Universität Stuttgart

IARIA

IARIA InfoSys 2023

Scientific Computing:

The future of data-centric computing

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Shortly about myself

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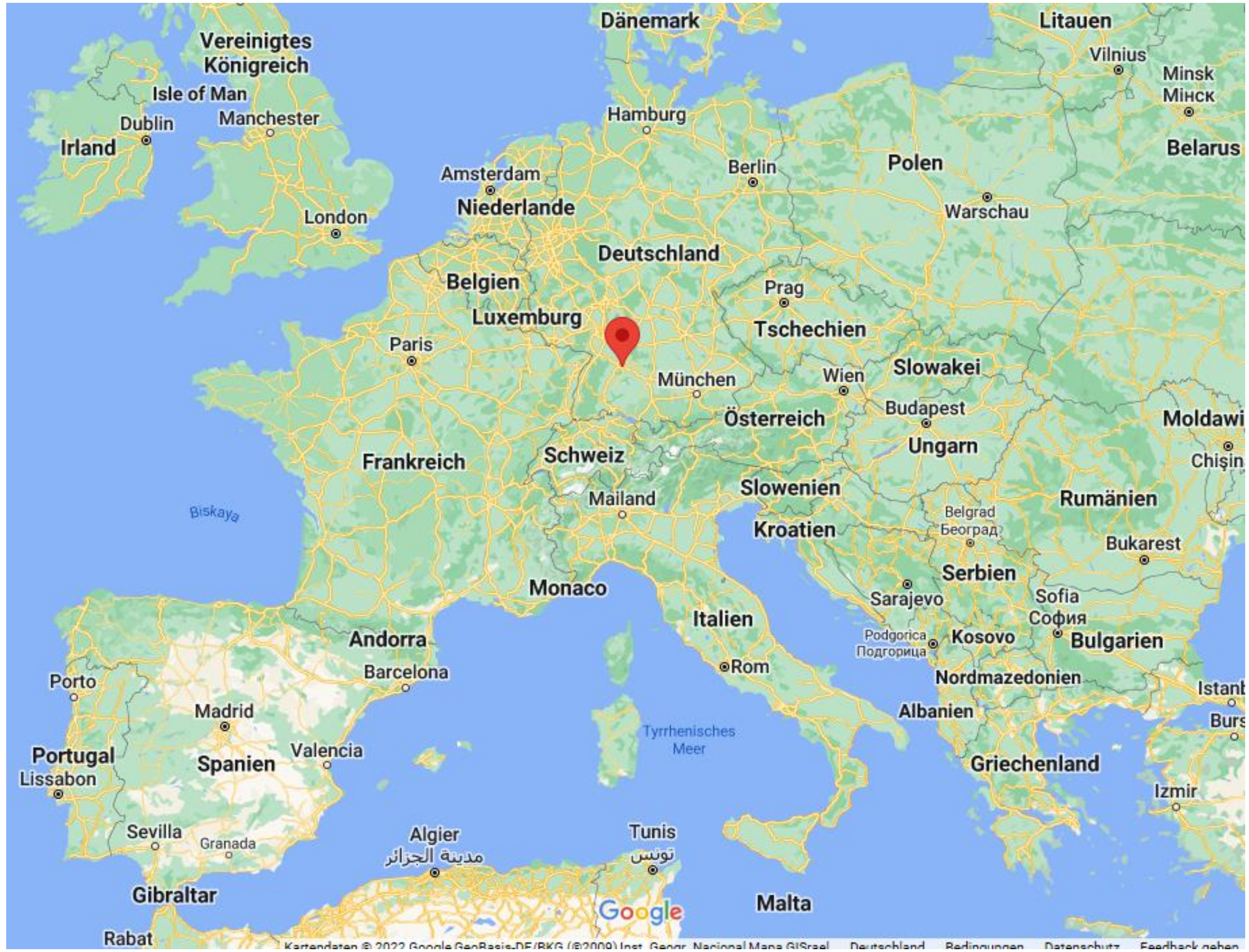
Head of Data Center and Cloud Technology @ TIK -
IT-service provider of the University of Stuttgart

- Founded 1829
  - Engineering
  - Nat. Science
- 10 faculties
- 28.000 students
- 270 professors
- 3.500 scientific & research staff



Industrial Background

KÄRCHER

Turnover: ~1-2 bil. €
Staff: ~8000

BOSCH

Turnover: ~50 bil. €
Staff: ~300.000

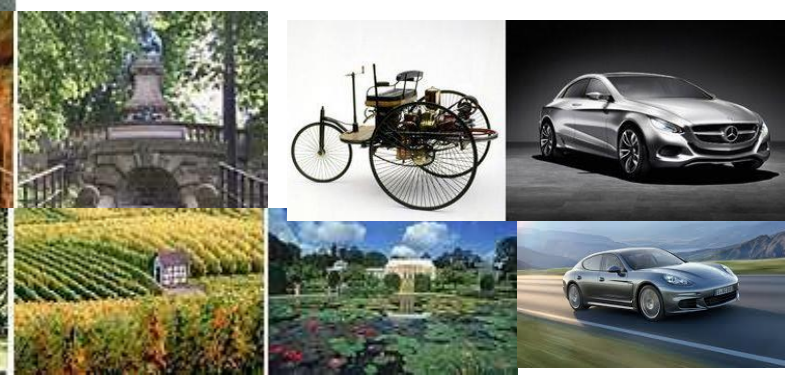
DAIMLER

Turnover: ~100 bil. €
Staff: 260.100

MAHLE

Driven by performance

Turnover: ~5 bil. €
Staff: ~50.000



STIHL

Turnover: ~2,5 bil. €
Staff: ~11.00

PORSCHE

Turnover: ~14 bil. €
Staff: ~19.000

OUTLINE

1. Introduction to High Performance Computing
   - What is HPC
   - How high is the high performance
   - Application examples
2. Data Science
   - Applications
   - Challenges
   - Cloud and Data Center technologies
3. Conclusion

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Performance: Definition

- **Number of operations for performing an algorithm**
  - Basic microprocessor operations such as ***Addition***, ***Substraction***, ***Multiplication***, and ***Division***.

$$\text{Performance} = \frac{\text{Nr. Operations}}{\text{Time [s.]}}$$

Performance: Measurement

- **Major metric – Flop/s**
  - Floating point (double precision – 64 bits) operations per second

196736893.993695017392

x

785.248915125826056 23

= ??? [Flop/s]

What‘s about the other systems‘ performance

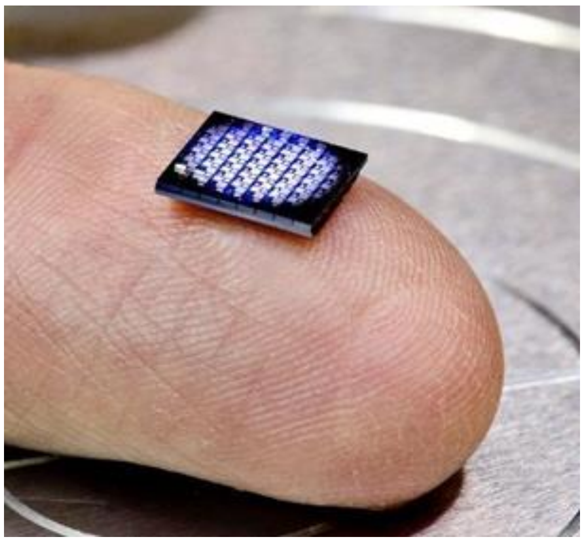
- **HAWK – a new-generation HPC system of HLRS**
  - HPL (High-Performance Linpack) – solver of a (random) dense system of linear equations in double precision

[Flop/s] 26 000 000 000 000 000

Peta

Performance: Way to increase

- **Increase the chip capacities**
  - IBM's Microprocessor as of 2018
  - Intel's Microprocessor Haswell

