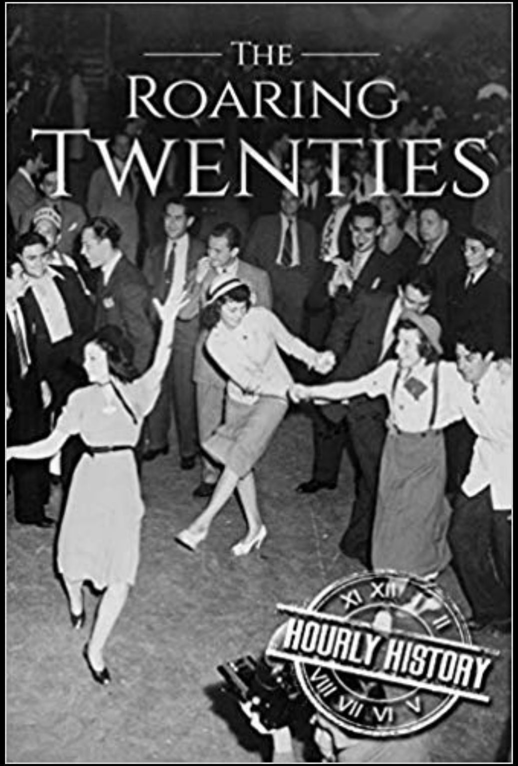
ICT to support the transformation of Science in the Roaring Twenties

Cees de Laat

Systems and Networking Laboratory
University of Amsterdam

ICT to support the transformation of Science in the Roaring Twenties



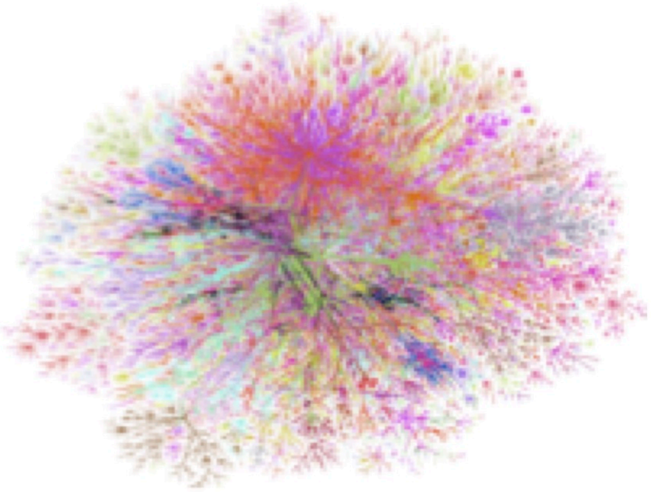
From Wikipedia: The Roaring Twenties refers to the decade of the 1920s in Western society and Western culture. It was a period of economic prosperity with a distinctive cultural edge in the United States and Western Europe, particularly in major cities such as Berlin, Chicago, London, Los Angeles, New York City, Paris, and Sydney. In France, the decade was known as the "années folles" ('crazy years'), emphasizing the era's social, artistic and cultural dynamism. Jazz blossomed, the flapper redefined the modern look for British and American women, and Art Deco peaked….

This period saw the large-scale development and use of automobiles, telephones, movies, radio, and electrical appliances being installed in the lives of thousands of Westerners. Aviation soon became a business. Nations saw rapid industrial and economic growth, accelerated consumer demand, and introduced significantly new changes in lifestyle and culture. The media focused on celebrities, especially sports heroes and movie stars, as cities rooted for their home teams and filled the new palatial cinemas and gigantic sports stadiums. In most major democratic states, women won the right to vote. The right to vote made a huge impact on society.

AIM

- Observe how the art of Science is transforming with AI & ML.
- Understand how the ICT world looks like in 2030.
- Understand what hinders Science, Industry, Society to progress.
- What is needed to obtain EU leadership
  - Why?
  - Where?
  - What?

In most applications, utilization of Big Data often needs to be combined with Scalable Computing.

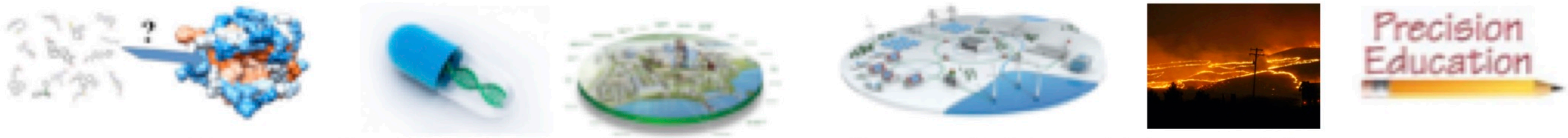


COMPUTING AT DIVERSE SCALES

"BIG" DATA

Enables dynamic data-driven applications

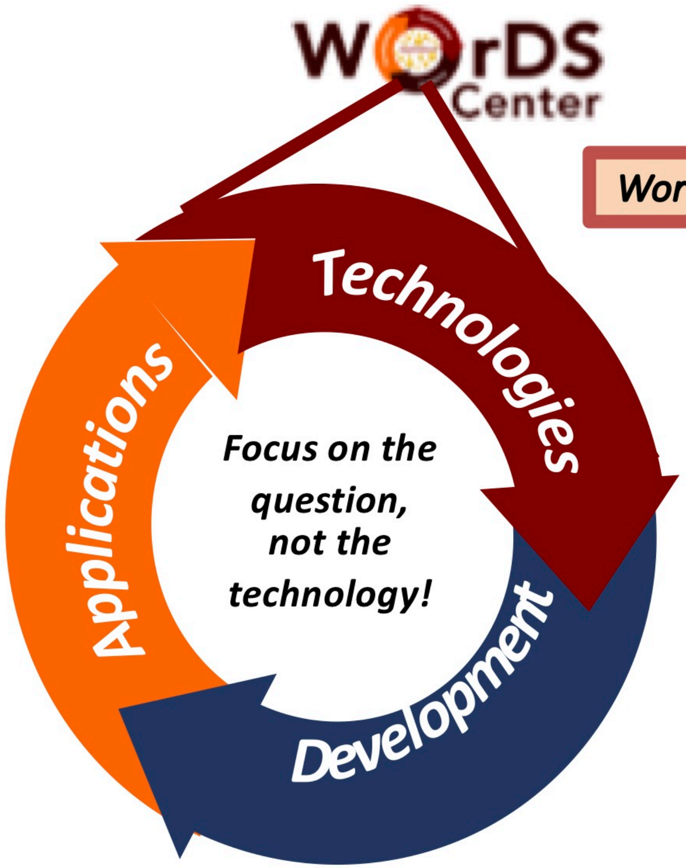
Computer-Aided Drug Discovery *Smart Cities* *Disaster Resilience and Response*



Smart Manufacturing *Personalized Precision Medicine* *Smart Grid and Energy Management*

İlkay ALTINTAŞ, Ph.D.
ialtintas@ucsd.edu

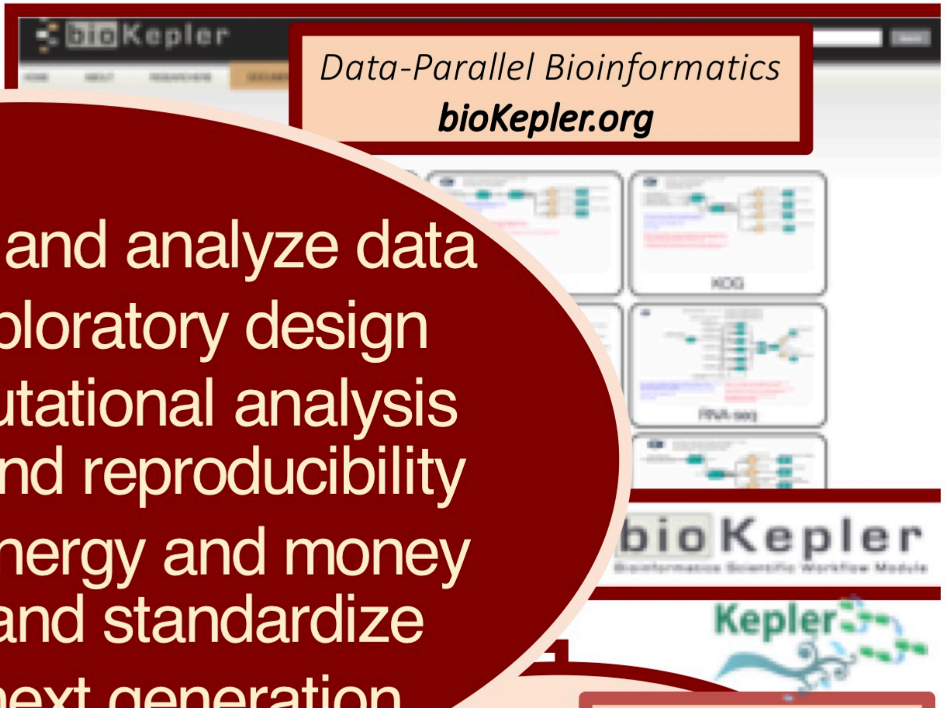
Workflows for Data Science Center of Excellence at SDSC



WorDS.sdsc.edu

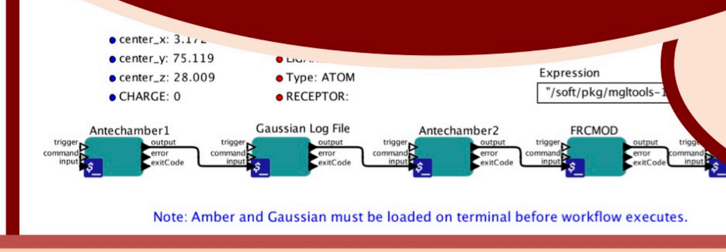
Real-Time Hazards Management
wifire.ucsd.edu

Data-Parallel Bioinformatics
bioKepler.org



- Find, access and analyze data
- Support exploratory design
- Scale computational analysis
- Fuel reuse and reproducibility
- Save time, energy and money
- Formalize and standardize
- Train the next generation

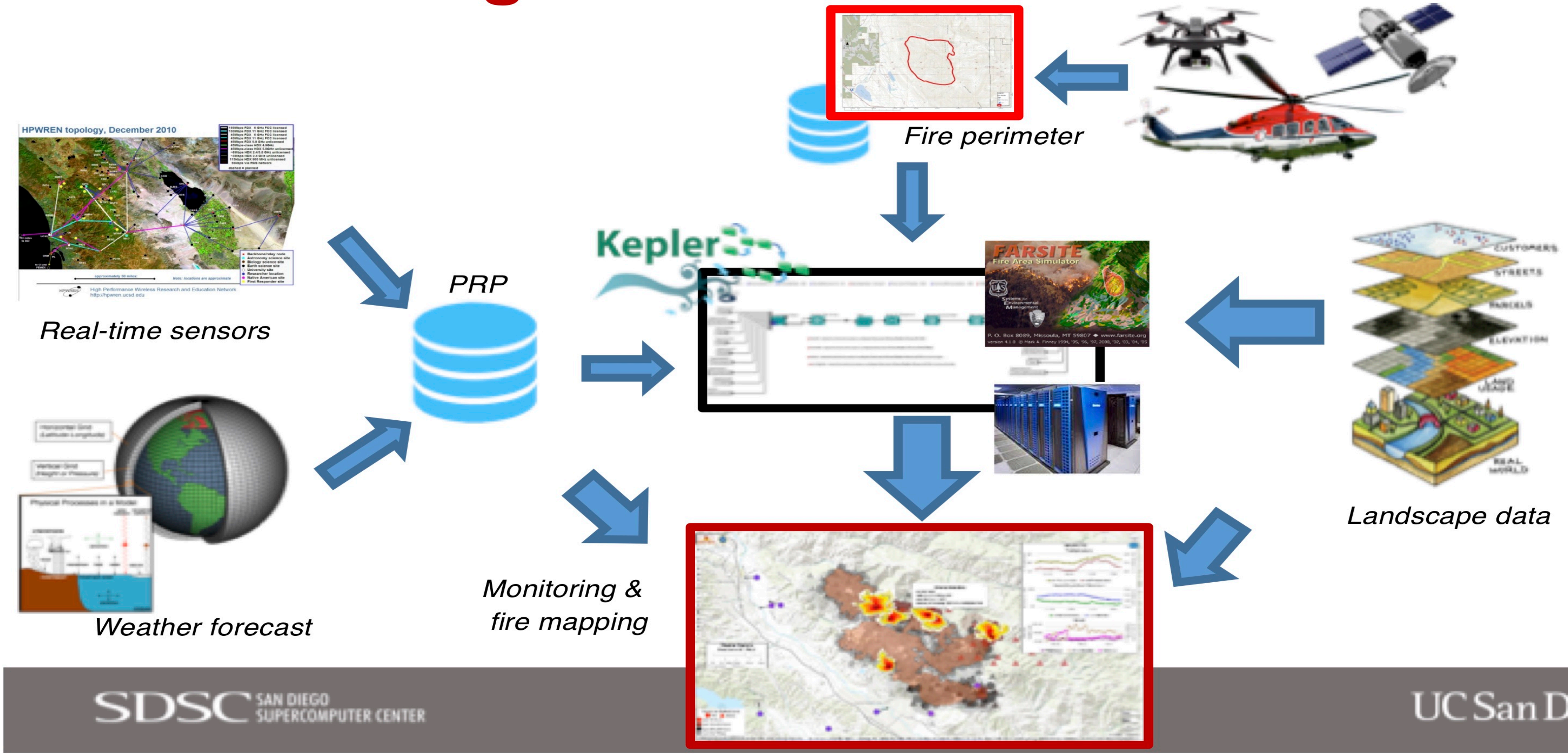
kepler-project.org



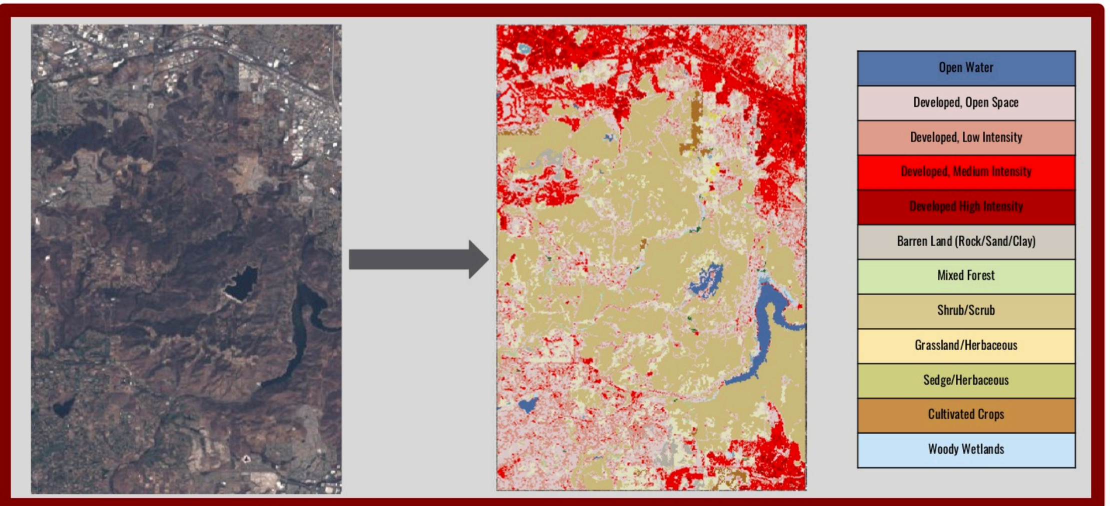
Goal: Methodology and tool development to build automated and operational workflow-driven solution architectures on big data and HPC platforms.

