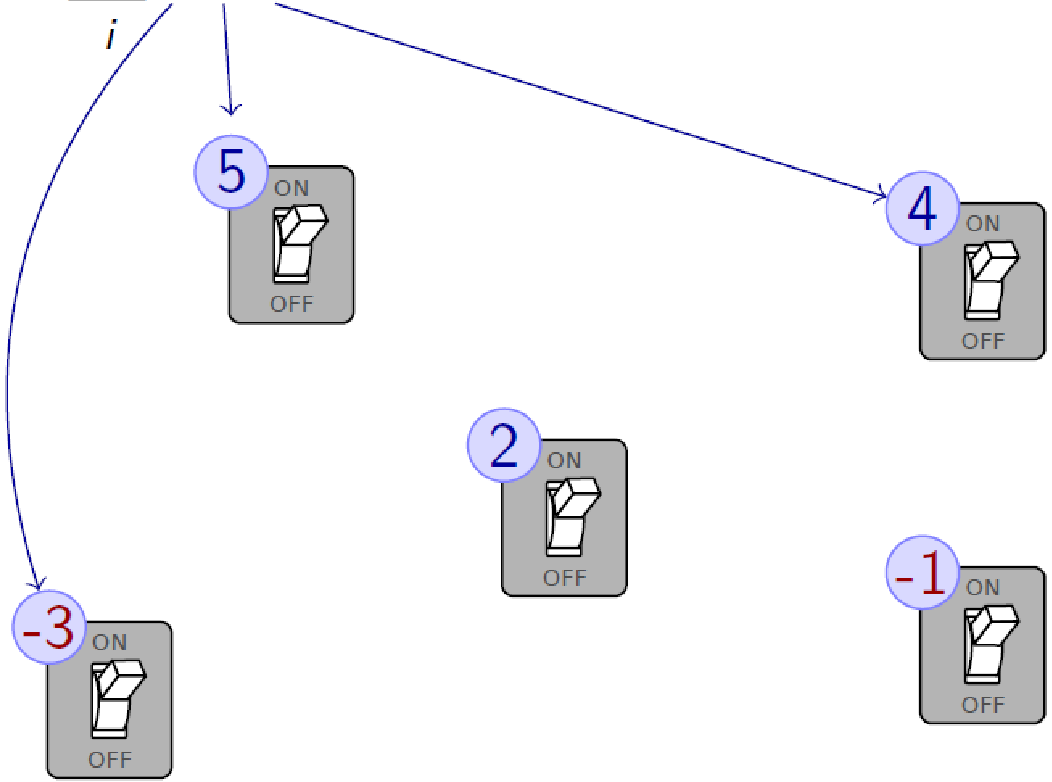

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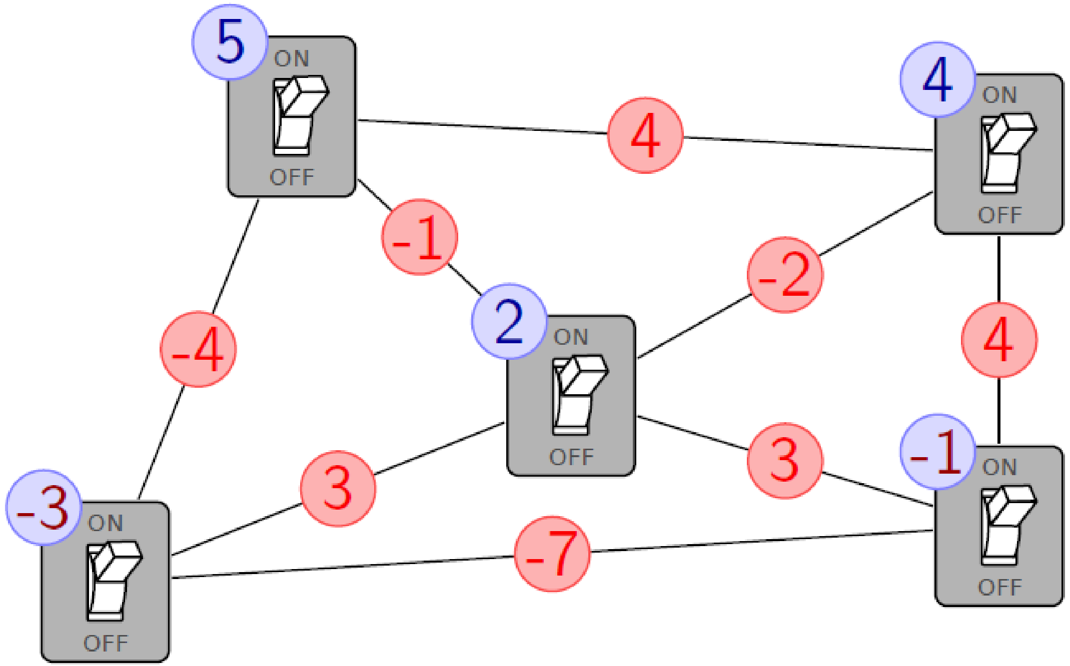
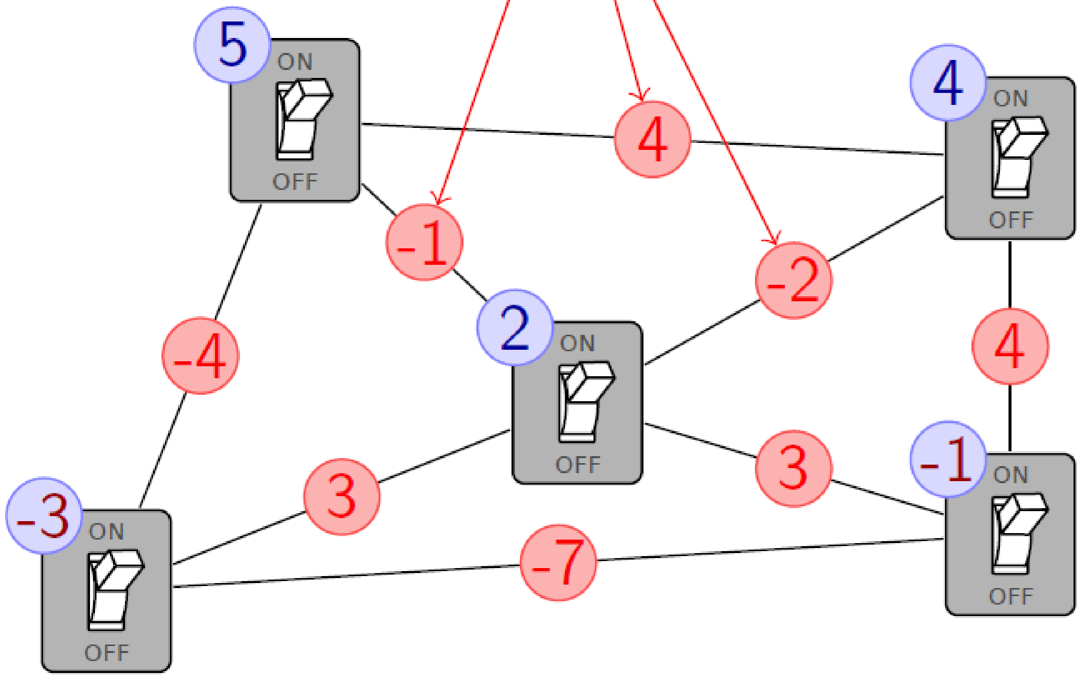


Adiabatic Quantum Computer

- Optimizer for quadratic unconstrained binary problems (QUBO)

$$E = \sum_{i} H_i \; x_i + \sum_{i \neq j} J_{ij} \; x_i x_j \qquad \text{with } x_i \in \{0,1\}$$