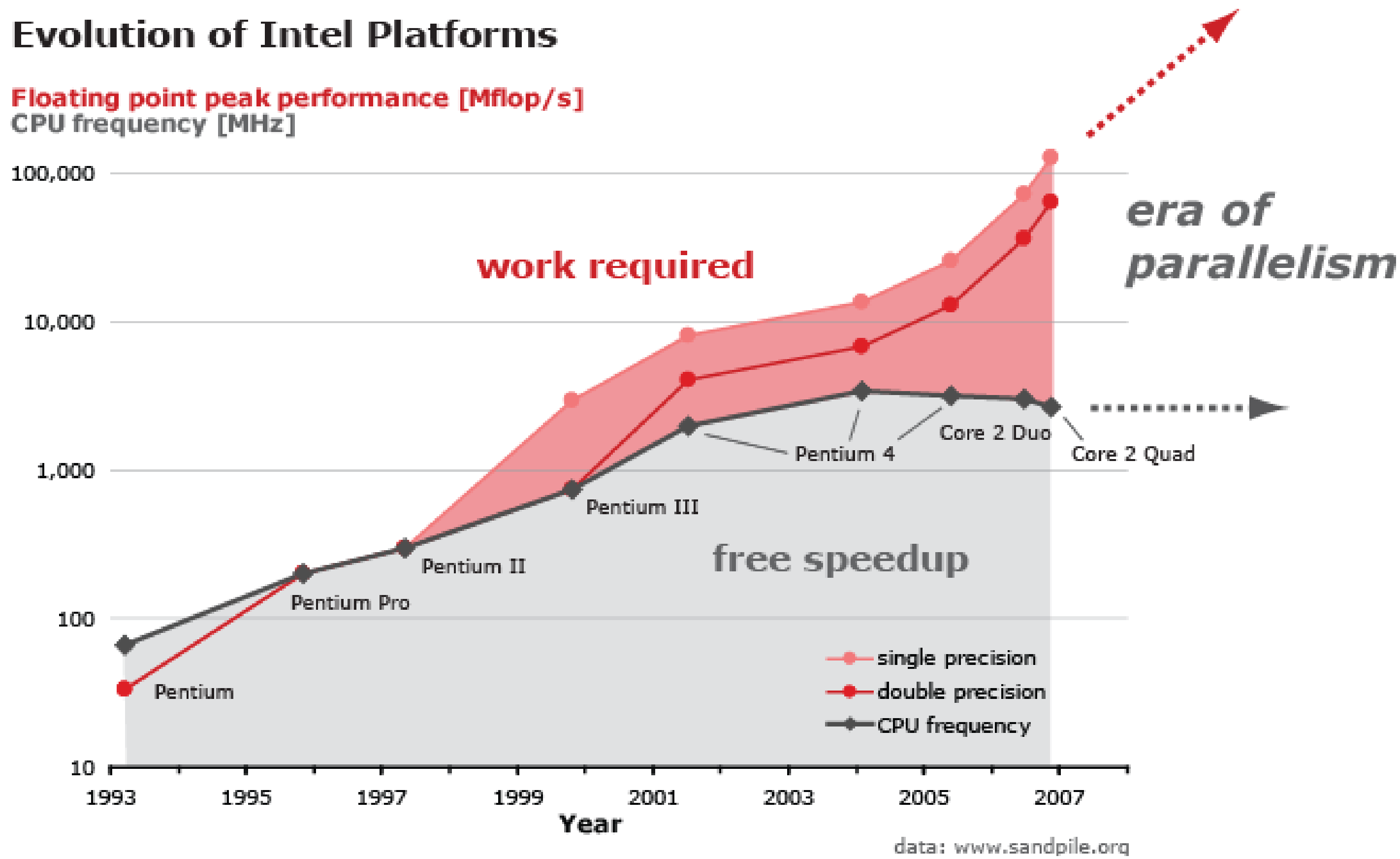


15 MFLOPs

480.000 MFLOPs

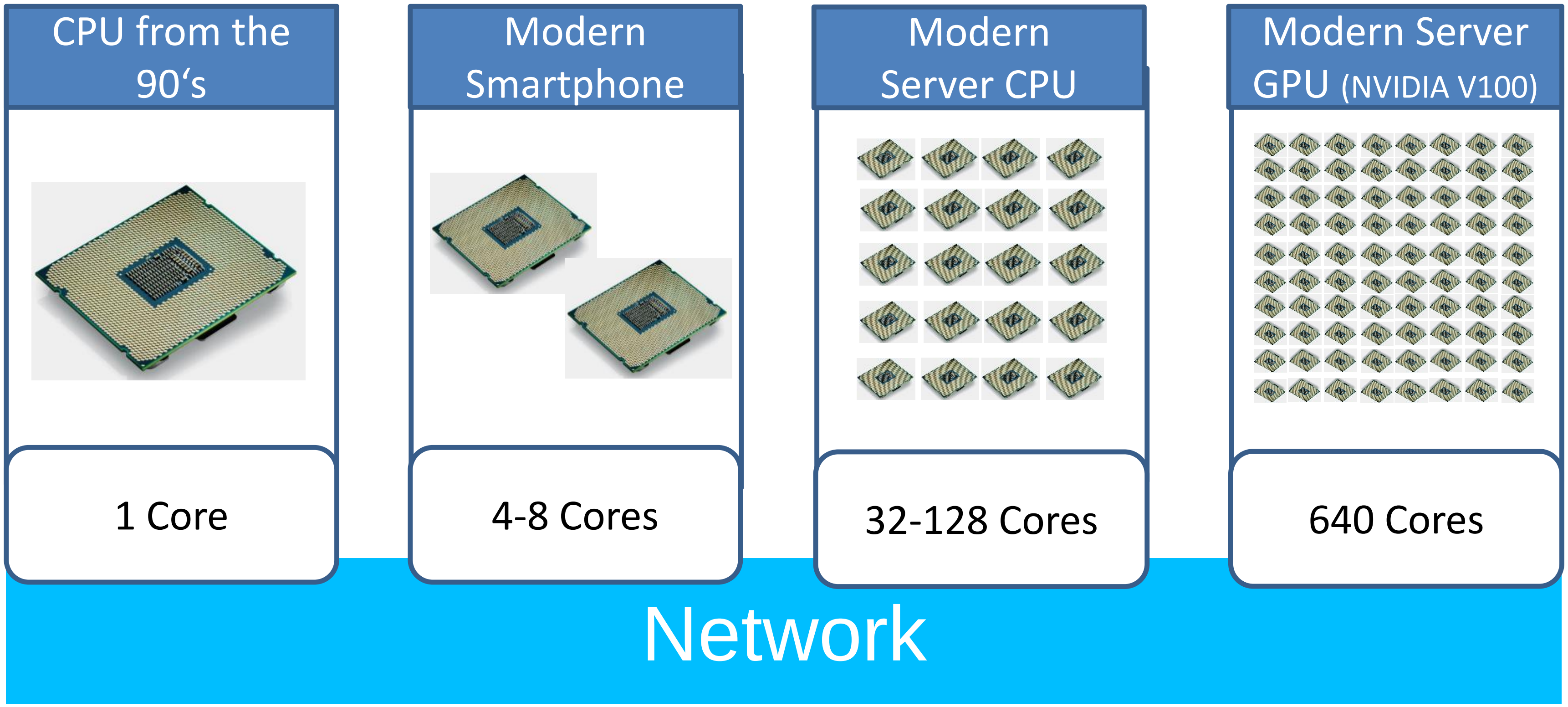
Performance: Way to increase

- **Increase the chip capacities: Limits**



Performance: Way to increase

- **Parallelisation**



Performance: Historical Development

- **Cray-2 (Stuttgart, 1986)**
  - 4 CPUs
  - 2 GFlop/s
  - 32GB RAM
  - 2,5 Tones
    (1/3 – cooling liquid)

Performance: Historical Development

- HLRS‘s Hawk (2021)
  - 5.632 Nodes / 2 CPUs/ 64 Cores
  - 720.896 Cores totally
  - 7,4 PFlop/s
  - 5 MW

Performance: Leaders

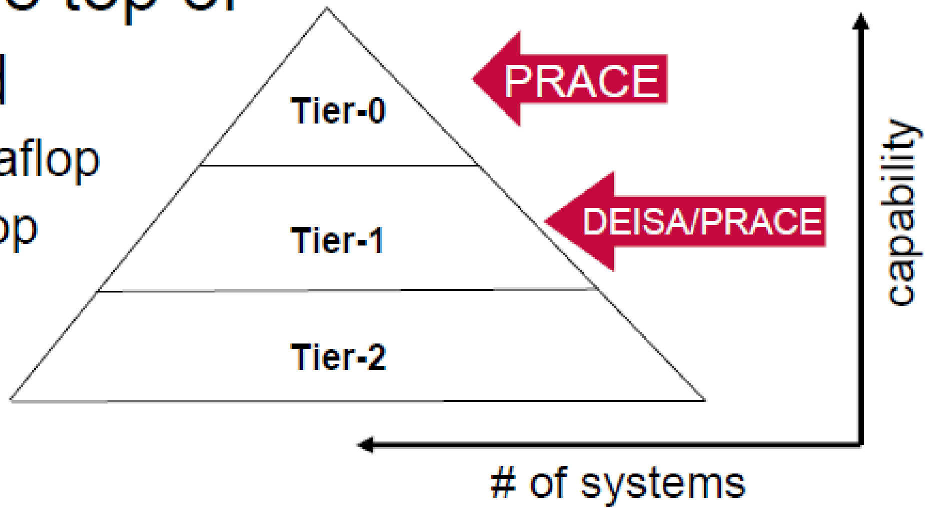
- **TOP500.org**

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory	8,730,112	1,102.00	1,685.65	21,100
	DOE/NNSA/LLNL United States				

10	**Adastra** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Grand Equipement National de Calcul Intensif - Centre Informatique National de l'Enseignement Suprieur (GENCI-CINES) France	319,072	46.10	61.61	921
11	**JUWELS Booster Module** - Bull Sequana XH2000 , AMD EPYC 7402 24C 2.8GHz, NVIDIA A100, Mellanox HDR InfiniBand/ParTec ParaStation ClusterSuite, Atos Forschungszentrum Juelich (FZJ) Germany	449,280	44.12	70.98	1,764

The EU-Vision of Supercomputing

- European HPC-facilities at the top of an HPC provisioning pyramid
  - Tier-0: 3-6 European Centres for Petaflop
  - Tier-0: ? European Centres for Exaflop
  - Tier-1: National Centres
  - Tier-2: Regional/University Centres
- Creation of a European HPC ecosystem