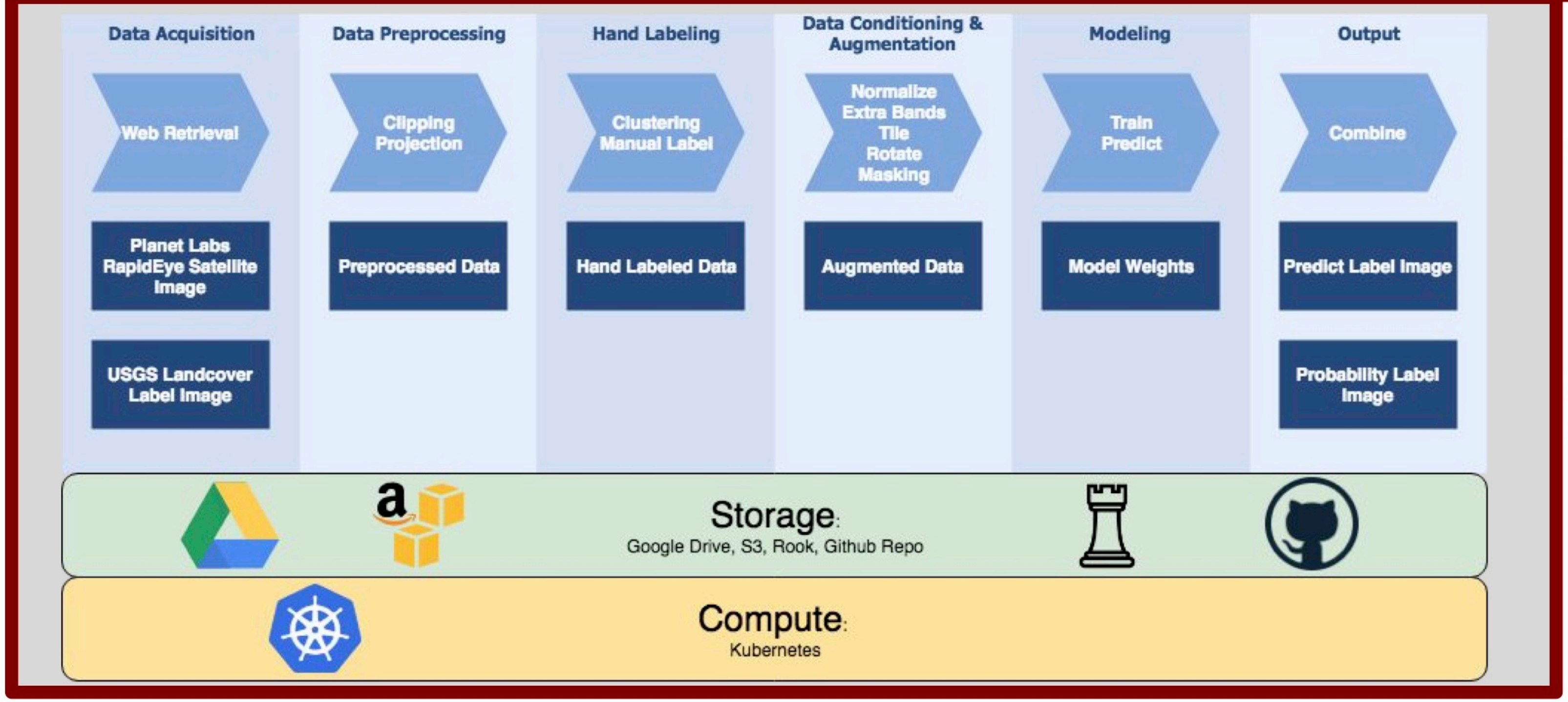
Scalable Automated Molecular Dynamics and Drug Discovery
nbcr.ucsd.edu

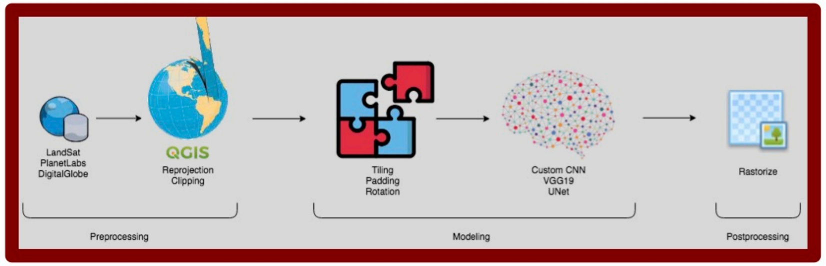
Fire Modeling Workflows in WIFIRE

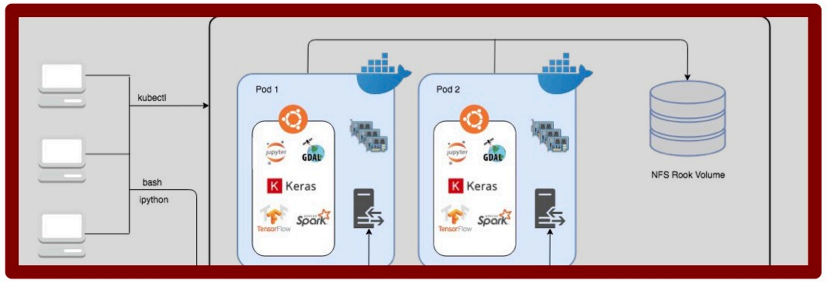


One Piece of the Puzzle: Vegetation Classification using Satellite Imagery









SDSC SAN DIEGO SUPERCOMPUTER CENTER

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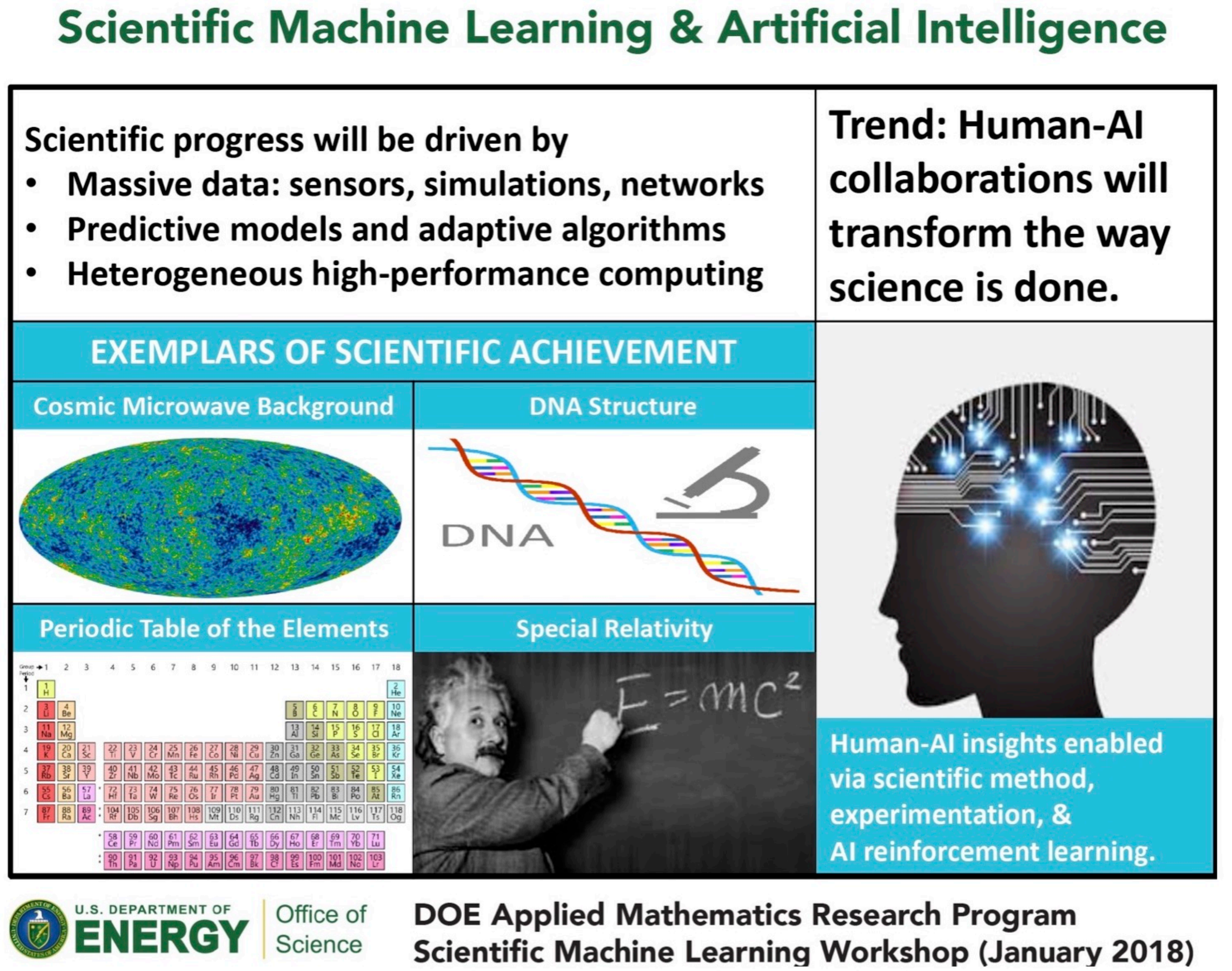
ialtintas@ucsd.edu

UC San Diego

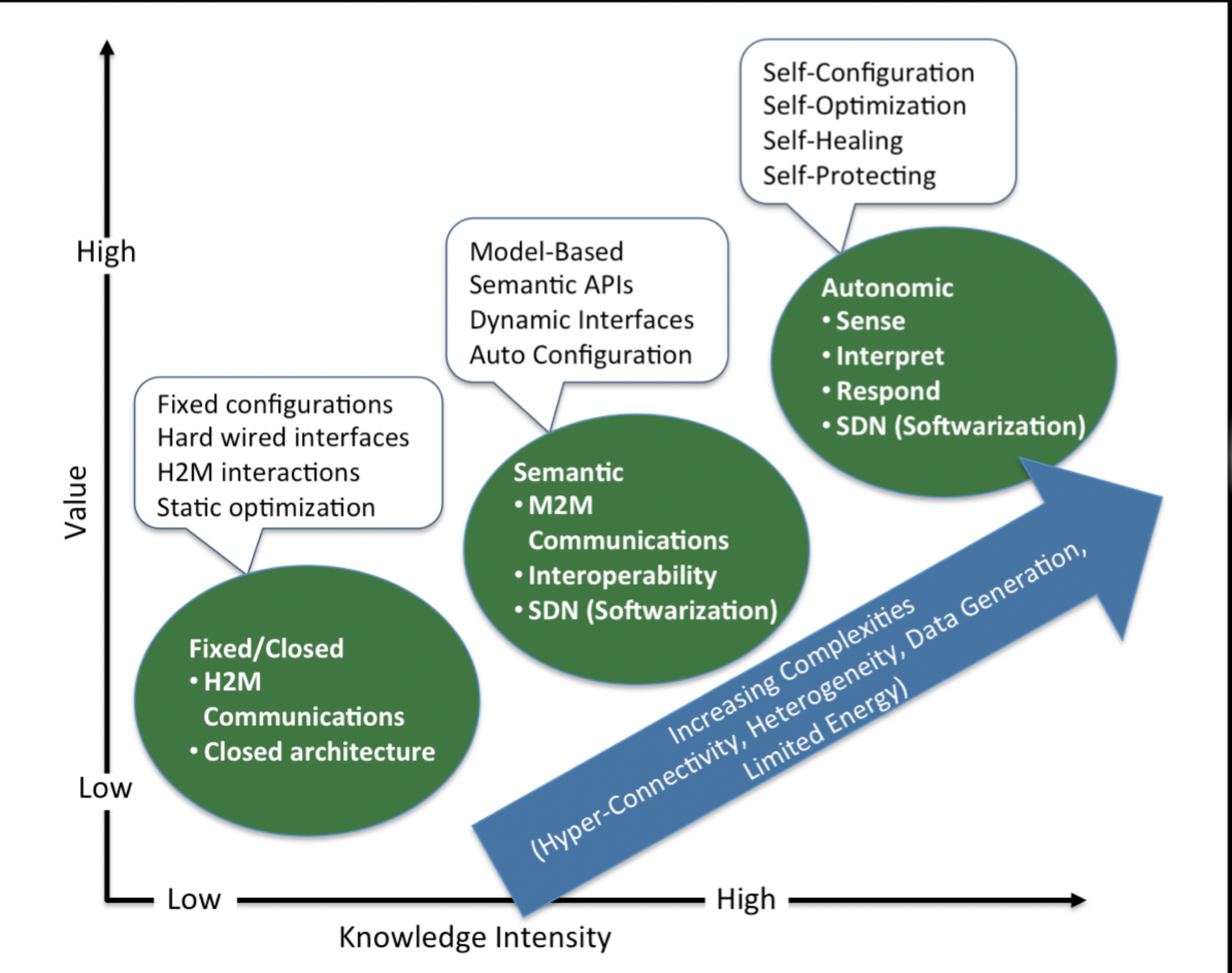


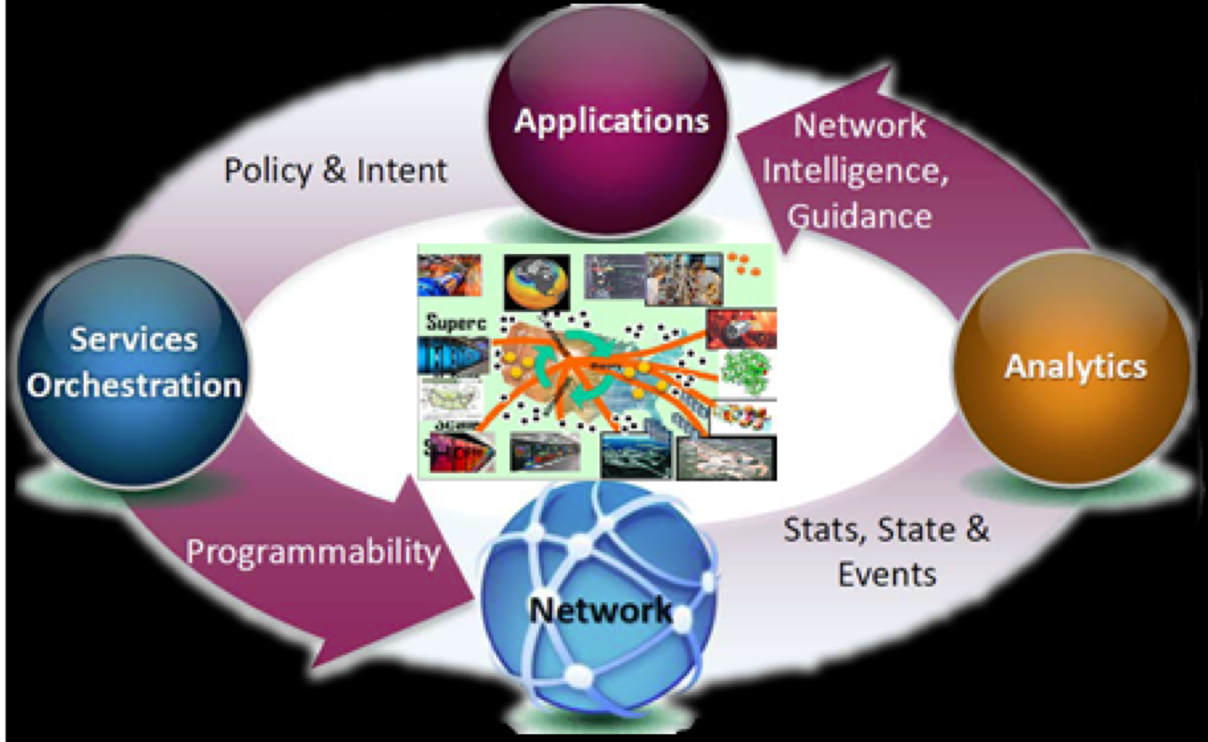
Workshop report:
https://www.osti.gov/biblio/1478744