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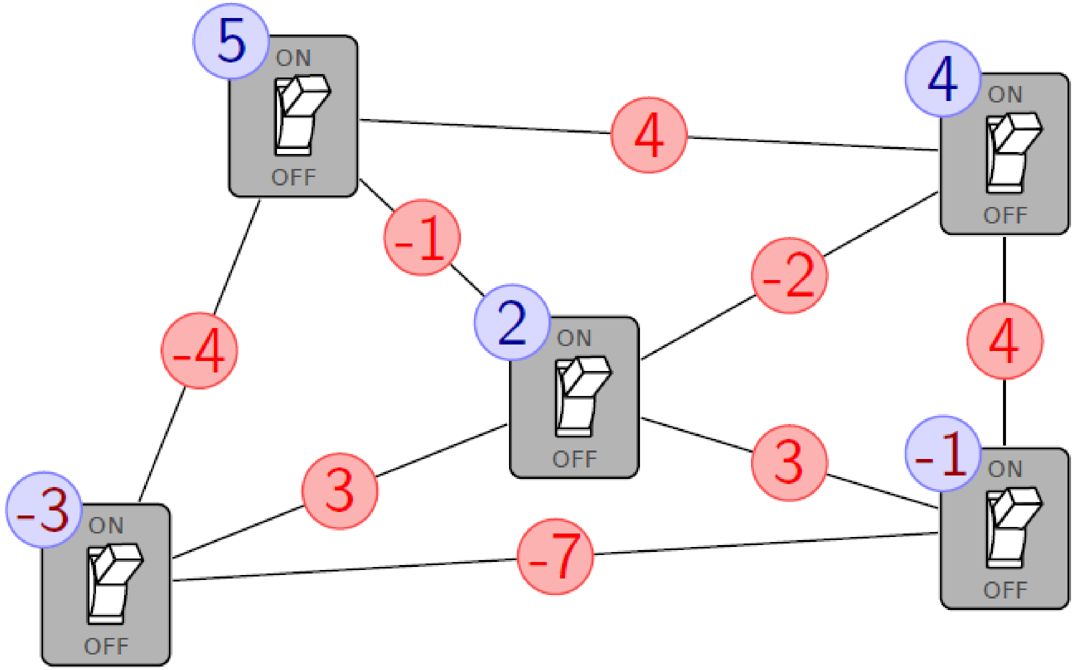
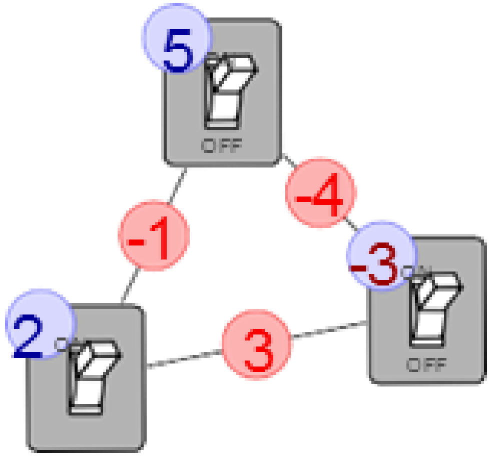


Adiabatic Quantum Computer

Example:

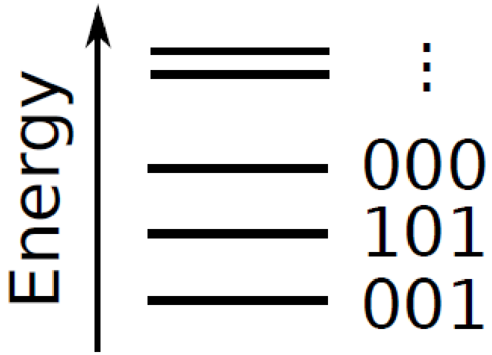


$$E = 5x_1 + 2x_2 - 3x_3 - x_1x_2 + 3x_2x_3 - 4x_3x_1$$

Lowest Energy: $E = -3$
at $(x_1, x_2, x_3) = (0, 0, 1)$

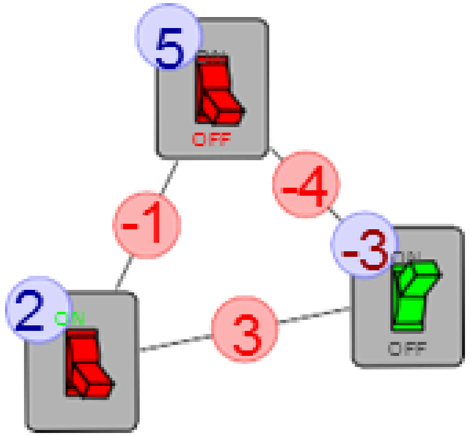
- Quantum systems have discrete energy levels (e.g. atom)

- Idea: Find system whose lowest energy state (ground state) corresponds to the solution of the optimization problem



Adiabatic Quantum Computer

Example:



$$E = 5x_1 + 2x_2 - 3x_3 - x_1x_2 + 3x_2x_3 - 4x_3x_1$$

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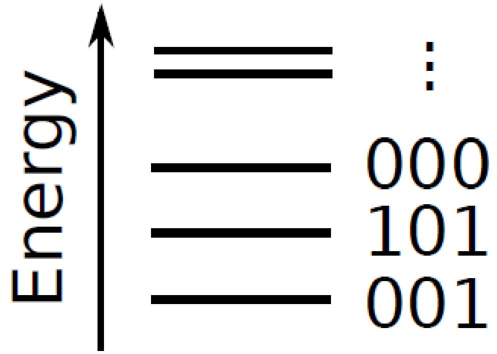