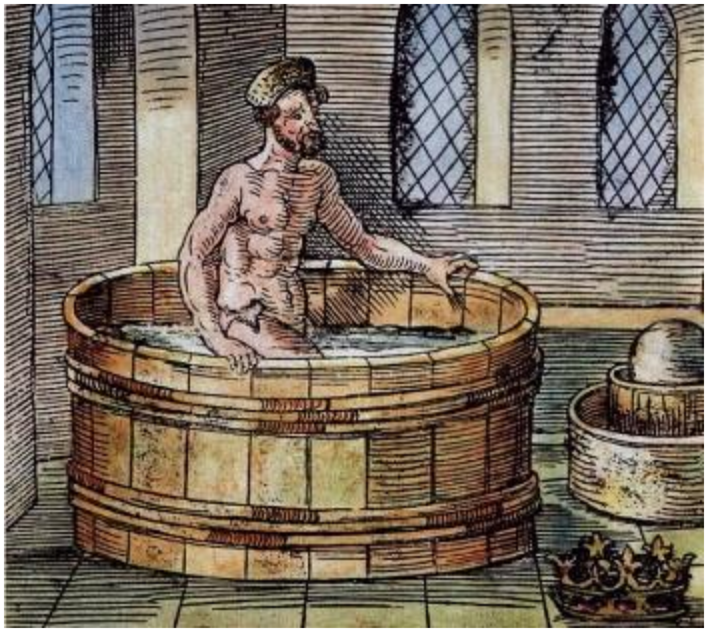


Evolution of Computational Science

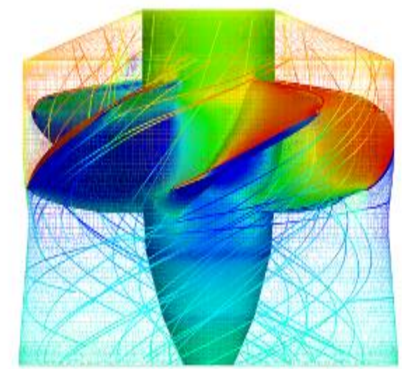
continuity: $\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$

x-momentum: $u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{1}{\rho}\frac{\partial p}{\partial x}+\nu\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right]$

y-momentum: $u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{1}{\rho}\frac{\partial p}{\partial y}+\nu\left[\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right]$



```
f = figure;
set(f,'Color', [0 0 0]);
sphere(200);
axis vis3d off;
h = findobj('Type','surface');
shading interp;
set(h,'FaceColor',[0.5 0.5 0.5]);
light('Position',[-3 -1 3]);
set(h,'DiffuseStrength',1.0);
set(h,'SpecularStrength',1);
set(h,'SpecularExponent',1);
set(h,'AmbientStrength',0.25);
set(h,'BackFaceLighting','lit')
```

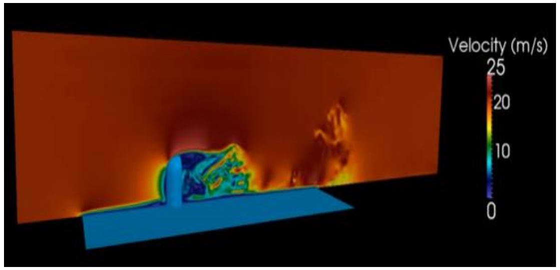


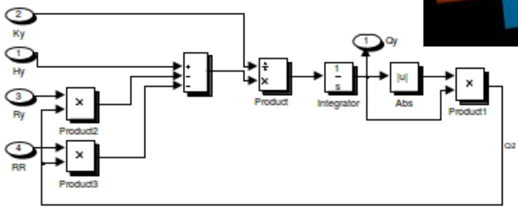
experimental — theory — computation — simulation

-1000 — **-100** — **-10** — **2010** Year, A.D.

Simulation: The Way

- Optimization
- Simulation Software
- Mathematical Model
- Abstract Model
- Simulation object





$$\rho\dot{\vec{v}} = \rho\left(\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\nabla)\vec{v}\right) = -\nabla p + \mu\Delta\vec{v} + \left(\zeta + \frac{\mu}{3}\right)\nabla(\nabla\cdot\vec{v}) + \vec{f}.$$

```
defineDynamics(lattice, lattice.getBoundingBox(),
               new CylinderShapeDomain3D<T>(cx,cy,radiu
               new BounceBack<T,DESCRIPTOR>);



createPoiseuilleBoundaries(lattice, parameters, *bounda
lattice.initialize();

// Main loop over time iterations.
for
    // Lattice Boltzmann iteration step.
    lattice.collideAndStream();
}

delete boundaryCondition;
```

Application Domains: Mathematical Background

- CFD – Computational Fluid Dynamics
- MD – Molecular Dynamics

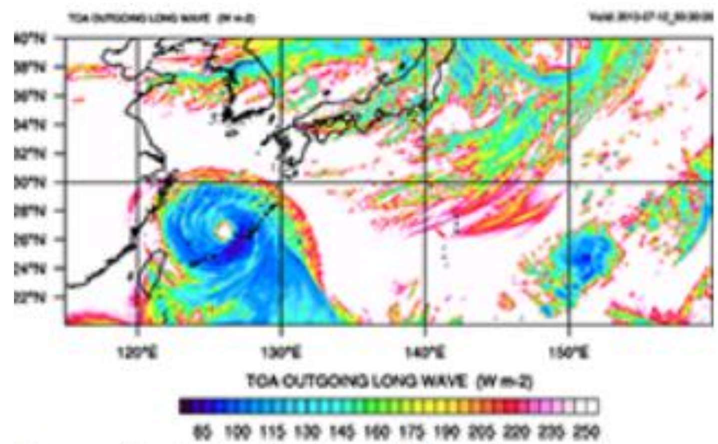
$$\frac{\partial \overline{\upsilon}}{\partial t} + \overline{\upsilon} \cdot (\nabla \overline{\upsilon}) = \overline{F} - \frac{1}{\rho} \nabla p + \nu \Delta \overline{\upsilon}$$

$$\nabla \cdot \overline{\upsilon} = 0$$

$$\rho S \cdot (1 + \xi) \cdot \left(\upsilon^2 \Big|_{S_2} - \upsilon^2 \Big|_{S_1} \right) = S \cdot \left(p \Big|_{S_1} - p \Big|_{S_{21}} \right) +$$
$$p \Phi dy - pS \frac{d\upsilon}{dt} dy - \frac{\rho \lambda S}{r} \upsilon^2 dy$$

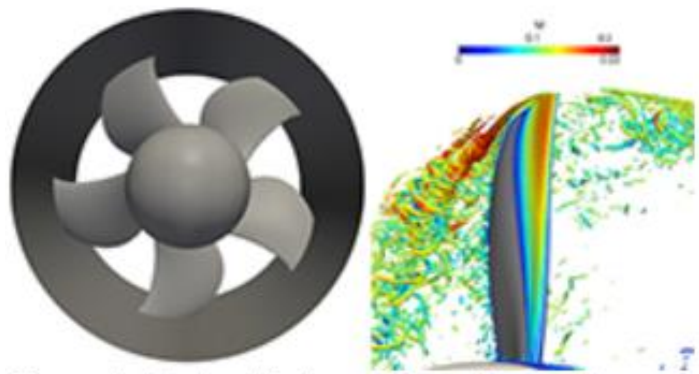
Applications: The XXL Portfolio

- Climate simulation on a high (a few kms) resolution
  - University of Hohenheim
  - 84.000 cores, 84 hours, 450 TB data



Copyright: *Institute of Physics and Meteorology, Universität Hohenheim*

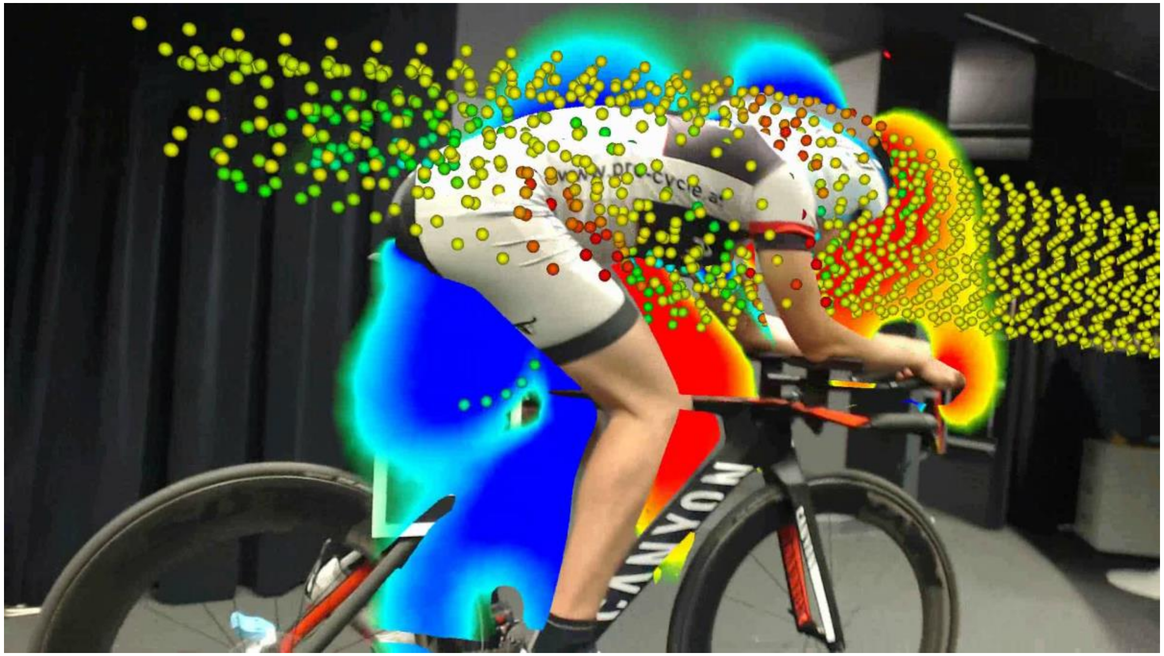
- Turbulent flow simulation for air- and gas dynamics analysis
  - RWTH Aachen University
  - 92.000 cores, 110 hours, 80 TB data