DoE workshop on smart networks

Bring AI in control plane to harness complexity

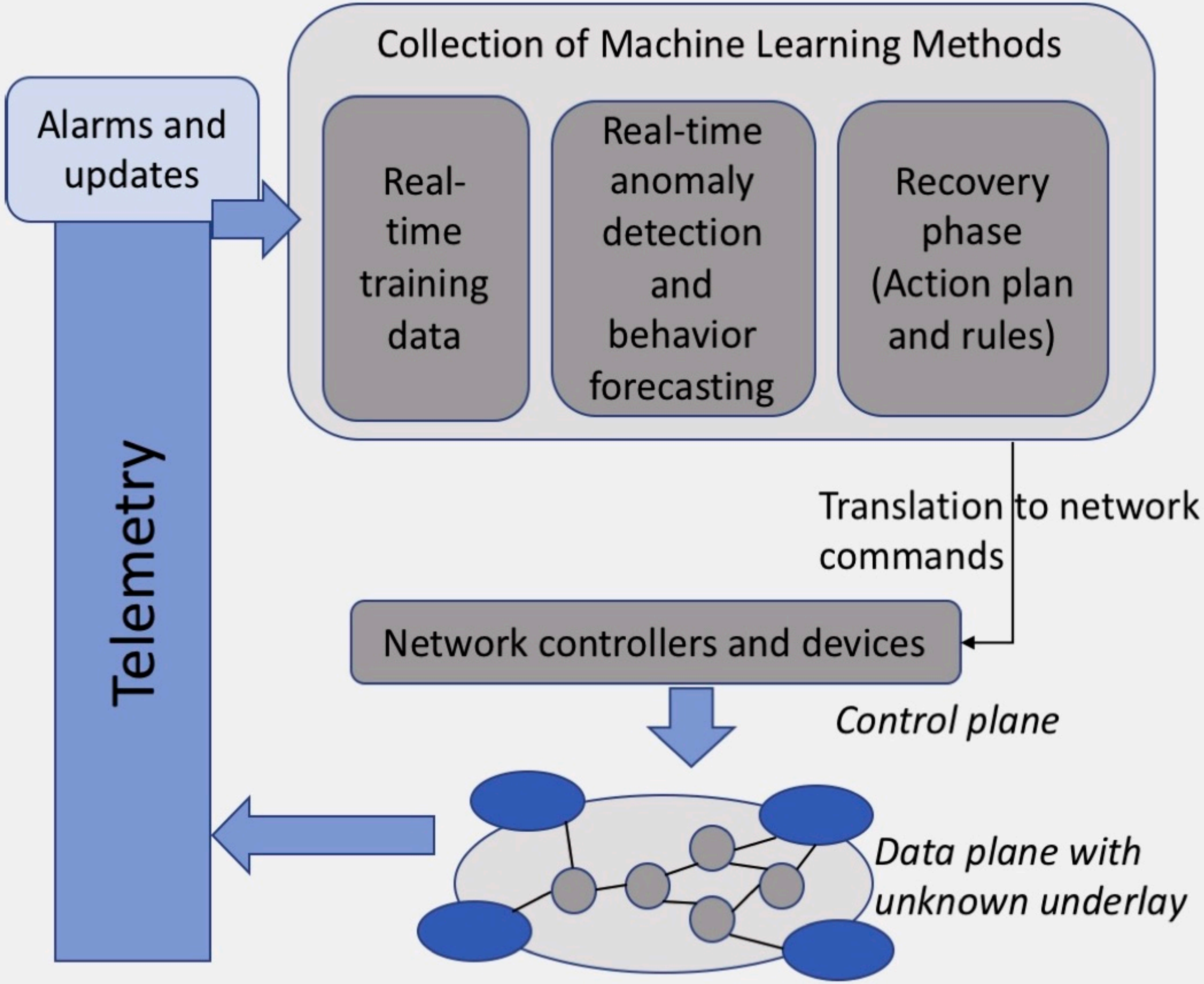
https://www.orau.gov/smarthp2016/





Example 1: Optimizing Network Traffic with Machine Learning

Exascale and increasingly complex science applications are exponentially raising demands from underlying DOE networks, such as traffic management, operation scale, and reliability constraints. Networks are the backbone to complex science workflows, ensuring data are delivered securely and on time for important computations to happen. To optimize these distributed workflows, networks are required to understand end-to-end performance needs in advance and be faster, efficient, and more proactive, anticipating bottlenecks before they happen. However, to manage multiple network paths intelligently, various tasks, such as pre-computation and prediction, must be done in near real time. ML provides a collection of algorithms that can add autonomy and assist in decision making to sup-

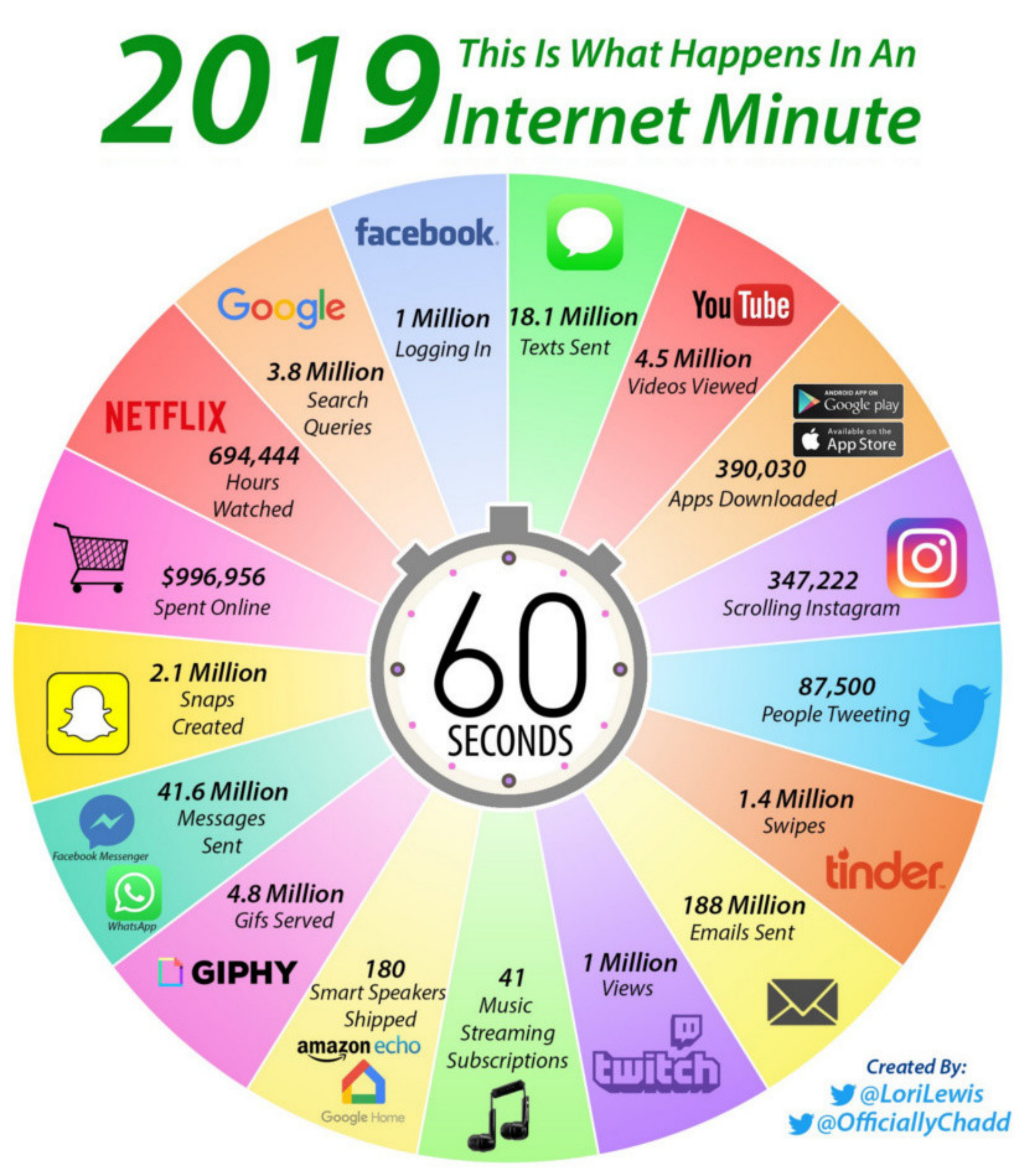


Initial debates about resource management and delivery options focused on expert personnel as a critical component of successful cyberinfrastructure delivery. Several examples such as Campus Champions (CC) or XSEDE's ECSS were described as critical to scientific advance but insufficient in numbers to meet demand. Regionally tasked staff might help to alleviate this shortfall. Benefits could include greater use of cloud or national resources if there was a local expert to help researchers with initial utilization. Along these lines, it was mentioned that the NSF CC* programs changed campus culture, spurring local networking expertise. A similar program to promote workforce development to incentivize local computational and data scientists could, for instance, result in the integration of otherwise isolated clusters on campuses with national resources. These key personnel, ranging from ECSS experts and developers to CCs, are often in careers that need professionalization.

Change in computing

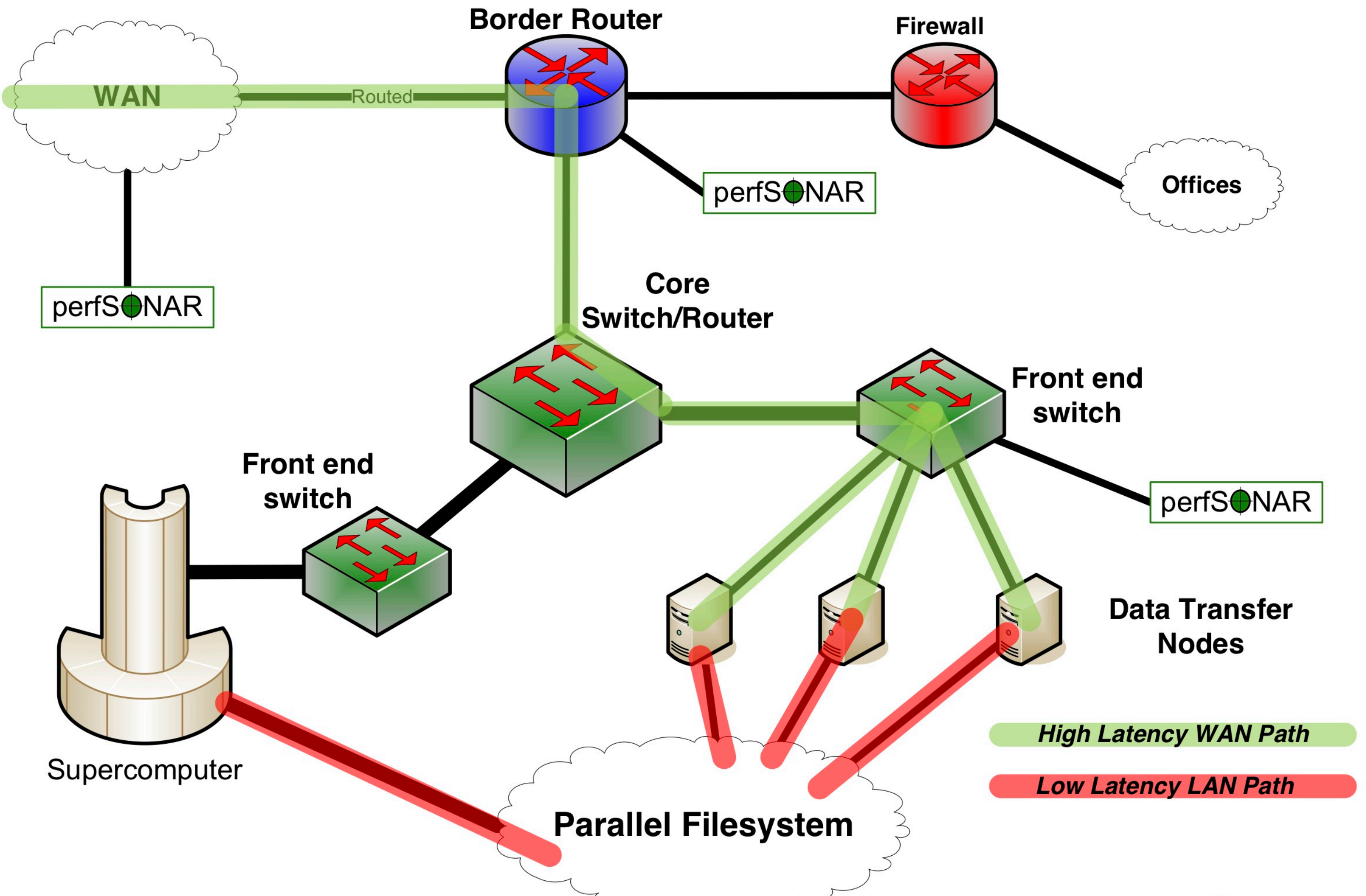
- Early days a few big Supercomputers
  - Mostly science domain
- Via grid to commercial cloud
  - AWS, Azure, Google Cloud, IBM, Salesforce
  - The big five: Apple, Alphabet, Microsoft, Facebook and Amazon
  - Computing has transformed into an utility
- Data => Information is the key

Now, how do we get and use data?