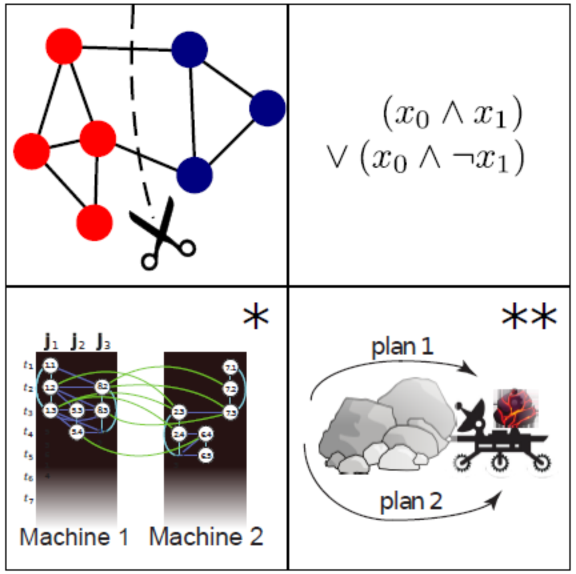
Applications for Quantum Annealers

Applications

Which problems can be mapped to QUBO?

$$E = \sum_i H_i x_i + \sum_{i \neq j} J_{ij} x_i x_j \qquad \text{with } x_i \in \{0, 1\}$$

- All NP-Complete Problems. E.g.
  - Graph Partitioning
  - Satisfiablity Problems
- Planning
  - Job-Shop Scheduling
  - Mars-Lander Operations
- Machine Learning

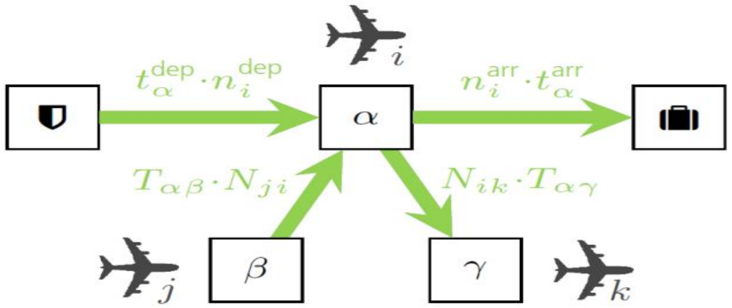


* Venturelli et. al. arXiv:1506.08479

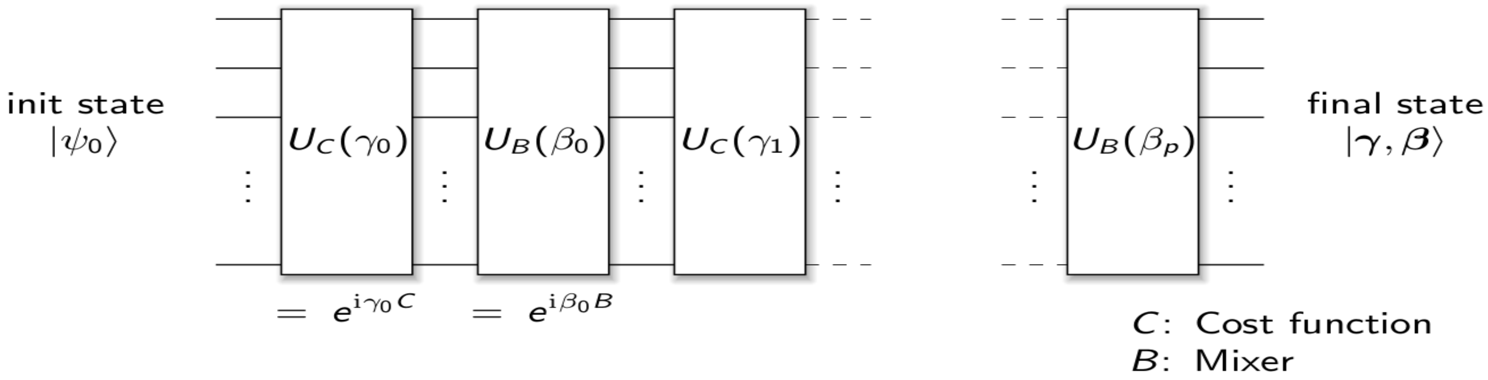
** Rieffel et. al. arXiv:1407.2887

Quantum Computing for Flight Gate Assignment

- Optimal assignment of flights to gates at airports
- Hard combinatorial optimization problem
- Amenable to D-Wave quantum annealer and gate based quantum computers (Google, IBM, etc.)
- Use real world data and perform experiments on hardware as well as simulations
- Collaboration with NASA Ames