Copyright: *Institute of Aerodynamics, RWTH Aachen University*

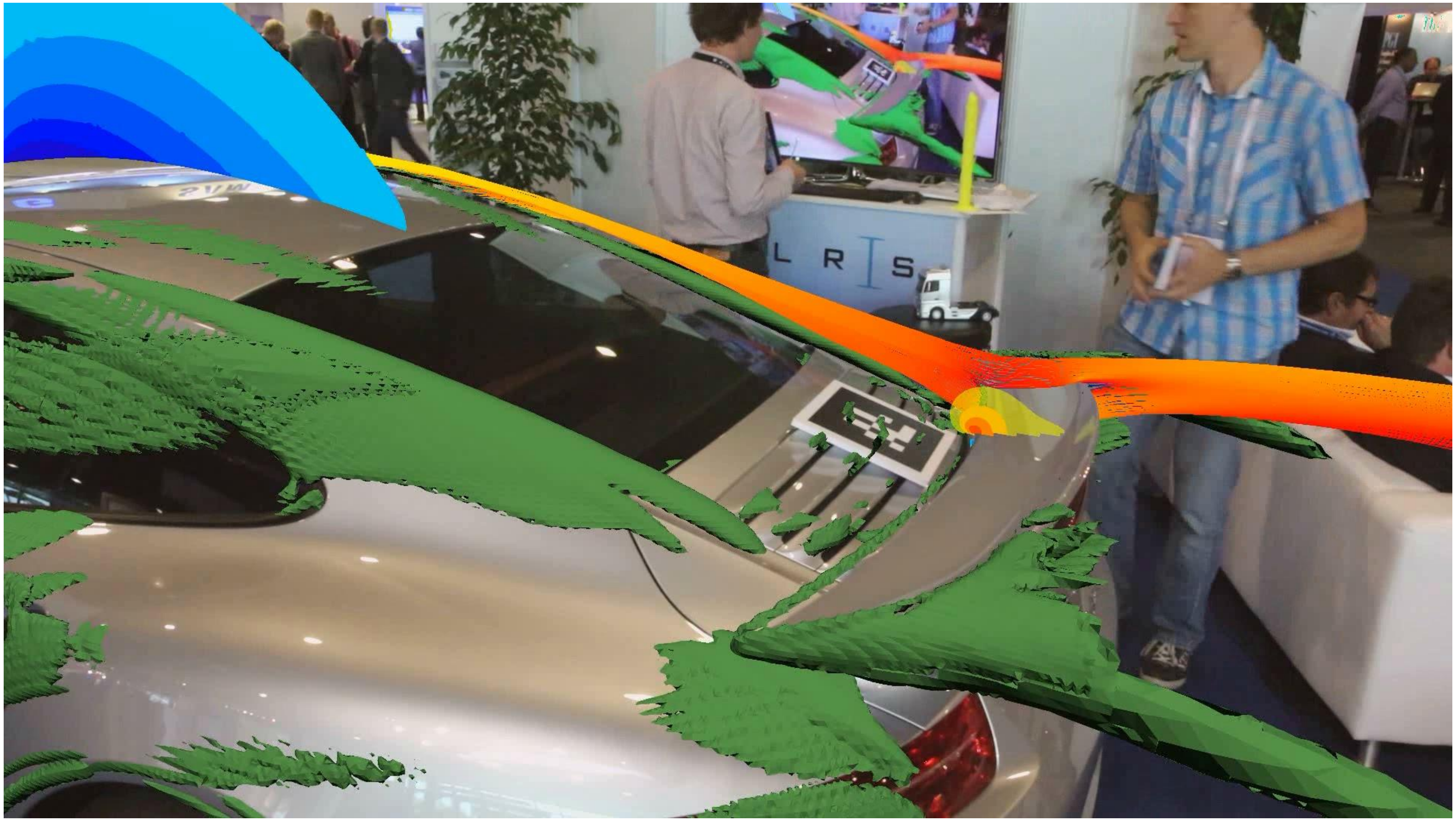
Further Use Cases

- Vehicle aerodynamics

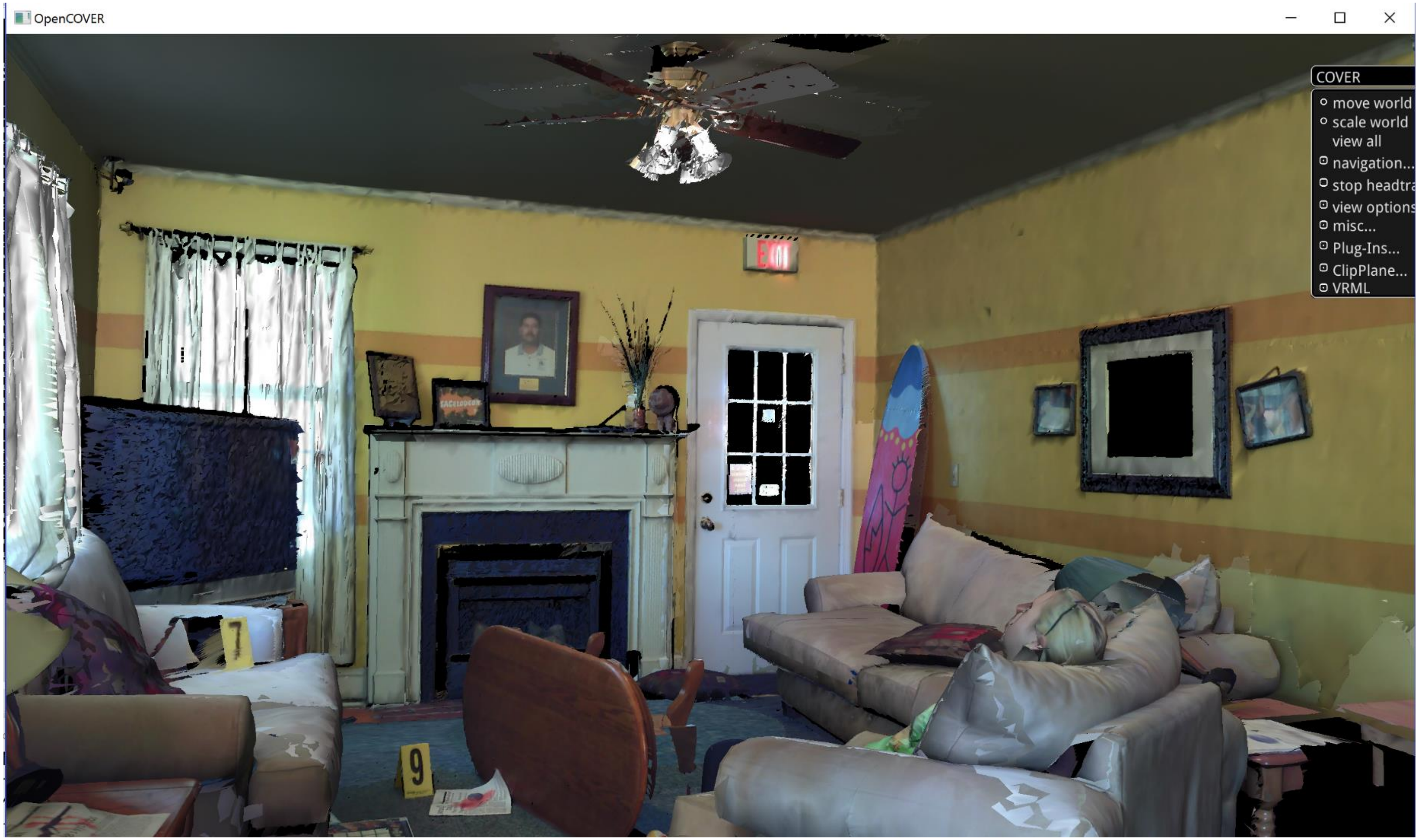


Further Use Cases

- Vehicle aerodynamics

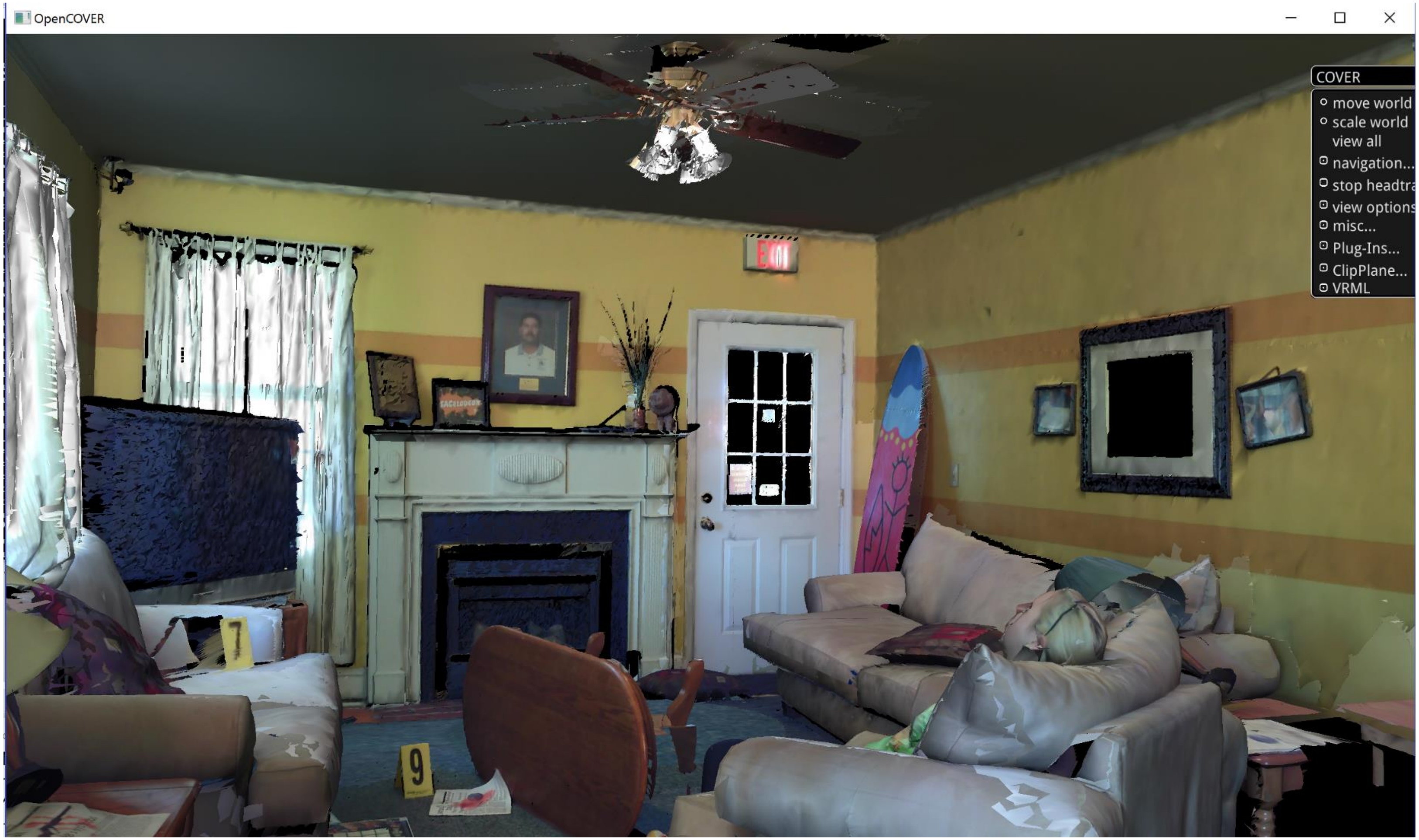


Further Use Cases



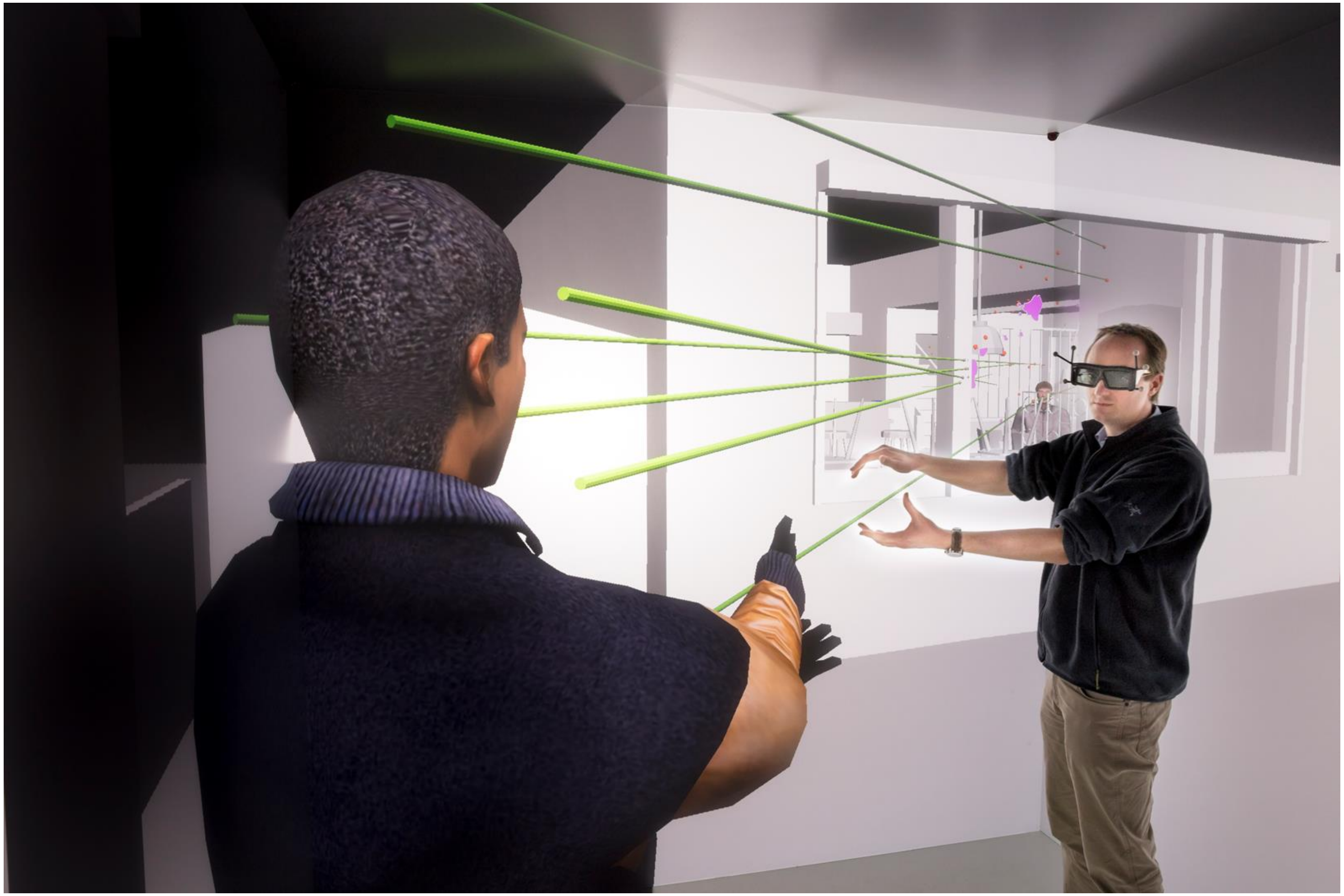
Further Use Cases

- **Crime Scene Reproduction**



Further Use Cases

- Crime Scene Reproduction