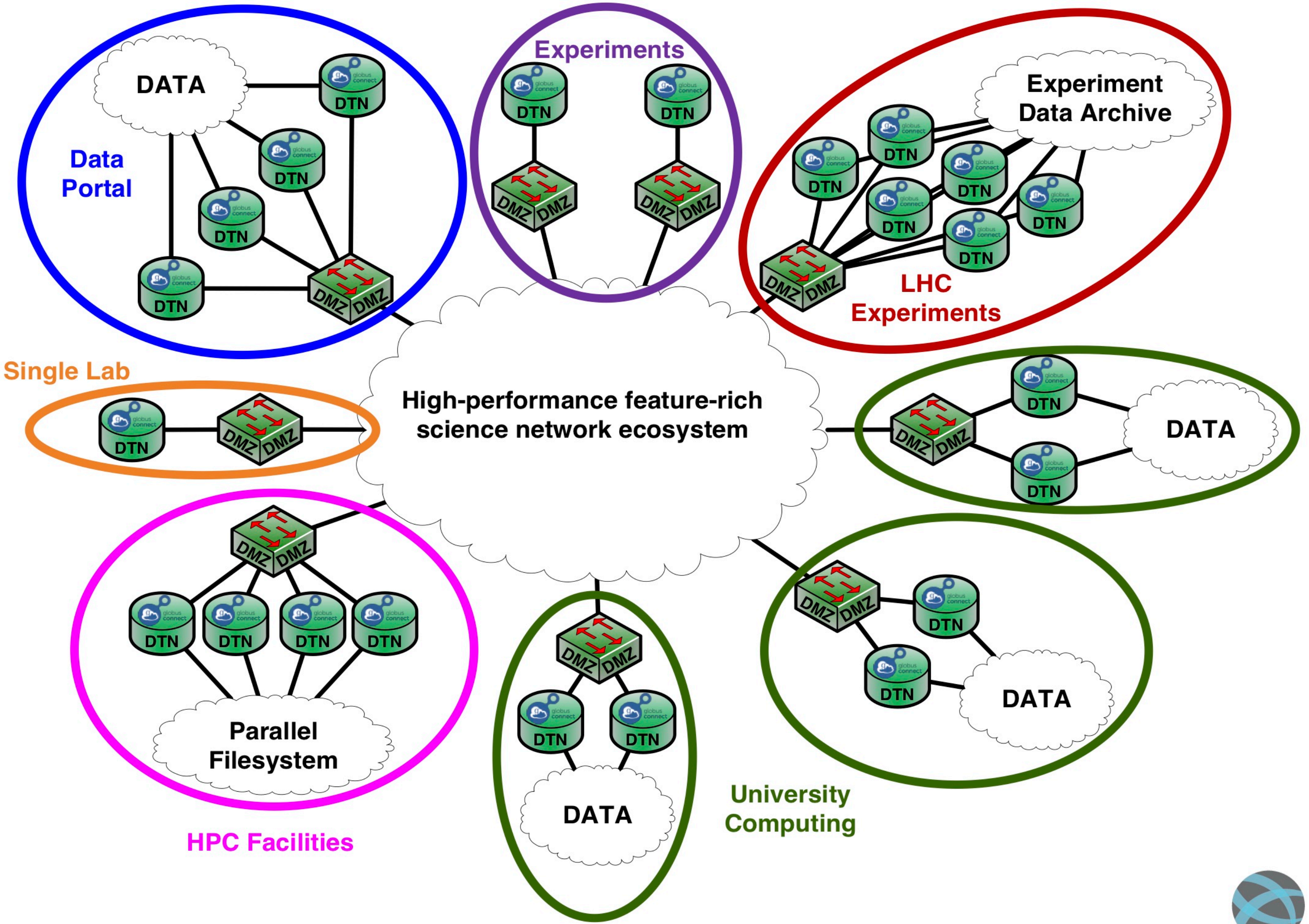
- Move towards streaming
  - Netflix
  - youtube
- Same in science world
  - SKA / LOFAR
  - Light Source
  - Environmental (Marine, Meteorology, …)
- Data is not always huge
  - Sometimes it is very complex
  - Some example:
    - biodiversity

Science DMZ – HPC Center DTN Cluster



Courtesy Eli Dart, ESnet

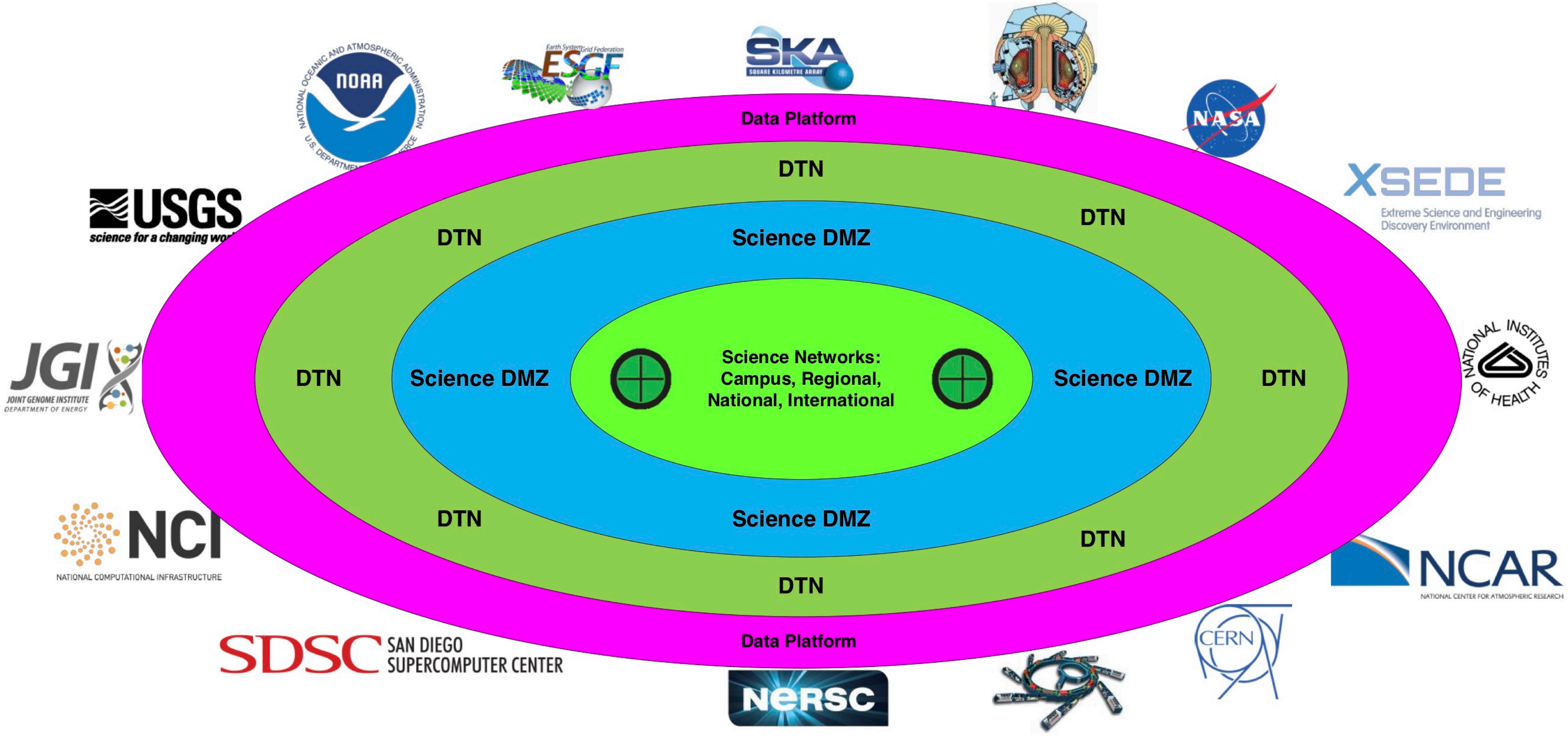
Science DMZs for Science Applications



ESnet

Courtesy Eli Dart, ESnet

Data Ecosystem – Concentric View



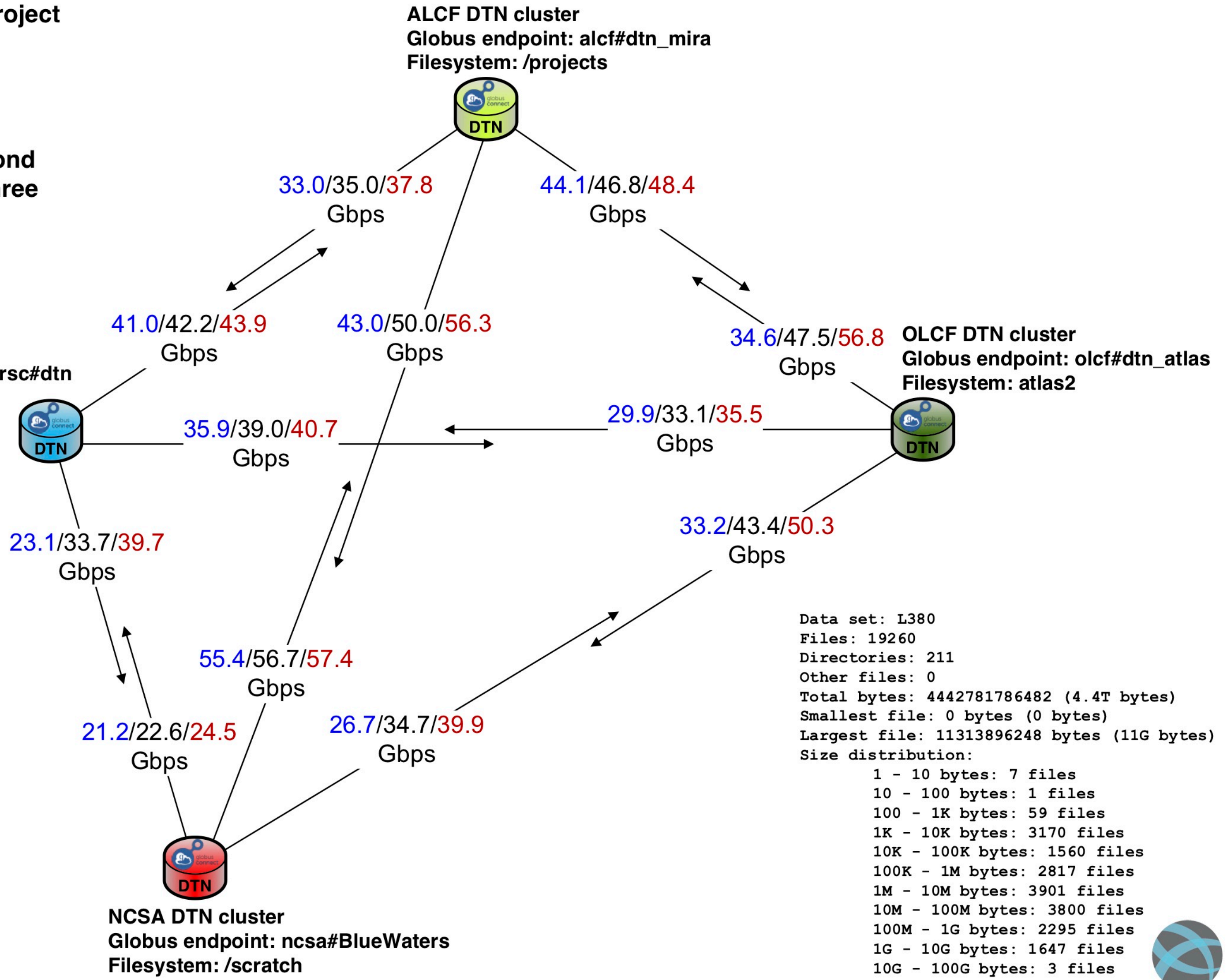
Courtesy Eli Dart, ESnet

DTN Cluster Performance – HPC Facilities (2017)

Petascale DTN Project

November 2017
L380 Data Set

Gigabits per second (min/avg/max), three transfers

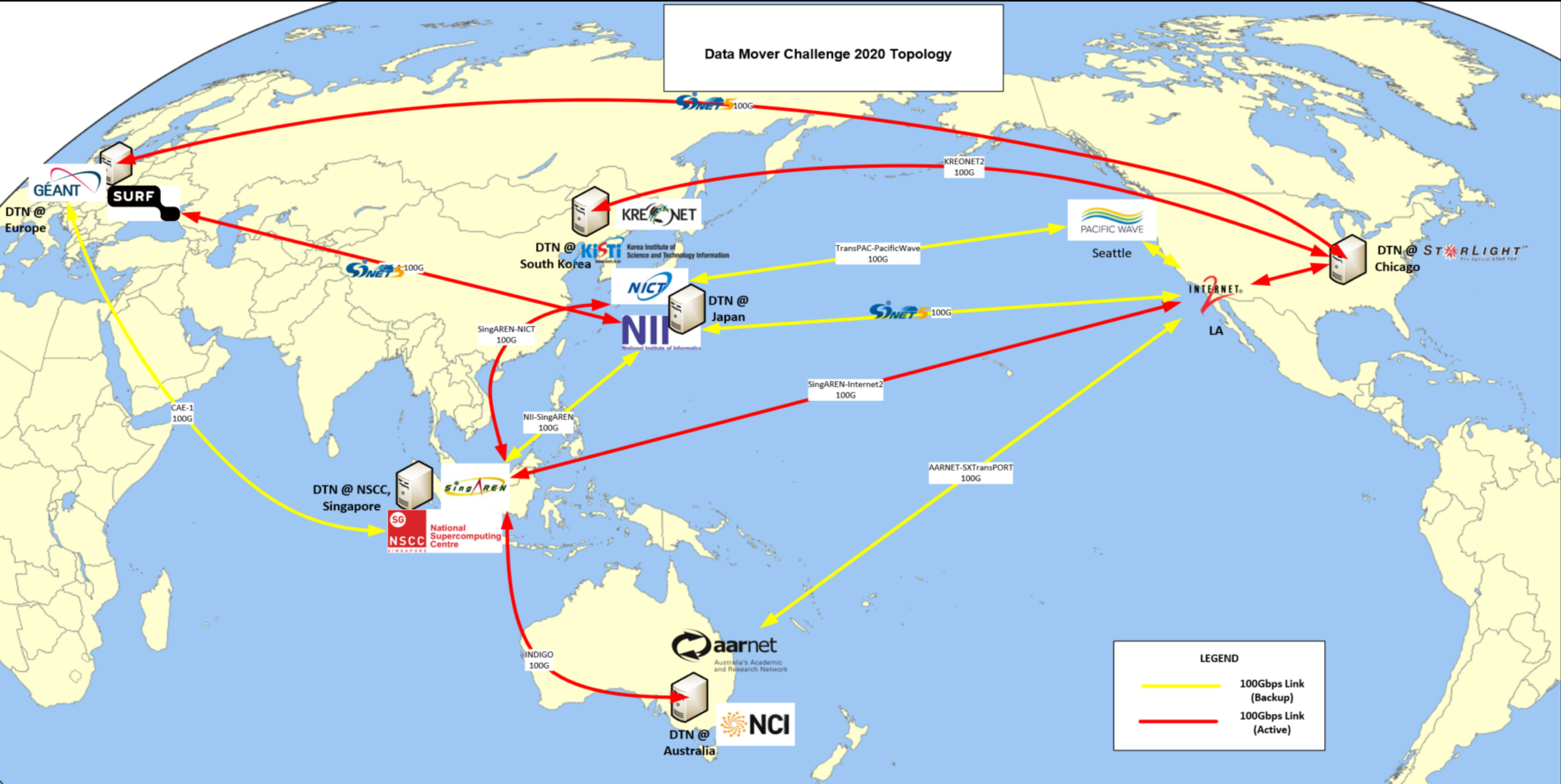



```
Data set: L380
Files: 19260
Directories: 211
Other files: 0
Total bytes: 4442781786482 (4.4T bytes)
Smallest file: 0 bytes (0 bytes)
Largest file: 11313896248 bytes (11G bytes)
Size distribution:
        1 - 10 bytes: 7 files
        10 - 100 bytes: 1 files
        100 - 1K bytes: 59 files
        1K - 10K bytes: 3170 files
        10K - 100K bytes: 1560 files
        100K - 1M bytes: 2817 files
        1M - 10M bytes: 3901 files
        10M - 100M bytes: 3800 files
        100M - 1G bytes: 2295 files
        1G - 10G bytes: 1647 files
        10G - 100G bytes: 3 files
```