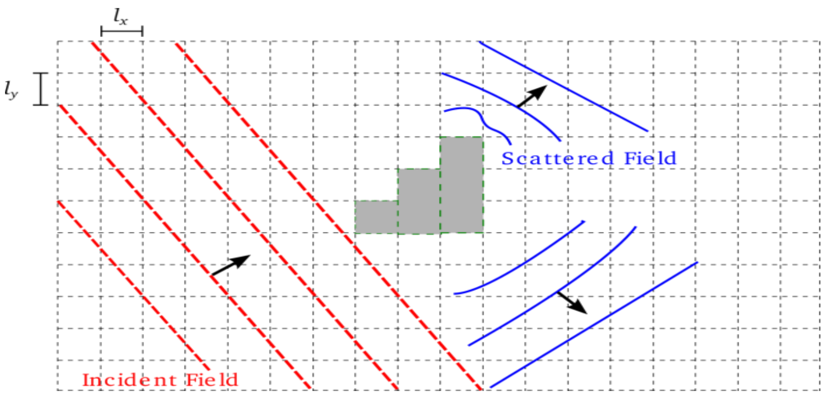
Flight Gate Assignment



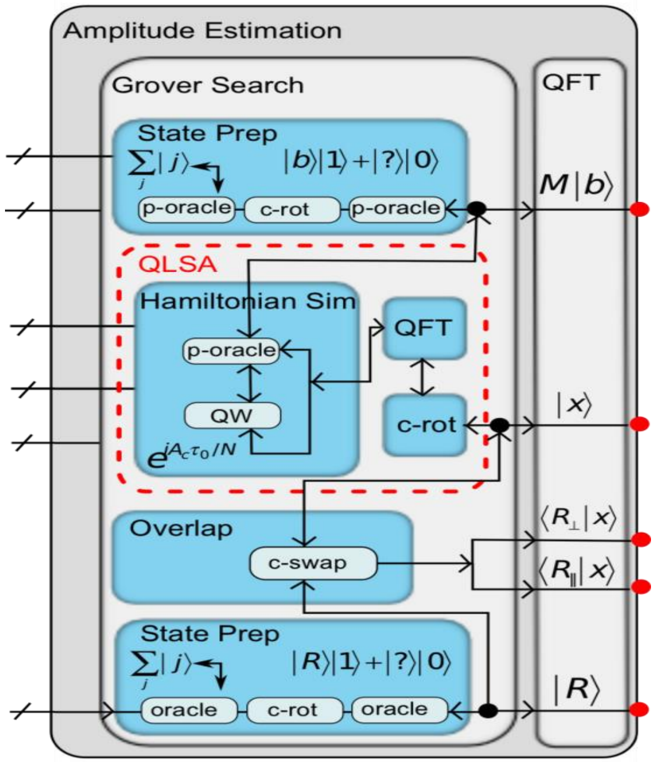
Optimization with gate-based QC (QAOA)

Quantum Computing for Radar Cross Section Calculation

- Algorithm for solving linear systems of equations (HHL)
- Amenable to large gate-based quantum computers
- Exponential speed-up over classical computers (if certain conditions are fulfilled)
- Goal: Resource estimation



FEM calculation for radar cross section
(Clader et.al. arXiv:1301.2340)



HHL Algorithm
(Clader et.al. arXiv:1301.2340)

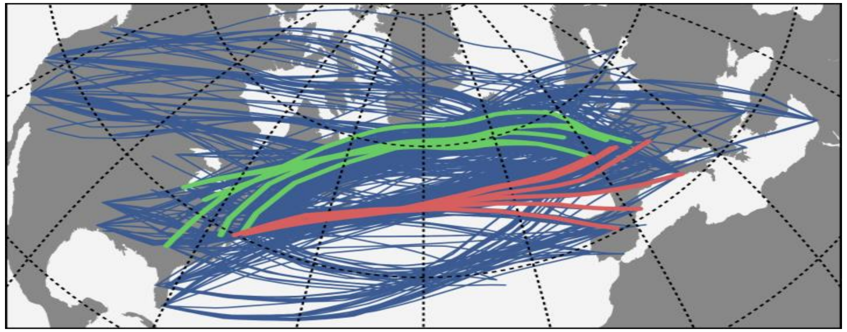
Quantum Computing for Earth Observation Data Acquisition Planning