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Further Evolution of Computational Science

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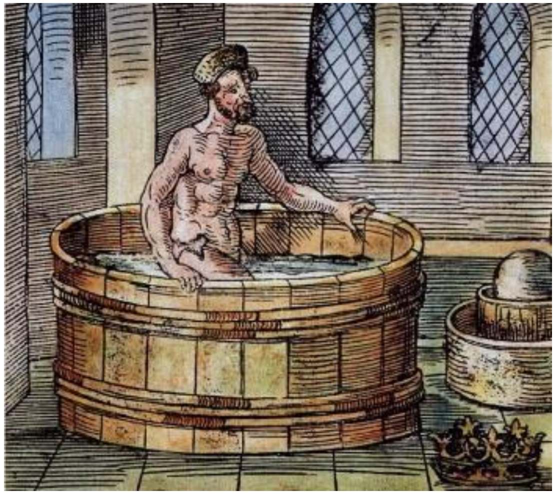

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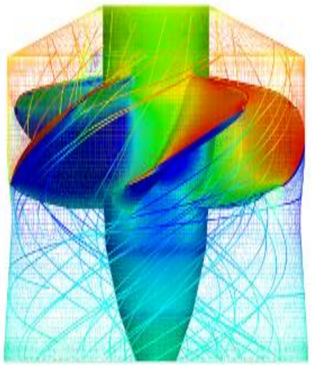
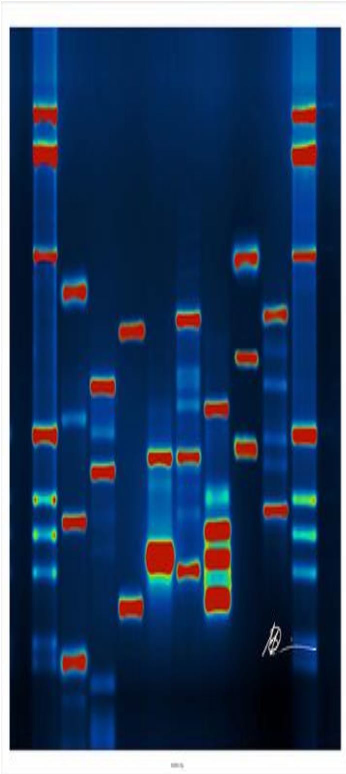


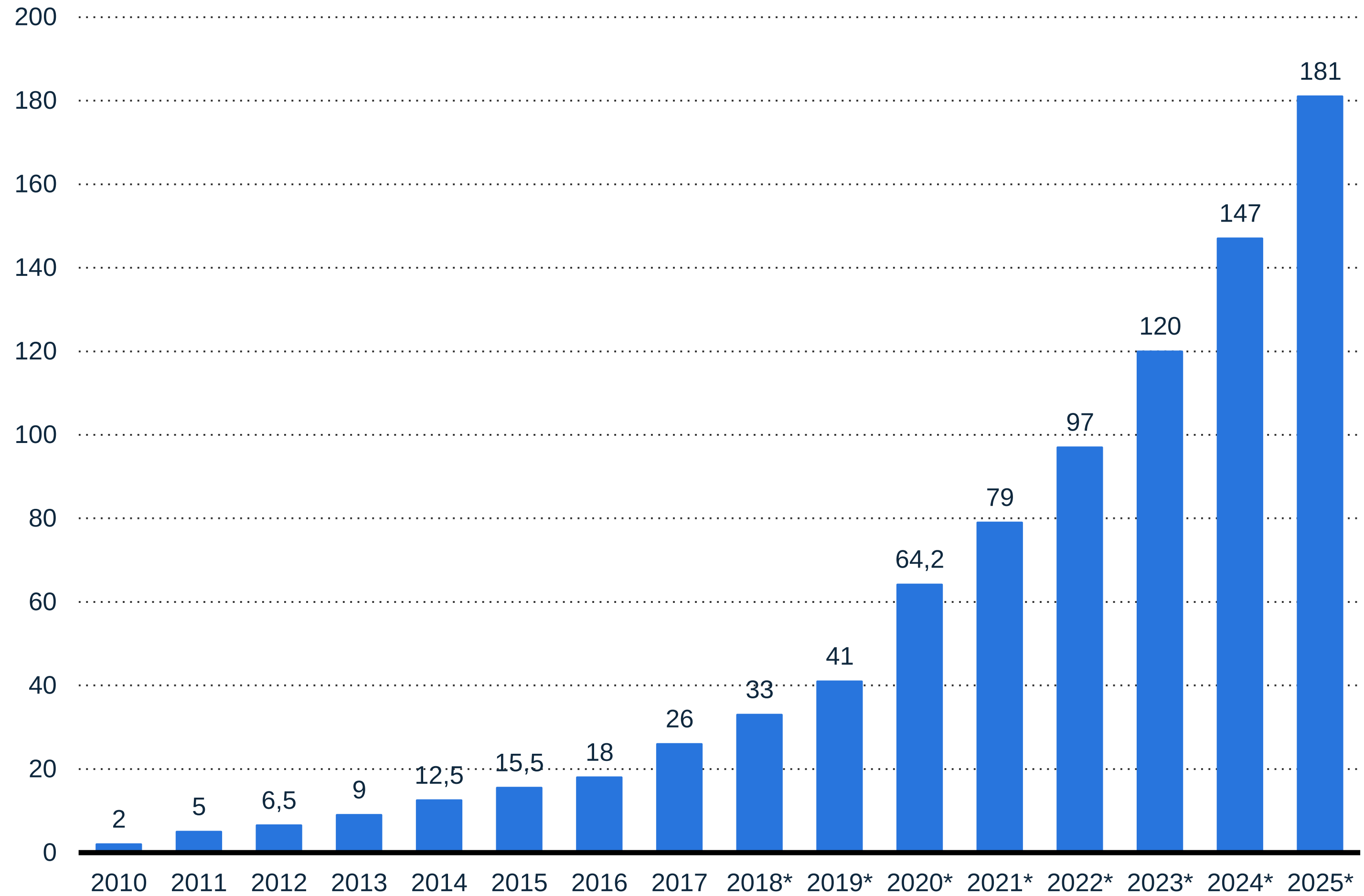


experimental | theory | computation | simulation | data-driven

-1000 | -100 | -10 | 2020 | Year, A.D.