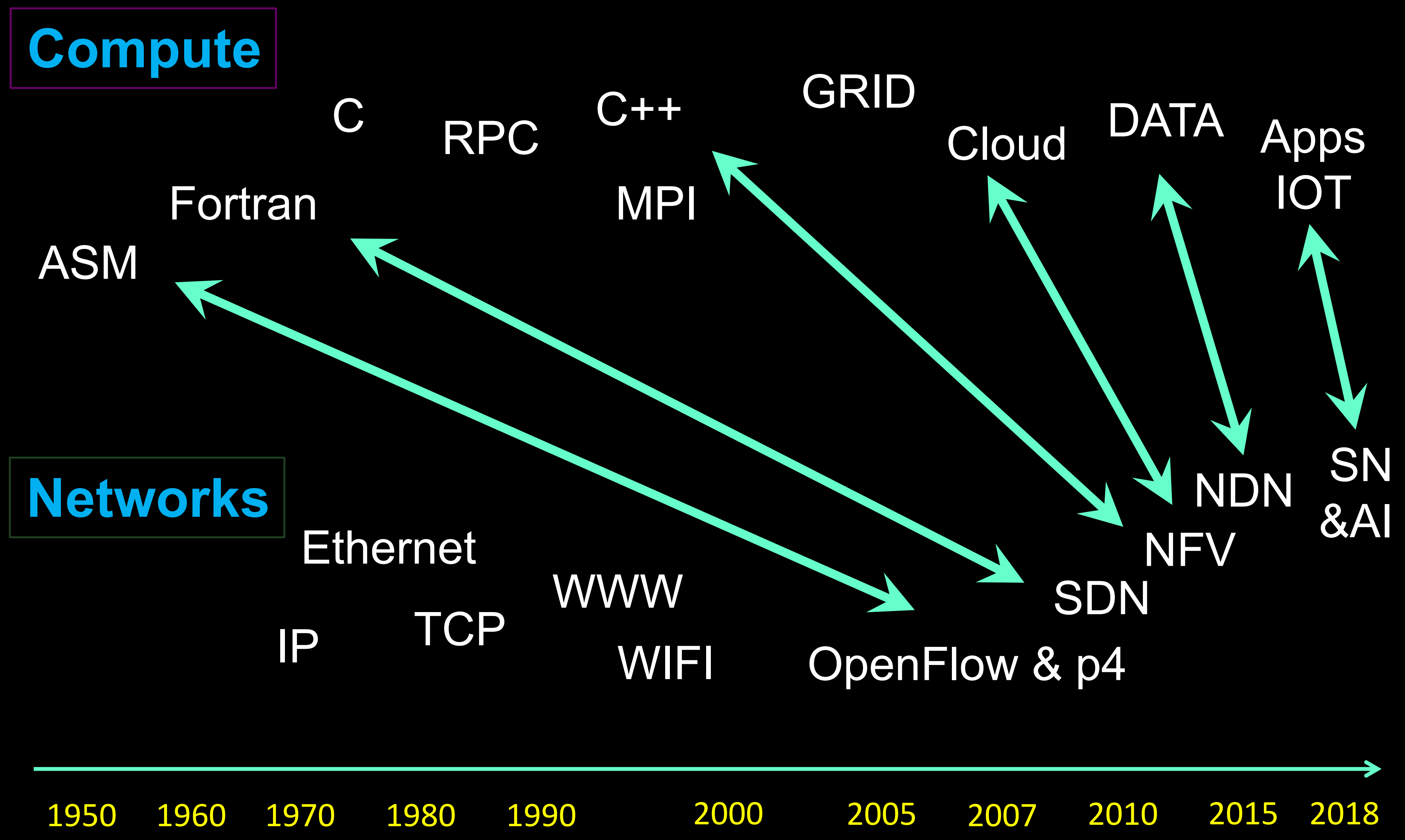
ESnet

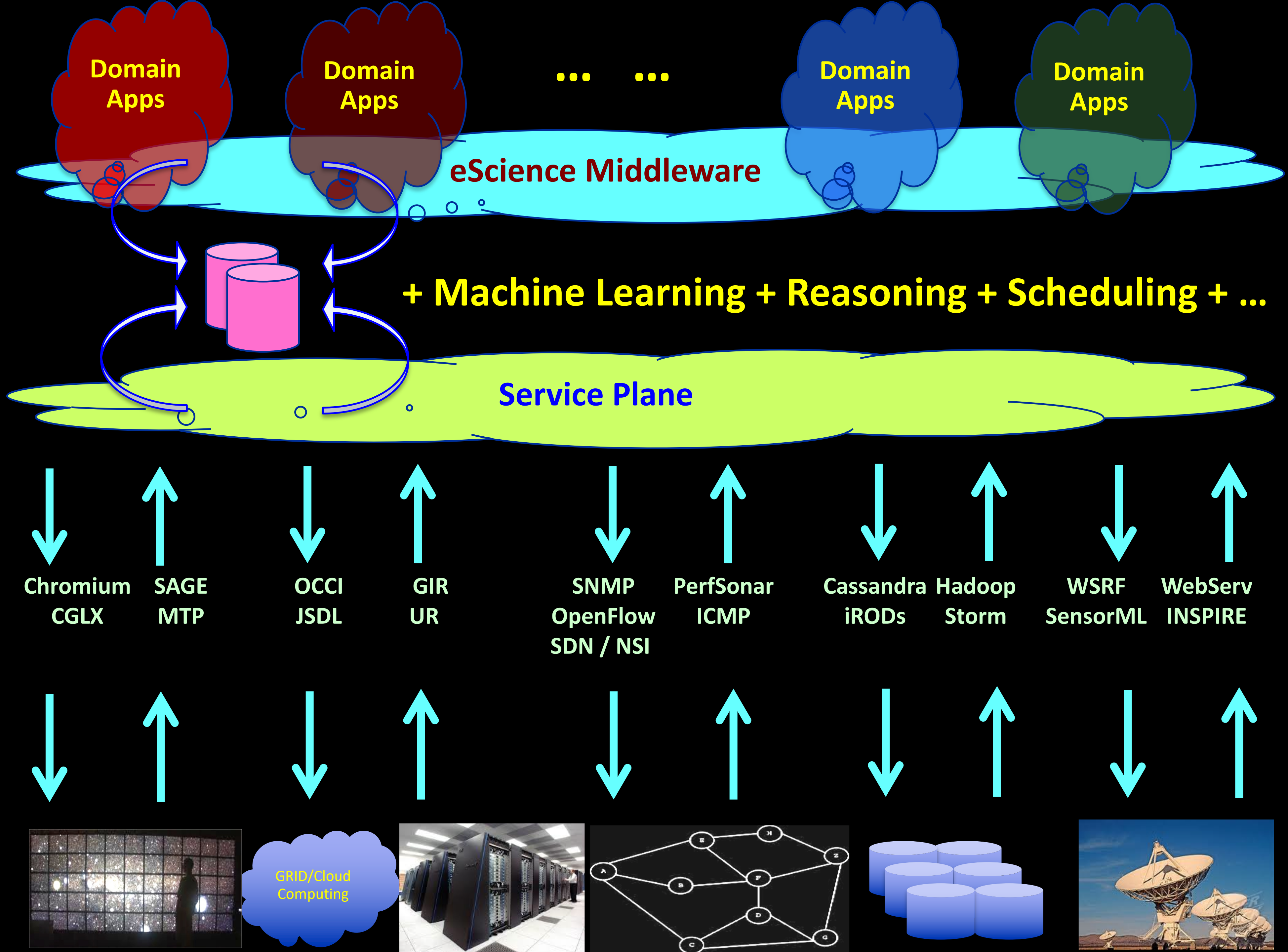
Courtesy Eli Dart, ESnet

https://www.sc-asia.org/data-mover-challenge/

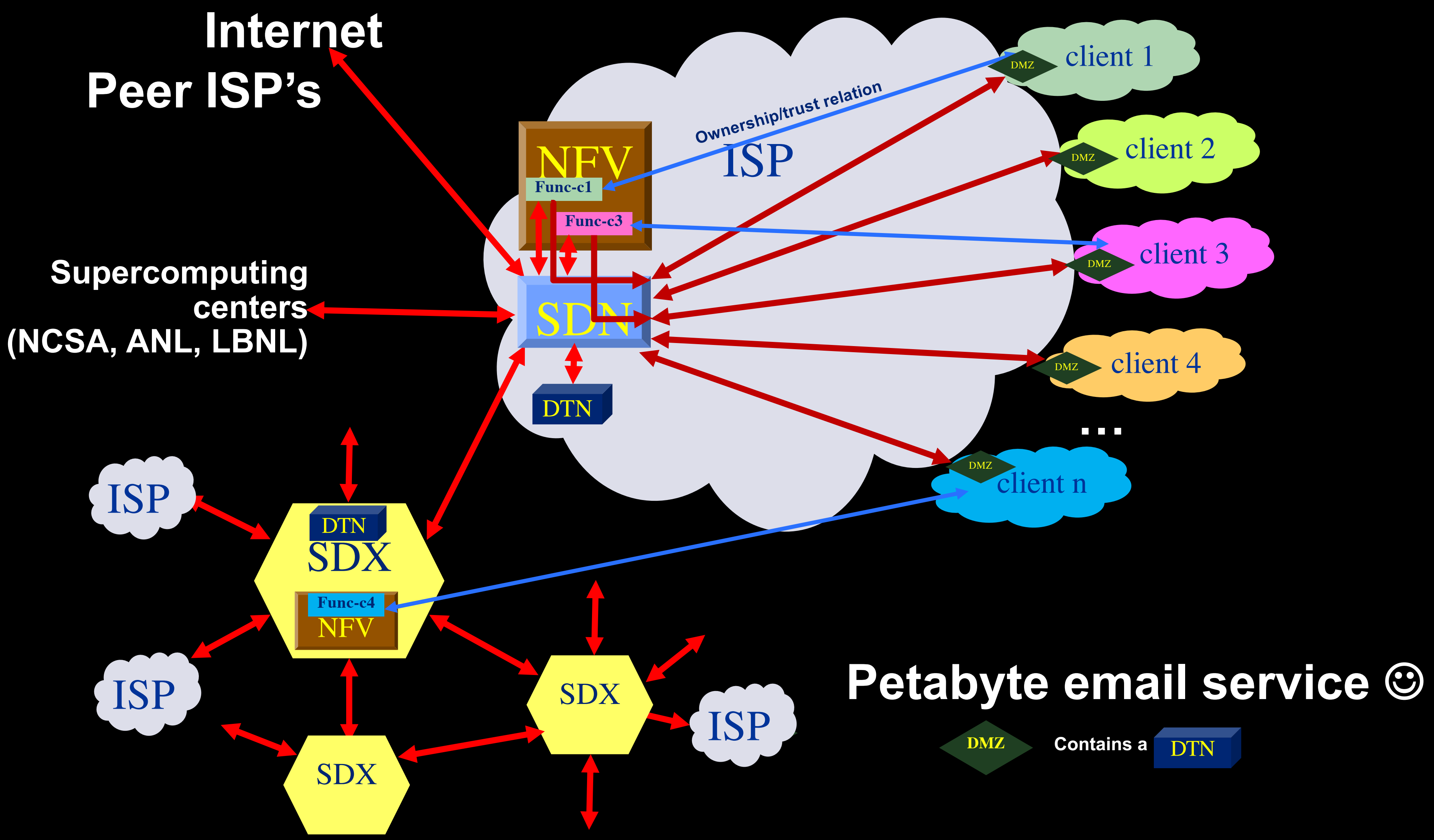


TimeLine

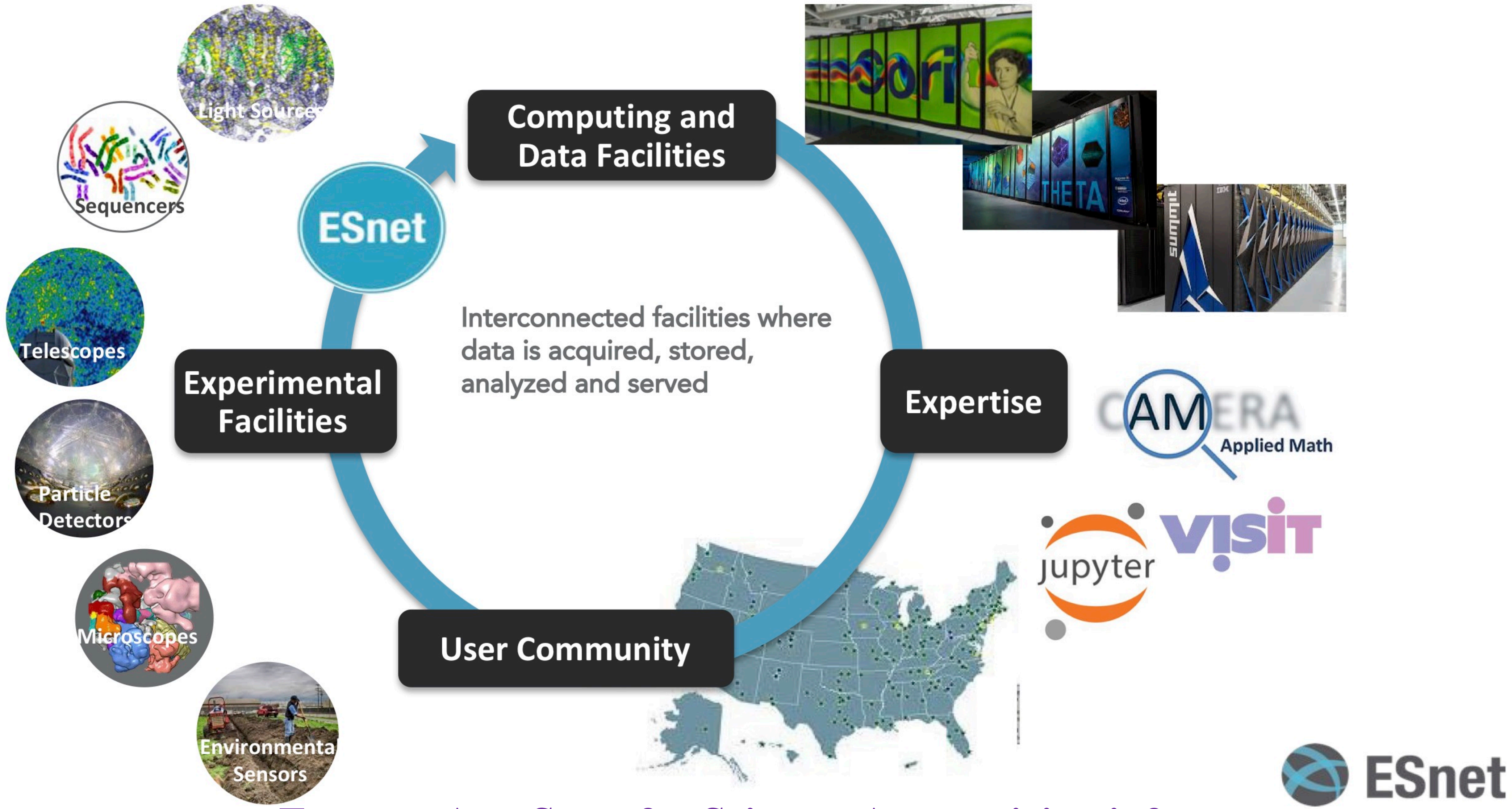

Compute
C
RPC
C++
GRID
Cloud
DATA
Apps
IOT
Fortran
MPI
ASM
Networks
Ethernet
WWW
IP
TCP
WIFI
OpenFlow & p4
SDN
NFV
NDN
SN
&AI
1950
1960
1970
1980
1990
2000
2005
2007
2010
2015
2018


Domain Apps
Domain Apps
… …
Domain Apps
Domain Apps
eScience Middleware
+ Machine Learning + Reasoning + Scheduling + …
Service Plane
Chromium
CGLX
SAGE
MTP
OCCI
JSDL
GIR
UR
SNMP
OpenFlow
SDN / NSI
PerfSonar
ICMP
Cassandra
iRODs
Hadoop
Storm
WSRF
SensorML
WebServ
INSPIRE
GRID/Cloud Computing

Networks of ScienceDMZ's & SDX's



Superfacility Model for Productive, Reproducible Science



Extreme App Store for Science; Amazonizing infrastructure

Data Sharing: Main problem statement

- Organizations that normally compete have to bring data together to achieve a common goal!
- The shared data may be used for that goal but not for any other!
- Data may have to be processed in untrusted data centers.
  - How to enforce that using modern Cyber Infrastructure?
  - How to organize such alliances?
  - How to translate from strategic via tactical to operational level?
  - What are the different fundamental data infrastructure models to consider?