- Optimal planning of earth observation imaging acquisition
- Hard combinatorial optimization problem
- Only solvable with heuristics
- Minor improvements to solutions would have strong impact
- Amenable to D-Wave Quantum Annealer and gate based quantum computers
- Collaboration with Airbus

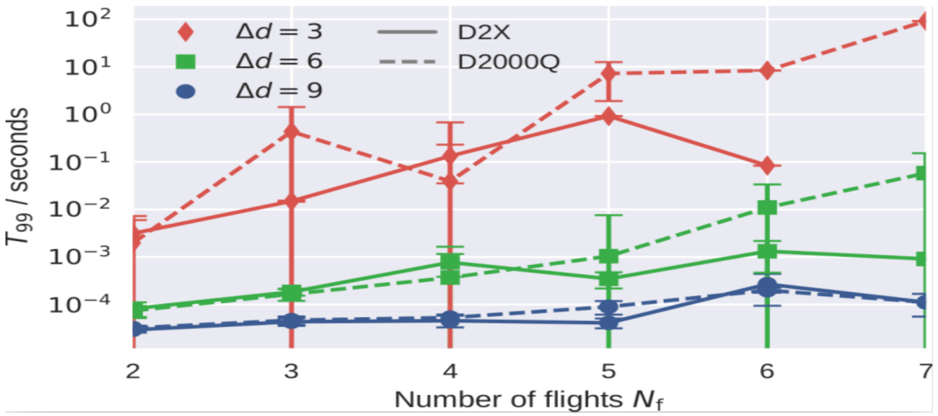
Earth Observation Satellite

Deconflicting Flights with Quantum Annealers

- Wind-optimal flight trajectories show conflicts
- Resolve these conflicts
- Reduce flight delays
- Amenable to D-Wave quantum annealer
- Collaboration with NASA Ames



Conflicts of transatlantic flights



Time-to-Solution on D-Wave
(arXiv:1711.04889)

Many thanks for your attention!

Questions?

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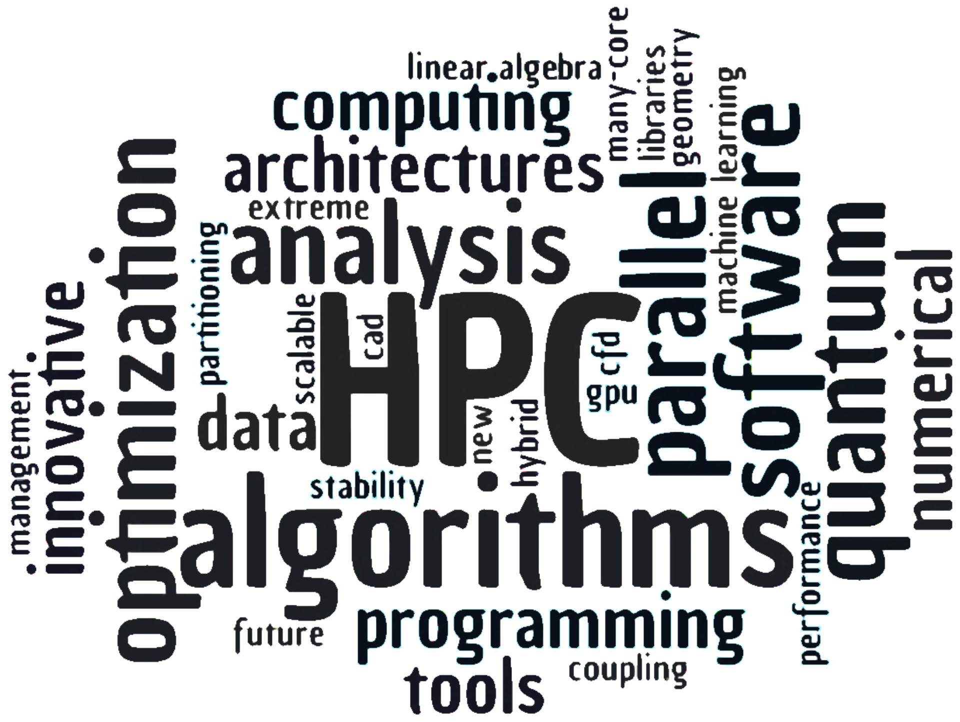
German Aerospace Center (DLR)

Simulation and Software Technology

Department Head High-Performance Computing

Achim.Basermann@dlr.de

http://www.DLR.de/sc



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