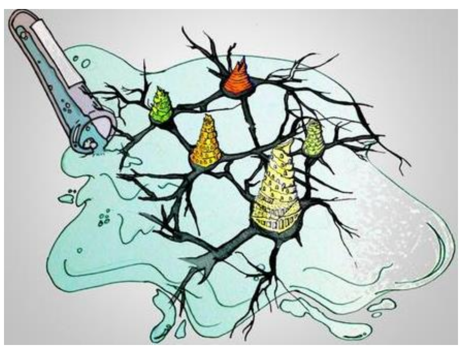
Digital Assets

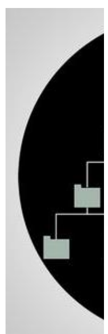
- Data Volume in Zetabytes (Gartner)

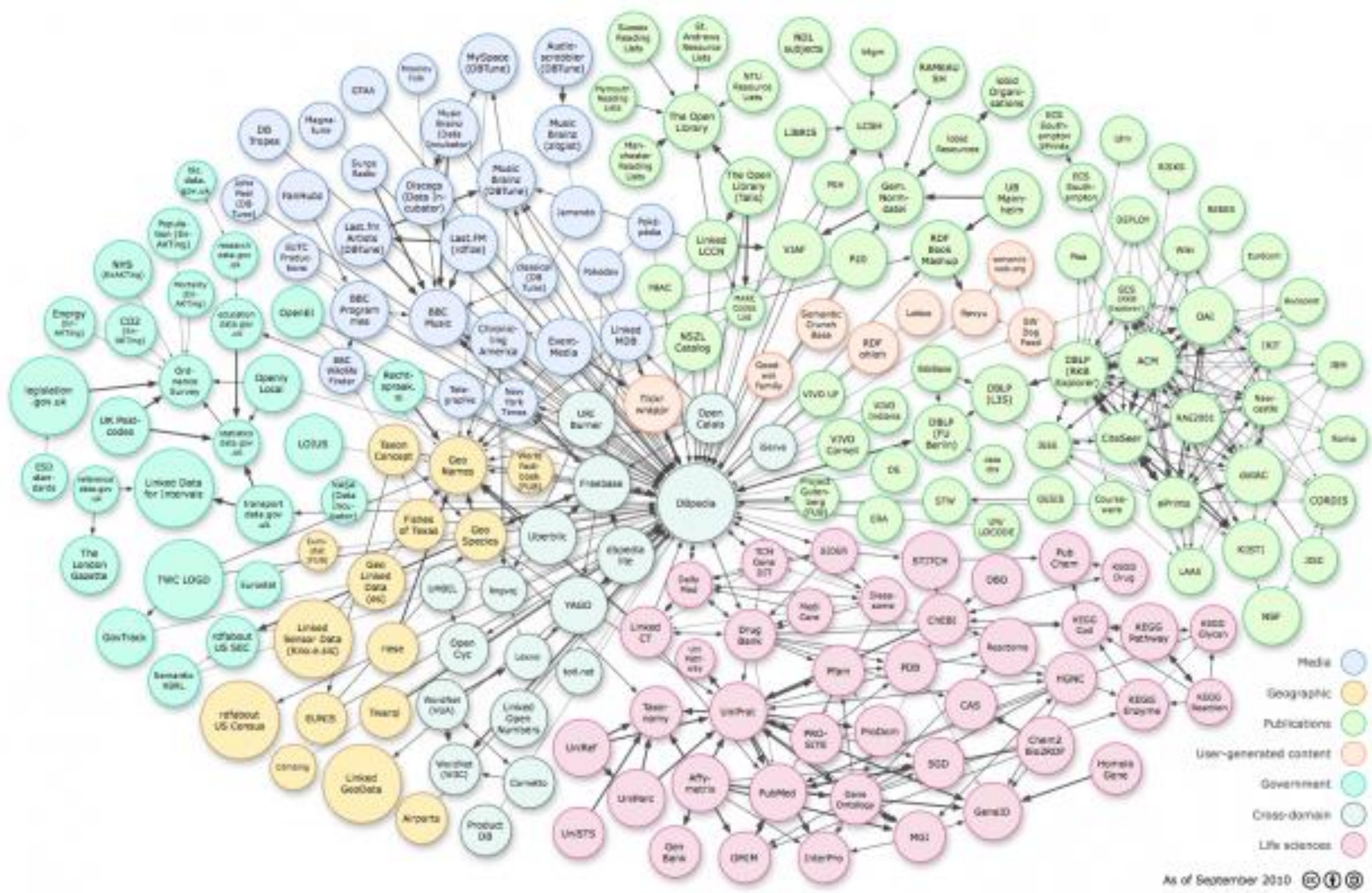


Digital Assets

- **Data Evolution**







unstructured data | ontologies | linked data | Semantic Web

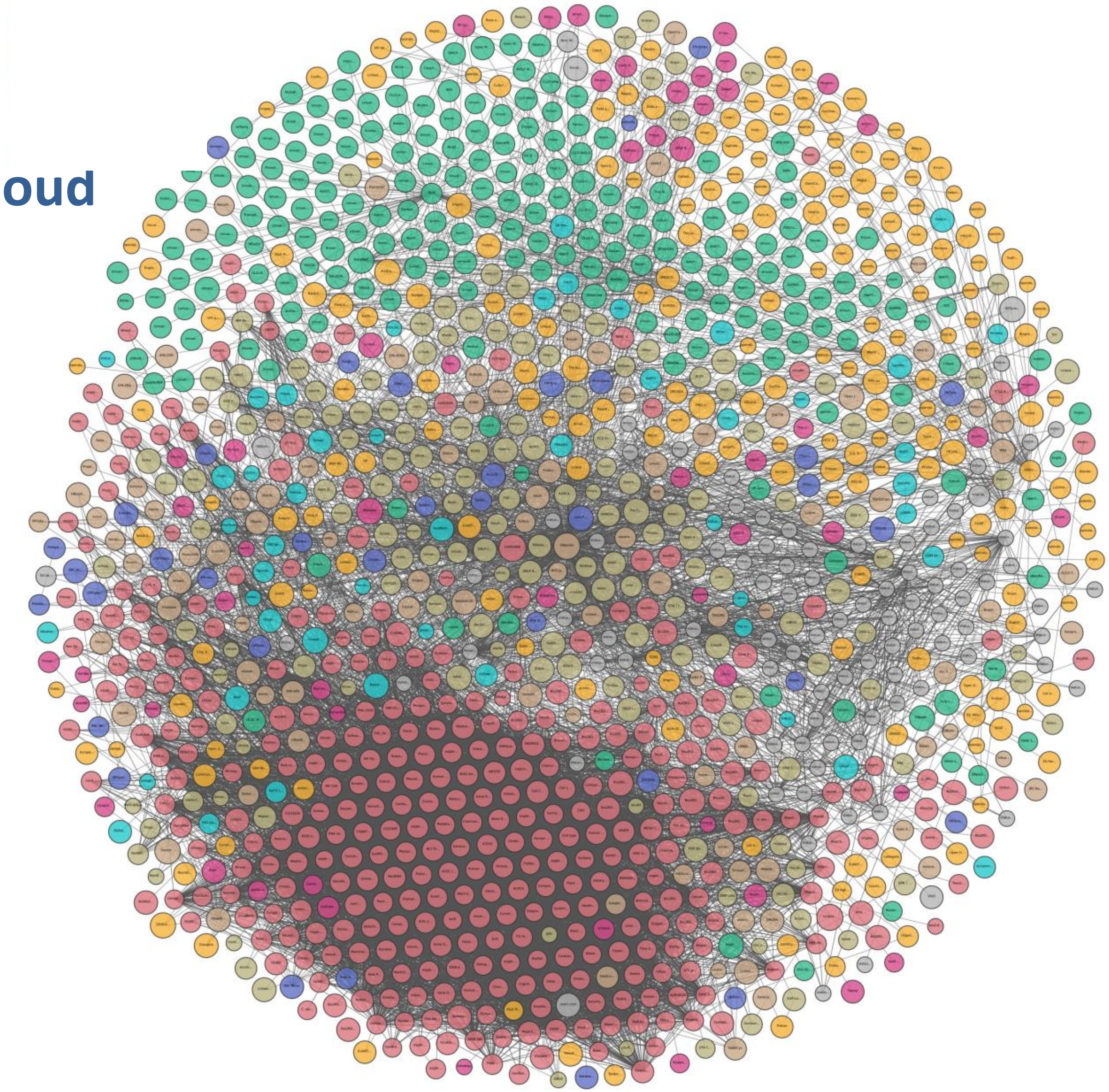
2000 | **2005** | **2010** | Year, A.D.