Big Data Sharing use cases placed in airline context

Global Scale

National Scale

City / regional Scale

Campus / Enterprise Scale

Aircraft Component Health Monitoring (Big) Data
NWO **CIMPLO project**
4.5 FTE

Cargo Logistics Data
(C1) DaL4LoD
(C2) Secure scalable policy-enforced distributed data Processing
(using blockchain)

NLIP iShare project

iSHARE
powered by NLIP

Cybersecurity Big Data
NWO COMMIT/
SARNET project
3.5 FTE

Harvard Business Review

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ECONOMY

Managing Our Hub Economy

by Marco Iansiti and Karim R. Lakhani

FROM THE SEPTEMBER–OCTOBER 2017 ISSUE

WHAT TO READ NEXT

The IT Transformation Health Care Needs

SUMMARY | SAVE | SHARE | 3 COMMENT | TEXT SIZE | PRINT | $8.95 BUY COPIES

THOMAS M. SCHEER/EYEEM/GETTY IMAGES

I. The Problem

The global economy is coalescing around a few digital superpowers. We see unmistakable evidence that a winner-take-all world is emerging in which a small number of "hub firms"—including Alibaba, Alphabet/Google, Amazon, Apple, Baidu, Facebook, Microsoft, and Tencent—occupy central positions. While creating real value for users, these companies are also capturing a disproportionate and expanding share of the value, and that's shaping our collective economic future. The very same technologies that promised to democratize business are now threatening to make it more monopolistic.

Data value creation monopolies

→

Create an equal playing field

→

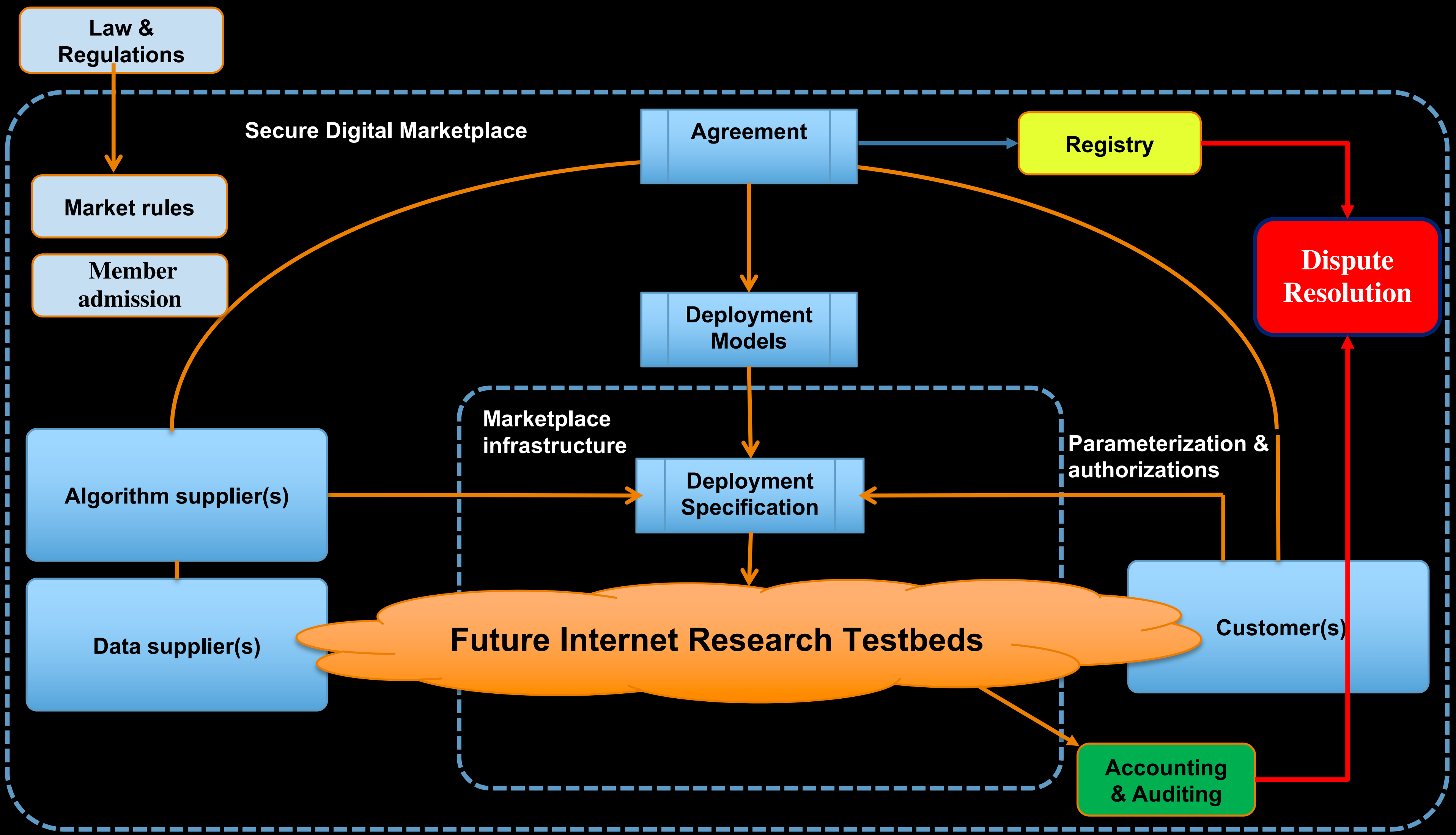
Sound Market principles

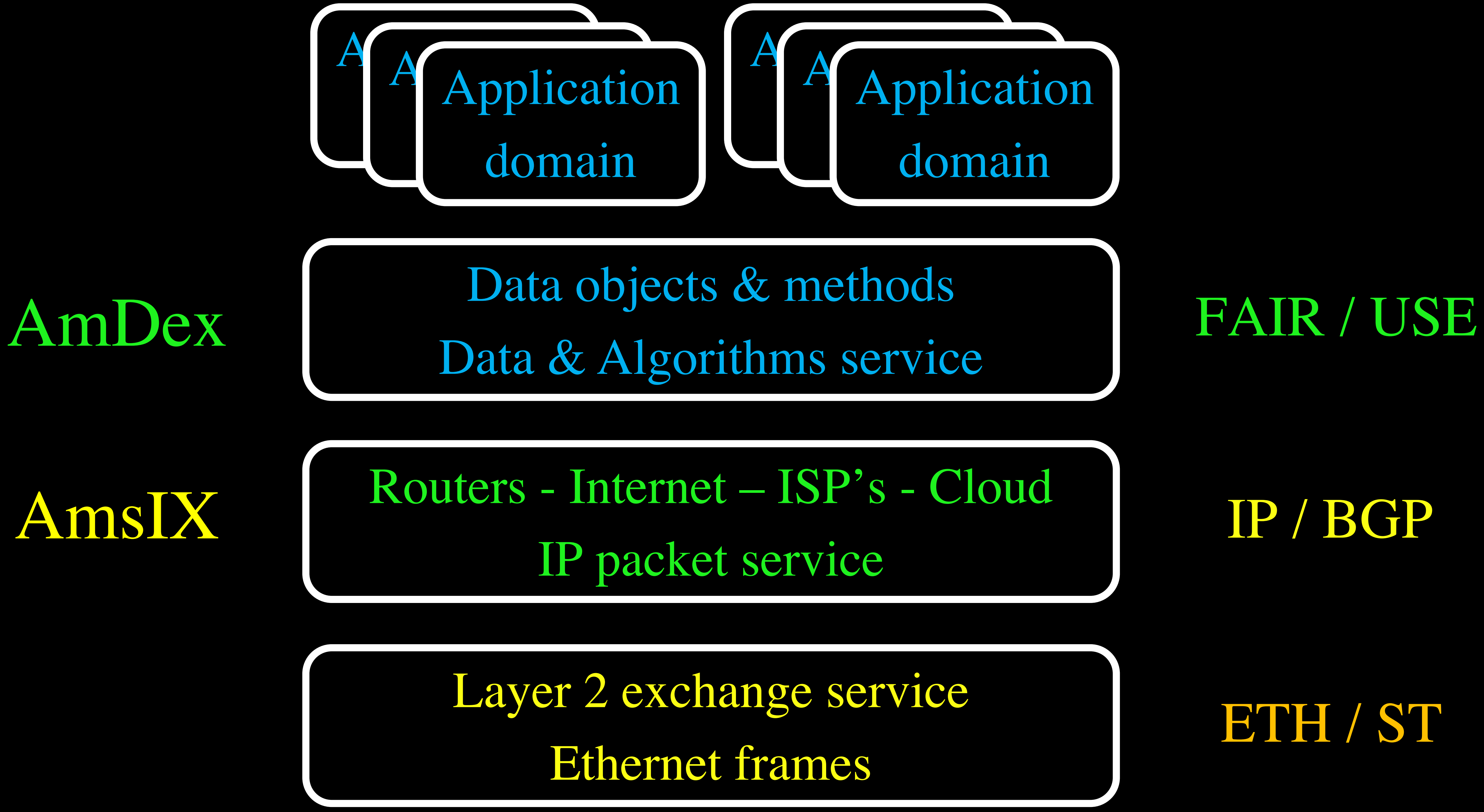
https://hbr.org/2017/09/managing-our-hub-economy

Approach

- Strategic:
  - Translate legislation into machine readable policy
  - Define data use policy
  - Trust evaluation models & metrics
- Tactical:
  - Map app given rules & policy & data and resources
  - Bring computing and data to (un)trusted third party
  - Resilience
- Operational:
  - TPM & Encryption schemes to protect & sign
  - Policy evaluation & docker implementations
  - Use VM and SDI/SDN technology to enforce
  - Block chain to record what happened (after the fact!)

Secure Digital Market Place Research

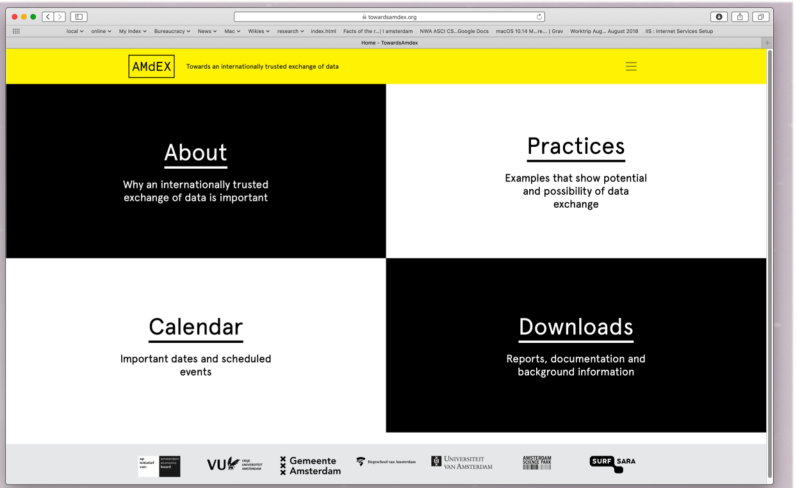


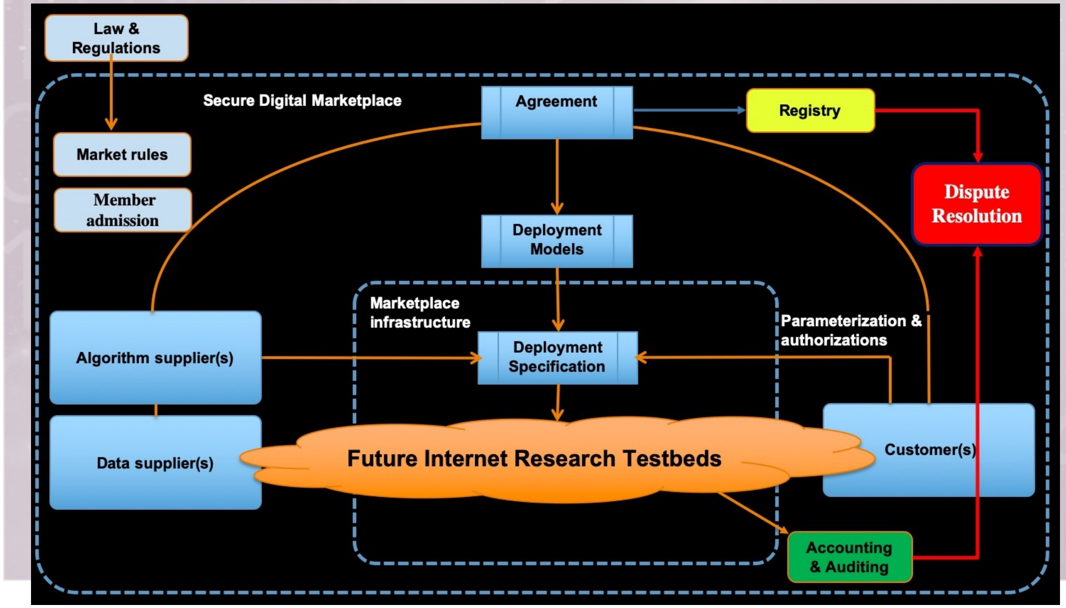


Application domain
Application domain
AmDex
Data objects & methods
Data & Algorithms service
FAIR / USE
AmsIX
Routers - Internet – ISP’s - Cloud
IP packet service
IP / BGP
Layer 2 exchange service
Ethernet frames
ETH / ST

AMdEX.eu

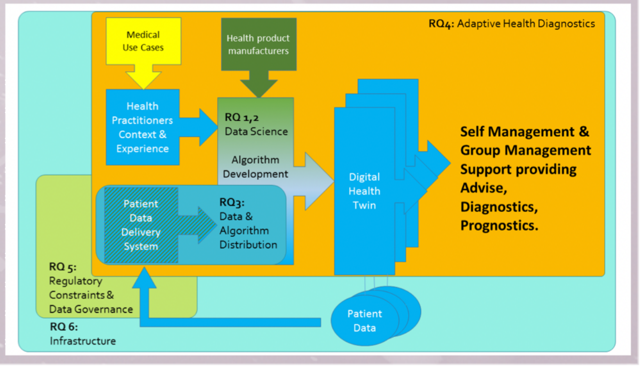
- Competing organisations, share data for common benefit
- Trust, Risk, data ownership & control
  - Industry: AF-KLM, Health, etc
  - Science: European Open Science Cloud
  - Society: Amsterdam Economic Board