Open Data

- **Linked Open Data Cloud**

<u>Legend</u>

- Cross Domain
- Geography
- Government
- Life Sciences
- Linguistics
- Media
- Publications
- Social Networking
- User Generated



The Linked Open Data Cloud from lod-cloud.net

Data Analytics Applications

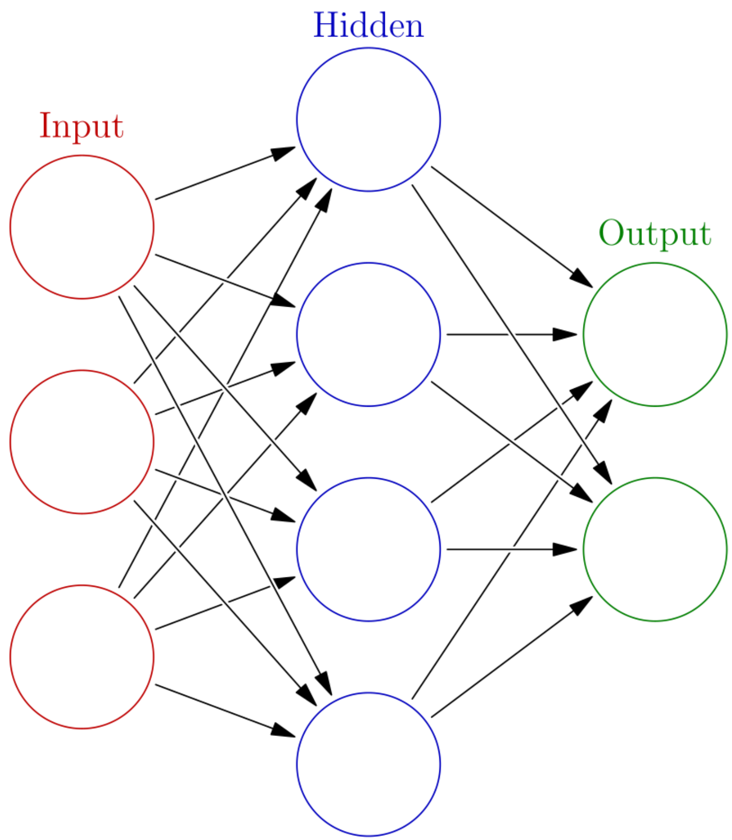
- **Semantic Web**
  - A common schema (RDF) for annotation and query of unstructured and unannotated data

- Google Knowledge Graph
  - **570 million** entities (nodes)
  - **500 billion** facts (connections)
  - **several petabytes** of files
- Facebook's Social Graph
  - **60 PB** of structured data
- Twitter's Interest Graph
  - **60 PB** of structured data

Data Analytics Applications

- **Artificial Intelligence**
  - Automated pattern recognition technology based on NN

- **Time to prepare**
- **Number of slides**
- **Duration of speech**

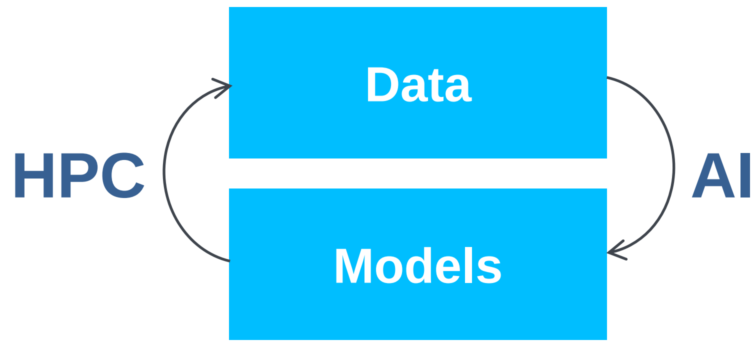


- **A perfect IARIA talk**
- **A very perfect IARIA talk**

Artifical Intelligence

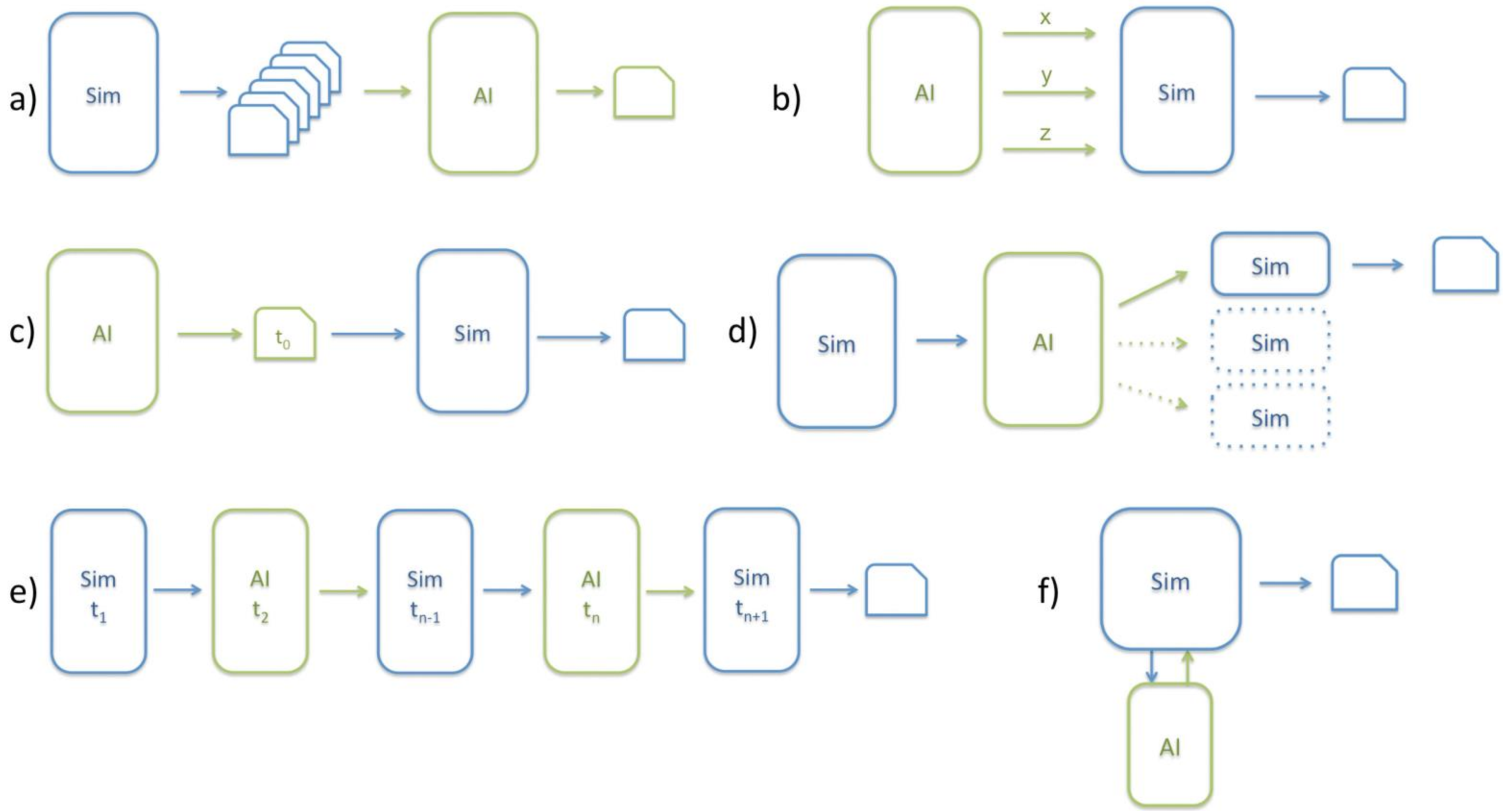
- **Role in Engineering**

  – Synthetic approach instead of precise mathematical model
  – Surrogate modelling – reproducing the relationship between the input and the output of data of the traditional model, mimicking its behavior
  – Fast, but less precise and reliable
  – A win-win strategy for AI and HPC