Aircraft Maintenance AF-KLM

Health: Enabling Personal Interventions



The Big Data Challenge

Doing Science

Wis
dom

Knowledge
to act

Information

Data
a.o. from ESFRI's

ICT to enable Science

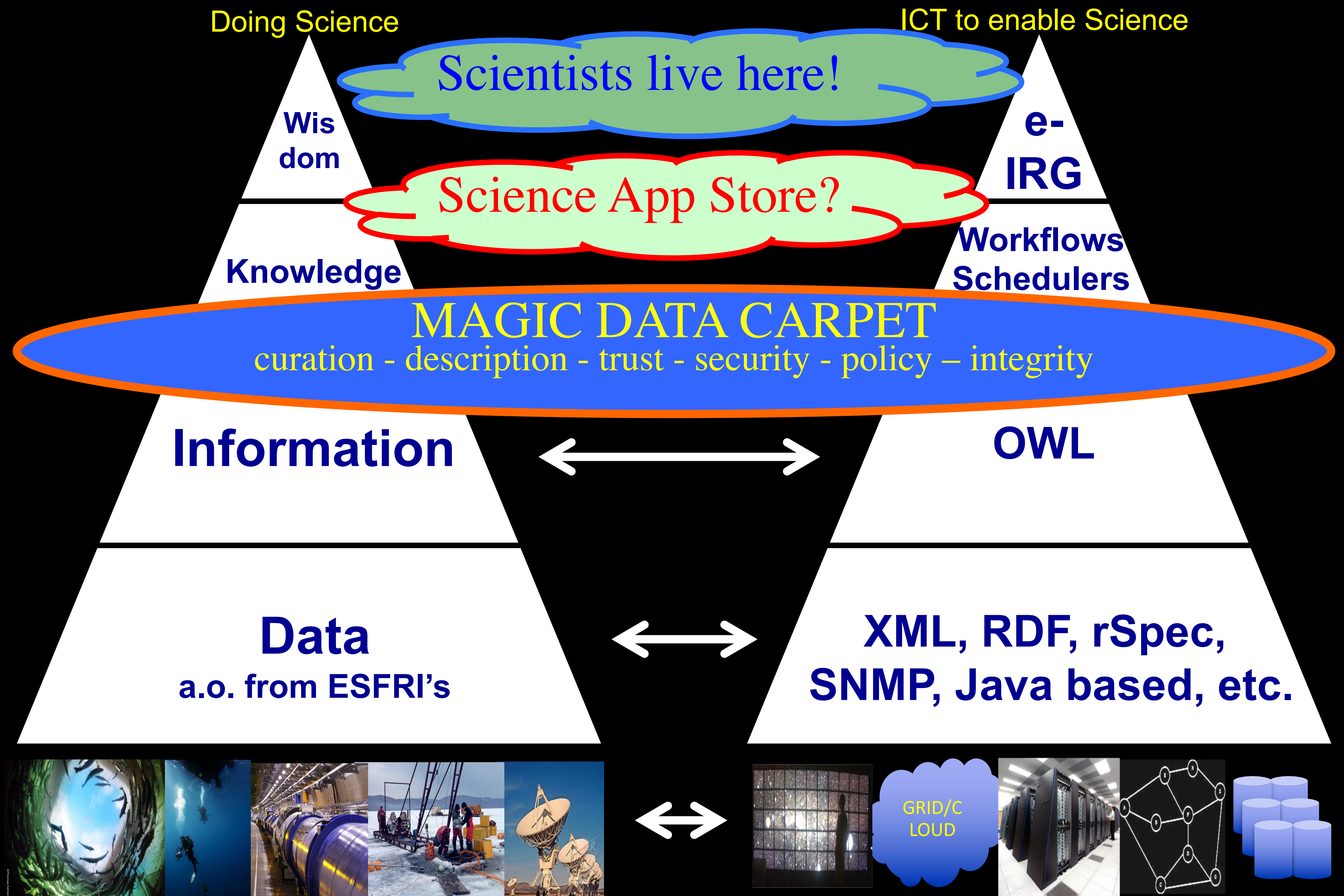
e-
IRG

Workflows
Schedulers
to act

OWL

XML, RDF, rSpec,
SNMP, Java based, etc.

The Big Data Challenge

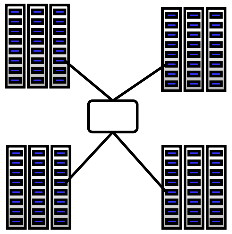


Past & future ICT research infrastructures

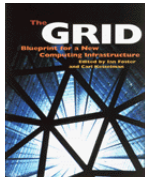
- TEN34 / TEN155
- Geant testbed & JRA’s
- FIRE
- Grid5000 (FR)
- DAS1-5 (NL)

Some years around 2010 connected by LightPath

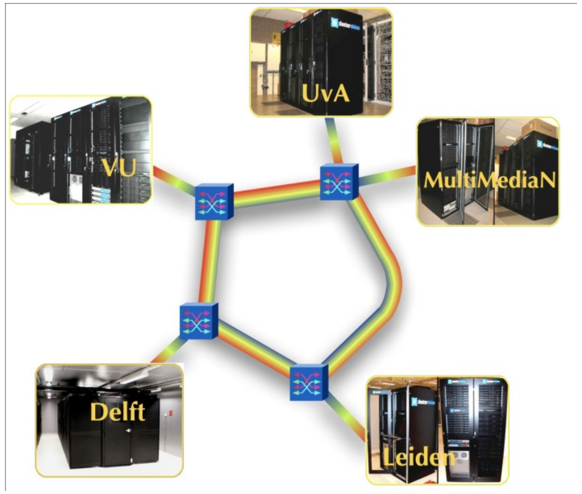
DAS generations: visions



- DAS-1: Wide-area computing (1997)
  - Homogeneous hardware and software



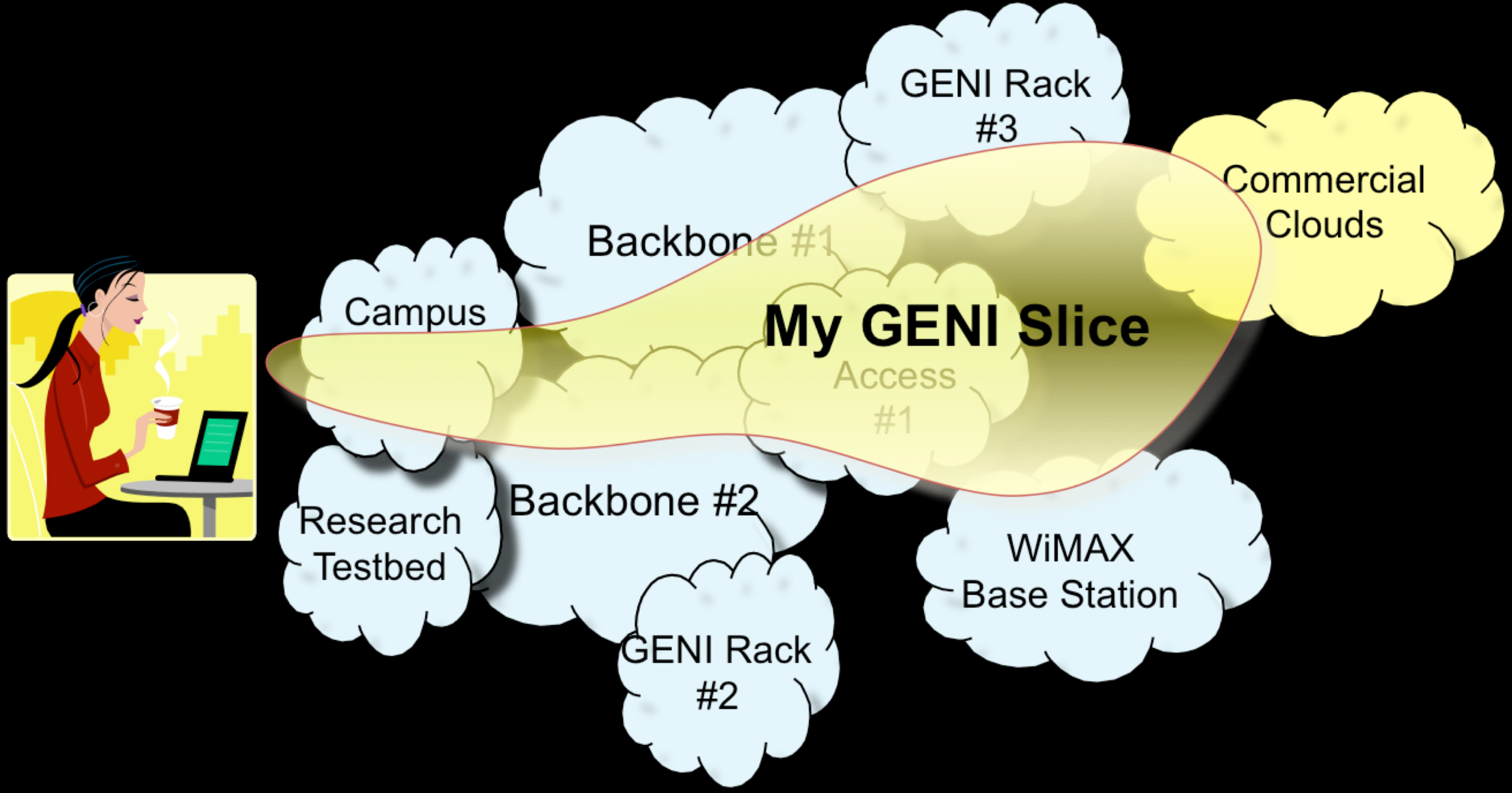
- DAS-2: Grid computing (2002)
  - Globus middleware
- DAS-3: Optical Grids (2006) StarPlane
  - Dedicated 10 Gb/s optical links between all sites



- DAS-4: Clouds, diversity, green IT (2010)
  - Hardware virtualization, accelerators, energy measurements
- DAS-5: Harnessing diversity, data-explosion (June 2015)
  - Wide variety of accelerators, larger memories and disks

Henri Bal, Dick Epema, Cees de Laat, Rob van Nieuwpoort, John Romein, Frank Seinstra, Cees Snoek, Harry Wijshoff, "The Distributed ASCI Supercomputer: a Long-term Computer Science Research Infrastructure.", IEEE Computer, Vol 49, Ed 5, pp 54-63, May 2016 (2015).

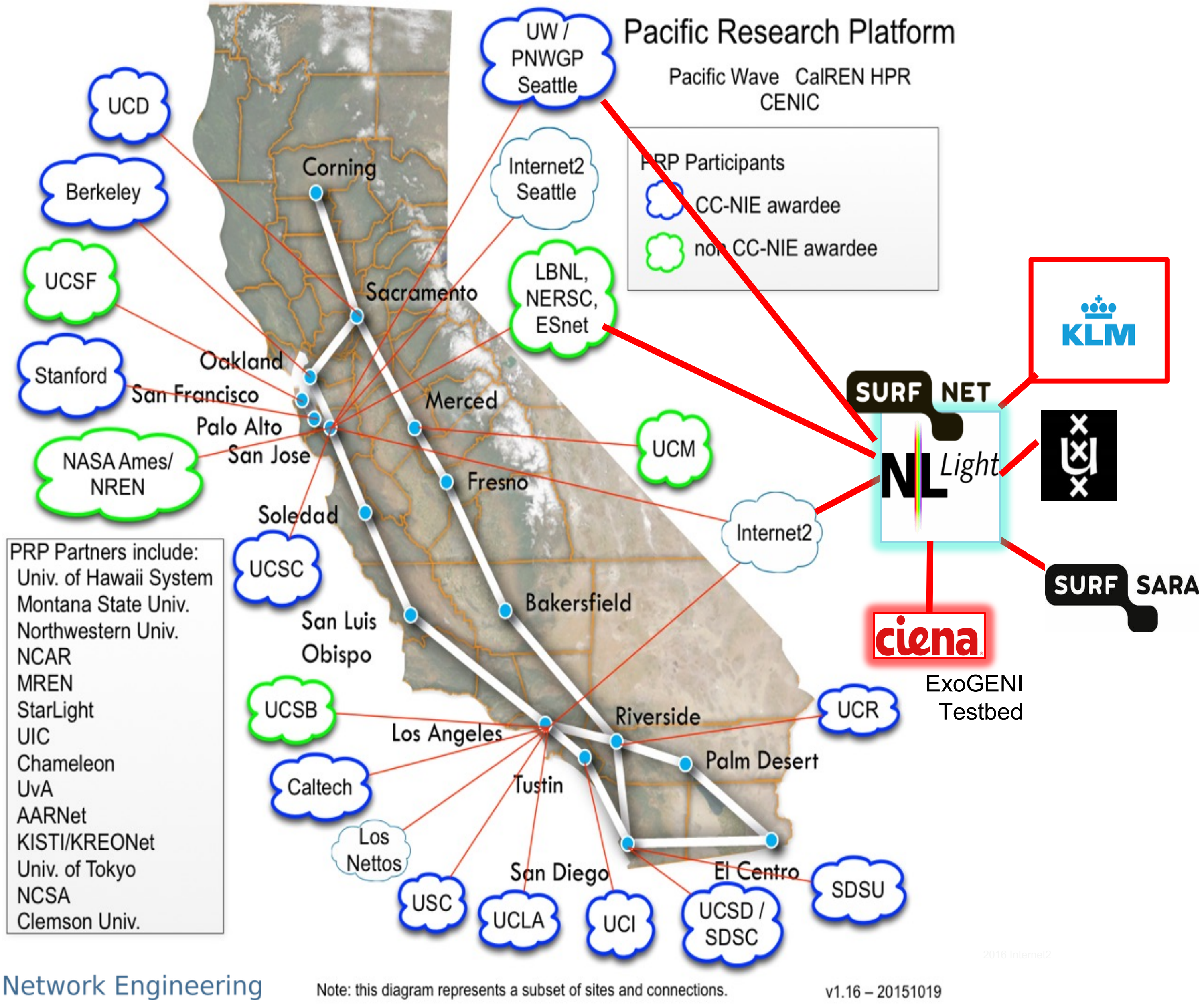
GENI: Virtualizing CI



Pacific Research Platform testbed involvement

Research goal:
Explore value of academic network research capabilities that enable innovative ways & models to share big data assets

PACIFIC RESEARCH PLATFORM



Past & future ICT research infrastructures

- TEN34 / TEN155
- Geant testbed & JRA's
- FIRE
- Grid5000 (FR)
- DAS1-5 (NL)

Was connected by LightPath around 2010!

- Need for breakable CS oriented testbed
- Must include: Programmable networks, Cloud, Exascale SC, DTN's, streaming, access to public services, IOT, Wireless
- Must include work on AI & ML, fundamental data security
- At Scale ➔ SILECS - https://www.silecs.net

SARNET: Security Autonomous Response with programmable NETworks

Marc Lyonnais, Leon Gommans, Rodney Wilson, Lydia Meijer, Frank Fransen Tom van Engers, Paola Grosso, Gauravdeep Shami, Cees de Laat,Ameneh Deljoo, Ralph Koning, Ben de Graaff, Gleb Polevoy, Stojan Travanovski.

Big Data: real time ICT for logistics

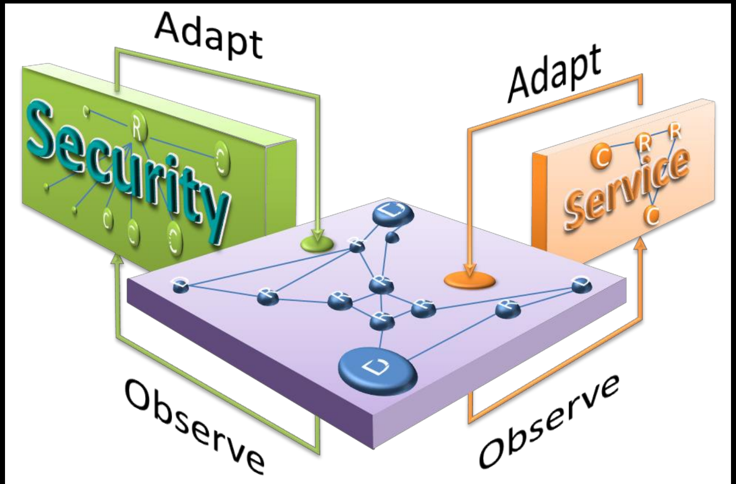
Data Logistics 4 Logistics Data (dl4ld)

Lydia Meijer (PI), Cees de Laat (Co-PI), Leon Gommans, Tom van Engers, Paola Grosso, Kees Nieuwenhuis.

EPI: Enabling Personalized Interventions

Cees de Laat(PI), Sander Klous (PL), Leon Gommans, Tom van Engers, Paola Grosso, Henri Bal, Anwar Osseyran, Aki Harma, Douwe Biesma, Peter Grünwald, Floortje Scheepers, Gertjan Kaspers.

Cyber security program SARNET



Research goal is to obtain the knowledge to create ICT systems that:

- model their state (situation)
- discover by observations and reasoning if and how an attack is developing and calculate the associated risks
- have the knowledge to calculate the effect of counter measures on states and their risks
- choose and execute one.

In short, we research the concept of networked computer infrastructures exhibiting SAR: Security Autonomous Response.

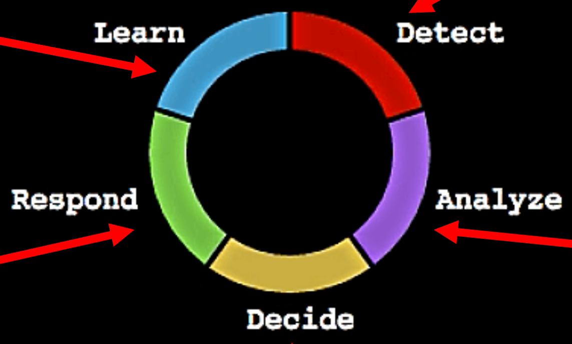
SARNET Publications (subset)

Laboratory: ExoGeni & PRP
Fieldlab with KLM & CIENA
OSA-Optical Forum Conference paper [1]

SC16 INDIS workshop paper [2]
TNC short paper [4]

Control loop

IEEE NetSoft paper [5]
efficiency of SDN mitigations [8]



SC16 demo/poster <delaat.net/sc16>
Salt Lake City (UT)
IEEE Sec-Virtnet 2016 paper [3]
Removing Undesirable Flows [6]

SC15 demo/poster <delaat.net/sc16>
Austin (TX)
Sec-Virtnet paper [3]
Computational Trust Model (SCTM) [7]

SC16 demo/poster <delaat.net/sc16>
Salt Lake City (UT)
CoreFlow: Enriching Bro security events [9]

1. Paper: R. Koning, A. Deljoo, S. Trajanovski, B. de Graaff, P. Grosso, L. Gommans, T. van Engers, F. Fransen, R. Meijer, R. Wilson, and C. de Laat, "Enabling E-Science Applications with Dynamic Optical Networks: Secure Autonomous Response Networks ", OSA Optical Fiber Communication Conference and Exposition, 19-23 March 2017, Los Angeles, California.
2. Paper: Ralph Koning, Nick Buraglio, Cees de Laat, Paola Grosso, "CoreFlow: Enriching Bro security events using network traffic monitoring data.", Special section on high-performance networking for distributed data-intensive science, SC16", Future Generation Computer Systems, <accepted for publication>
3. Paper: Ralph Koning, Ben de Graaff, Cees de Laat, Robert Meijer, Paola Grosso, "Analysis of Software Defined Networking defenses against Distributed Denial of Service attacks", The IEEE International Workshop on Security in Virtualized Networks (Sec-VirtNet 2016) at the 2nd IEEE International Conference on Network Softwarization (NetSoft 2016), Seoul Korea, June 10, 2016.
4. Short paper: Nick Buraglio, Ralph Koning, Cees de Laat, Paola Grosso, "Enriching network and security events for event detection", Conference proceedings TNC2017, https://tnc17.geant.org/core/presentation/30.
5. Paper: Ralph Koning, Ben de Graaff, Robert Meijer, Cees de Laat, Paola Grosso, "Measuring the effectiveness of SDN mitigations against cyber attacks", IEEE Conference on Network Softwarization (Netsoft 2017 - SNS 2017), Bologna, Italy, July 3-7, 2017.
6. Paper: Gleb Polevoy, Stojan Trajanovski, Paola Grosso and Cees de Laat, "Removing Undesirable Flows by Edge Deletion.", COCOA'2018 conference, December 15 - 17, 2018, Atlanta, Georgia, USA, Springer-Verlag.
7. Paper: Ameneh Deljoo , Tom van Engers, Leon Gommans, Cees de Laat, "Social Computational Trust Model (SCTM): A Framework to Facilitate Selection of Partners". In: Proceedings of 2018 IEEE/ACM Innovating the Network for Data-Intensive Science (INDIS), Dallas, TX, USA, 2018
8. Paper: R. Koning, B. de Graaff, G. Polevoy, R. Meijer, C. de Laat, P. Grosso, "Measuring the efficiency of SDN mitigations against attacks on computer infrastructures", Future Generation Computer Systems 91, 144-156.
9. Ralph Koning, Nick Buraglio, Cees de Laat, Paola Grosso, "CoreFlow: Enriching Bro security events using network traffic monitoring data.", Special section on high-performance networking for distributed data-intensive science, SC16", Future Generation Computer Systems

EPI Project goals

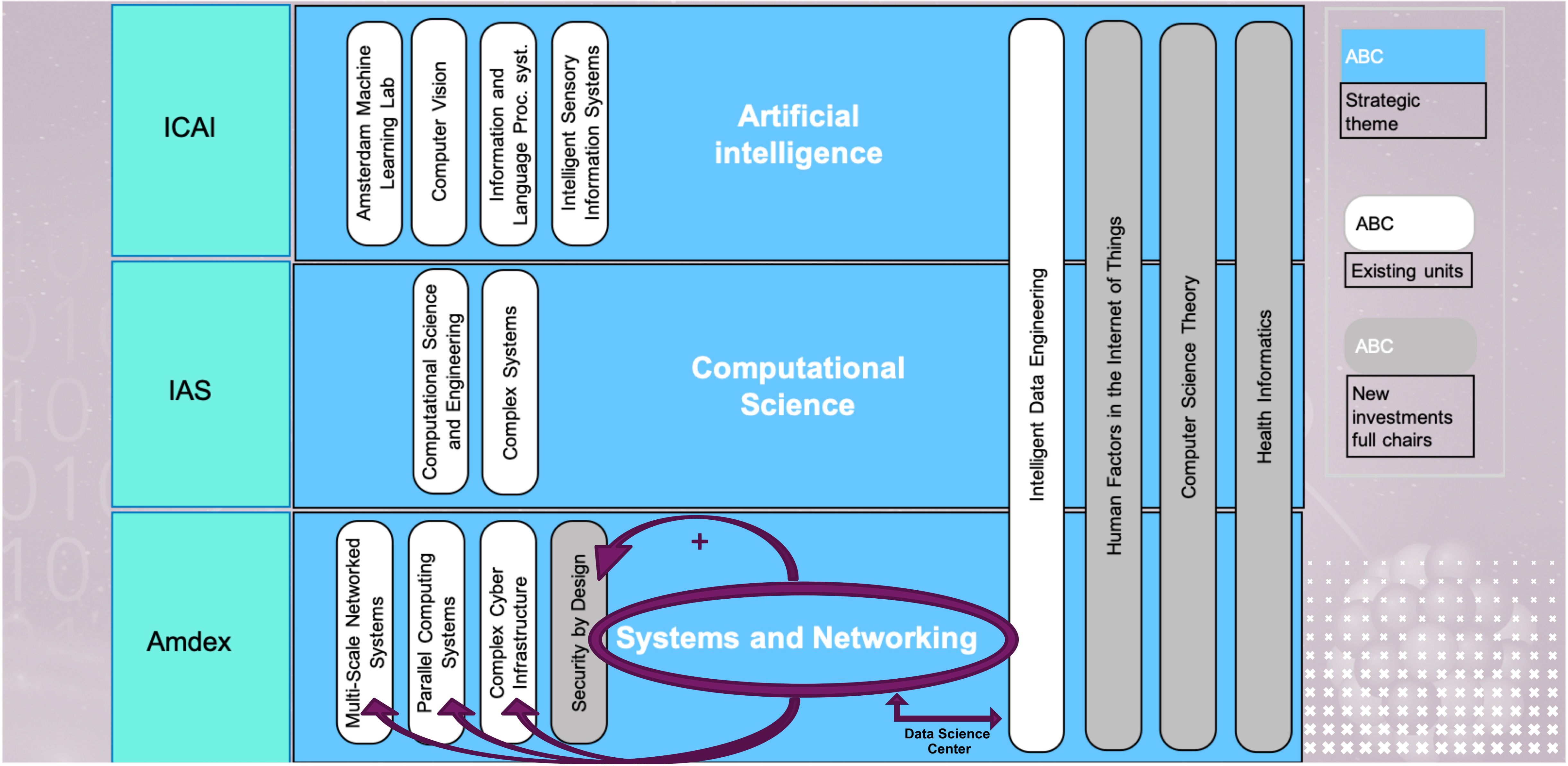
“The overall aim of this project is to explore the use and effectiveness of data driven development of scientific algorithms, supporting personalized self- and joint management during medical interventions / treatments.

The key objective is to use data science promoting health practically with data from various sources to formulate lifestyle advice, prevention, diagnostics, and treatment tailored to the individual, and to provide personalized, effective, real-time feedback via a concept referred in this proposal as a digital health twin.”

Research questions

- **RQ1: Dynamically Analyzing Interventions based on Small Groups: how can we determine, based on as little data as possible, whether an intervention does or does not work for a small group or even an individual patient?**
- **RQ2: Dynamically Personalizing the Group: how can we identify effective intervention strategies and optimize personalization strategies applicable for different patient and lifestyle profiles via dynamic (on-line) clustering of patients? Can those clusters be adapted as new data about patients and results of interventions come in and as other data may be removed or modified?**
- **RQ3: Data and Algorithm Distribution: what are the consequences of a distributed, multi-platform, multi-domain, multi-data-source big data infrastructure on the machine learning algorithms and what are potential consequences on performance?**
- **RQ4: Adaptive health diagnosis leading to optimized intervention: how can we enhance self- / joint management by dynamically integrating updated models generated from machine learning from various data sources in state of the art health support systems that based on personal health records, knowledge of health modes and effective interventions?**
- **RQ5: Regulatory constraints and data governance: how can we create scalable solutions that meet legal requirements and consent or medical necessity-based access to data for allowed data processing and preventing breaches of these rules by embedded compliance, providing evidence trails and transparency, thus building trust in a sensitive big data sharing infrastructure?**
- **RQ6: Infrastructure: how can the various requirements from the use-cases be implemented using a single functional ICT-infrastructure architecture?**

Position in the Instituut



CONCLUSIONS

- Observations:
  - parallels energy world and internet developments
    - move to micromarkets
    - IOT alike security treats
  - trend: ML & AI replaces Visualization
  - Illinois governor (1998) noting: canals - railroads - cars - fibers, and now we add trusted data exchange driving economy and markets
  - San Diego Super Center aligns with data science and portal for sustainability in RNE
  - LEGO model for CI & Data & Methods
  - Industry recognized need for new data related approaches
  - Data Value creates an economy for data sharing.

CONCLUSIONS

- Overal advice
  - It is about people & knowledge
  - Base on society relevant applications
  - Get faculty drivers from each campus
  - Governance model is essential
  - align with education (soft&hard money)
- Applications
  - Health
  - Instrumenting IOT
  - Energy transition/critical infrastructures IT
  - CyberSecurity

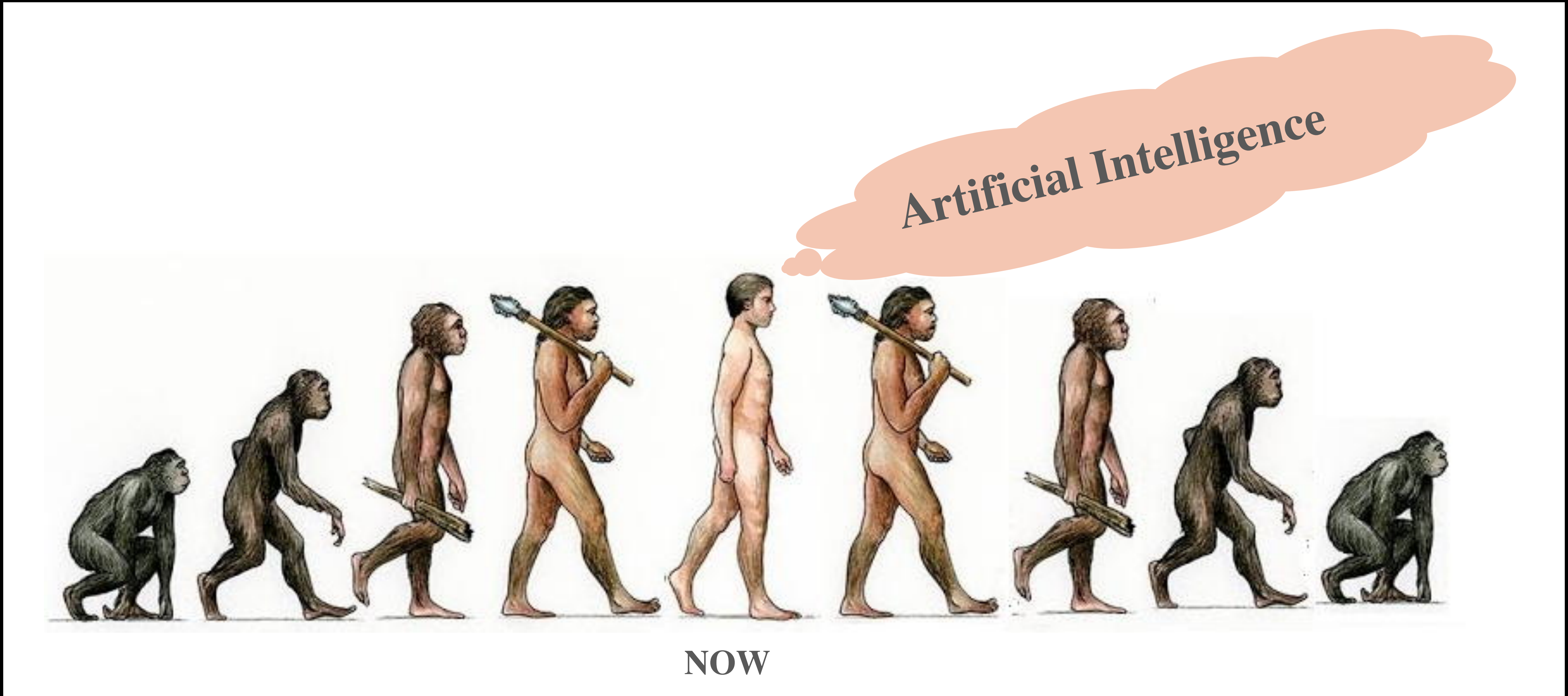
CONCLUSIONS

- Themes
  - global data & methods ecosystem supporting applications
  - Explainable AI to aid managing CI
  - Security
  - Super-facility
  - revisiting Internet standards with current technology in mind
  - Quantum compute and networking

Remarks, Quotes:

- Wouter Los: Considering the list of conclusions, it comes in my mind that any future data infrastructure should accommodate the preferred governance model. And this is related to the cultural dimension. What kind of data market do we foresee, what are checks and balances, and who decides (has power) on what? How is this framed in the context of (self regulating) micro markets, when billions of agents interact.
- Tom Defanti: ML is like training your dog without knowing how the dog works.
- Larry Smarr: Manage the exponential.
- Mike Norman: It is not about hardware, it is about the people!!!
- Inder & me: The kids of today are the decision makers tomorrow and have no feeling for classic CI.

AI forking off



Conclusion, Q&A

Need for Network to Data level experimental Infrastructure.

Europe's own DTN infra, CC program, CI Ambitions

Data at scale.

P.S. I did not mention Quantum Compute & Networking; See:

- https://www.orau.gov/quantumnetworks2018/default.htm
- https://science.energy.gov/%7E/media/ascr/pdf/programdocuments/docs/2019/QNOS_Workshop_Final_Report.pdf
- https://delaat.net/qn
- https://delaat.net/
  - https://delaat.net/sarnet
  - https://delaat.net/dl4ld
  - https://delaat.net/epi

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