Application Areas

- **AI + HPC**

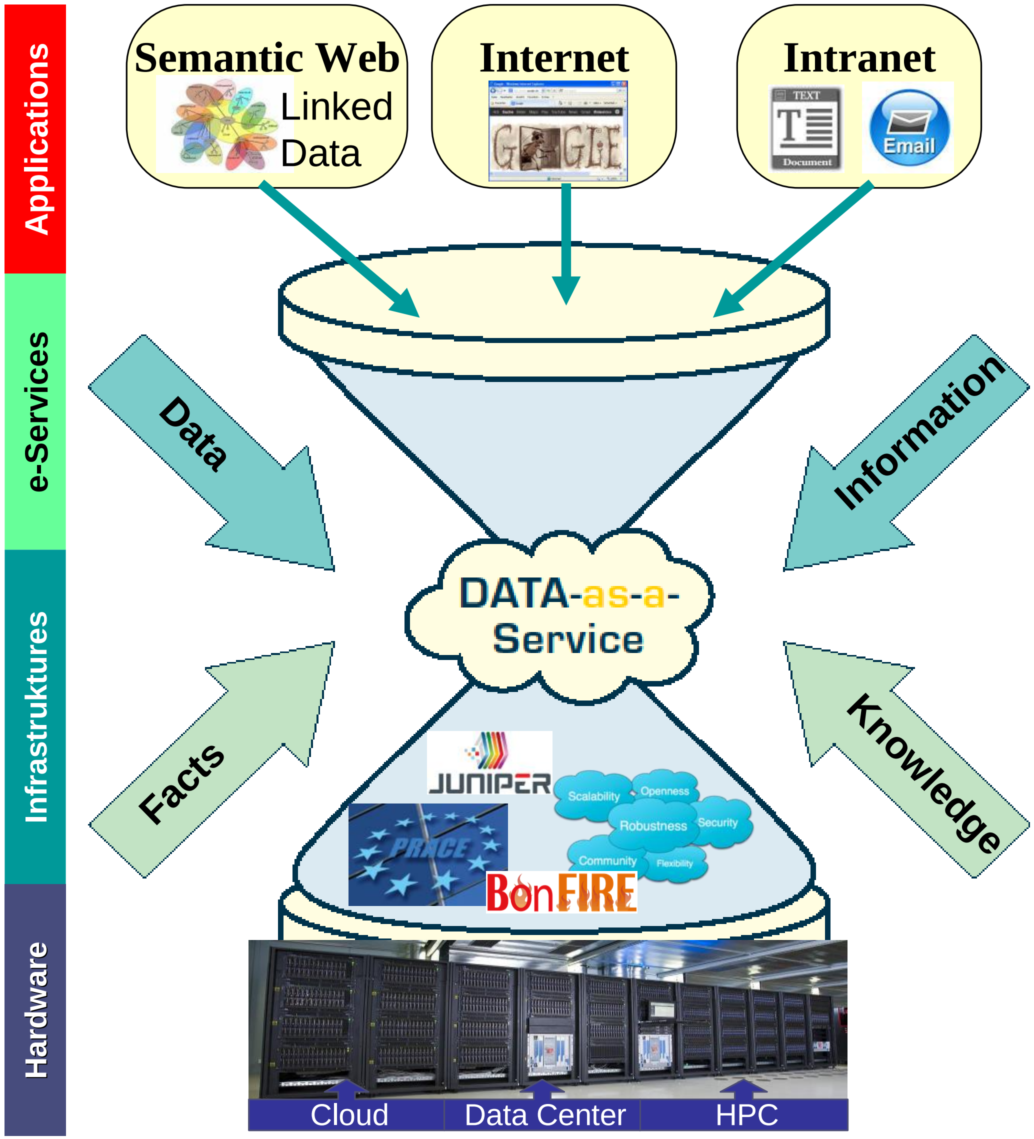


Various interaction patterns between AI and simulations: a) generation of data for AI training from simulations; b) finding simulation parameters by AI; c) generation of initial solutions by AI; d) choosing the right path by AI; e) replacing iterations in simulation by AI; f) replacing specific functions/equations by AI.

Data Science Applications

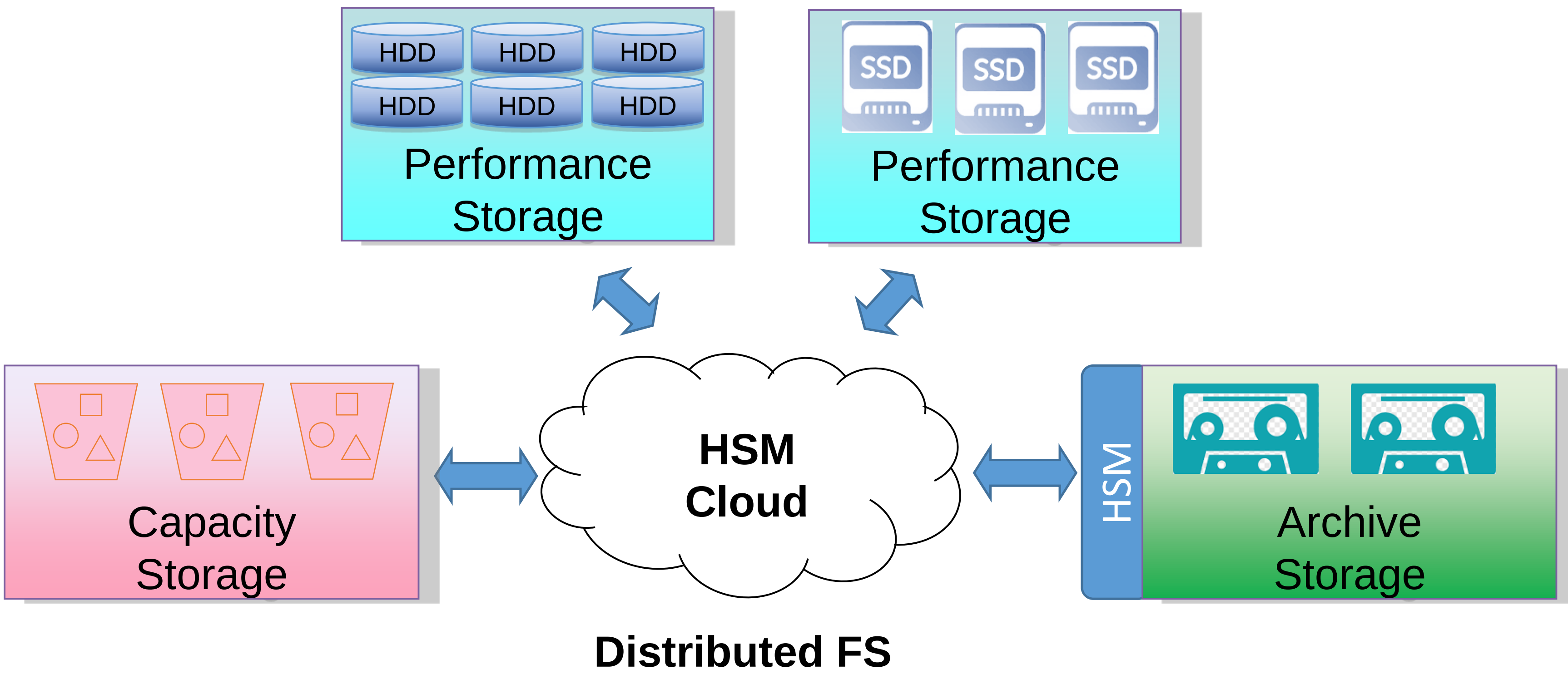
	Traditional Computational Sciences	Data-Intensive Sciences
Structure	static	dynamic
Locality	spatially and temporally local	no or little
Volume	fit into memory	do not fit into memory
Arithmetical Complexity	High Precision Arithmetic	variable precision or integer based

Challenges and Bottlenecks



Data Science Infrastructure

- **Hierarchical Storage Management**



Data Science Infrastructure

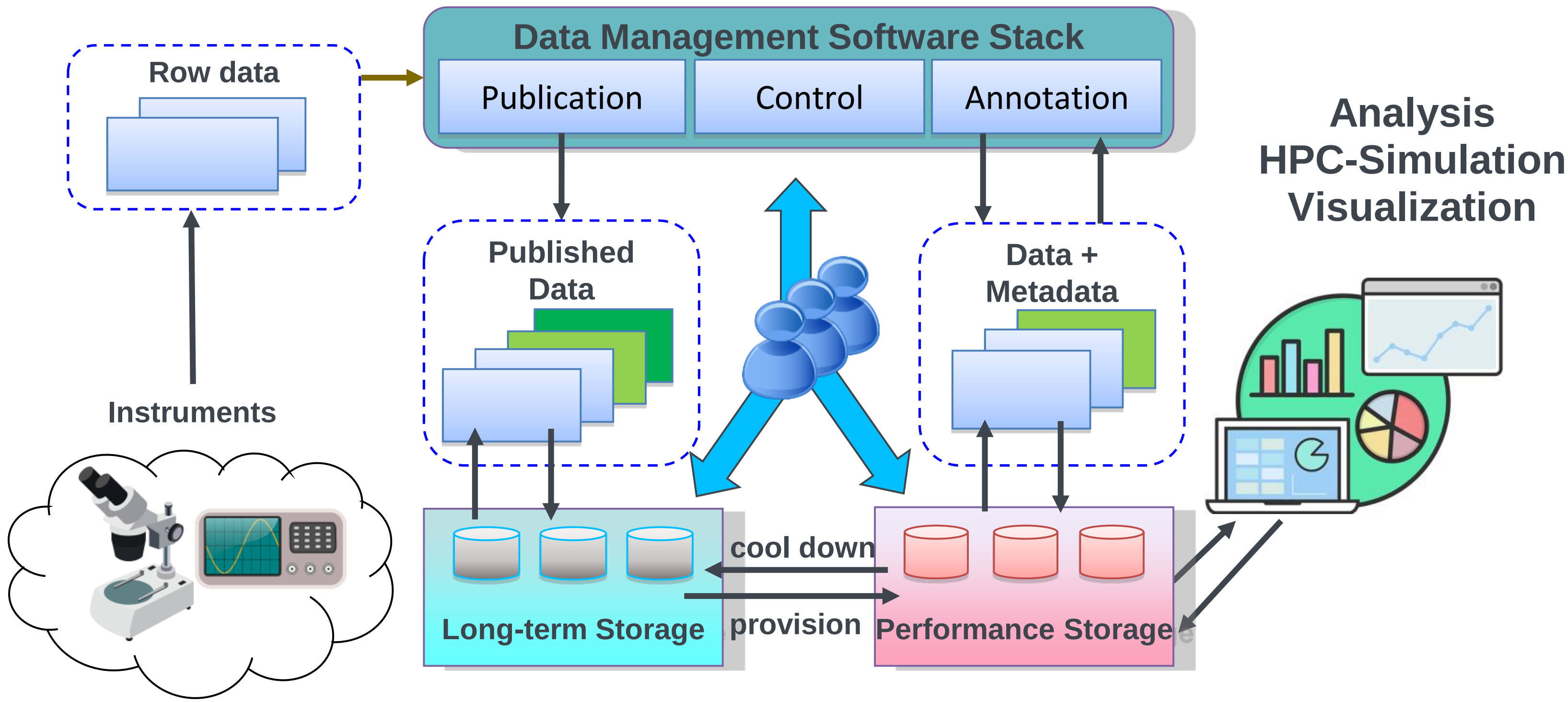
- ## Special Requirements

  - Redundancy over multiple locations
  - Data backup and recovery
  - Hybrid Cloud – on-demand infrastructure
  - Data Lifecycle Workflows support

Scientific Data Management

- ## Typical Workflow

Data Infrastructure	Data Management Framework	Application



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Conclusion

- **HPC and Data Science have to find a common language**
  - A lot of integration is required
  - Virtualization infrastructure (*-a-a-S) are beneficial
  - Lack of a common software technology

- **Qualification of researchers**
  - HPC as a curriculum discipline

Thank You!