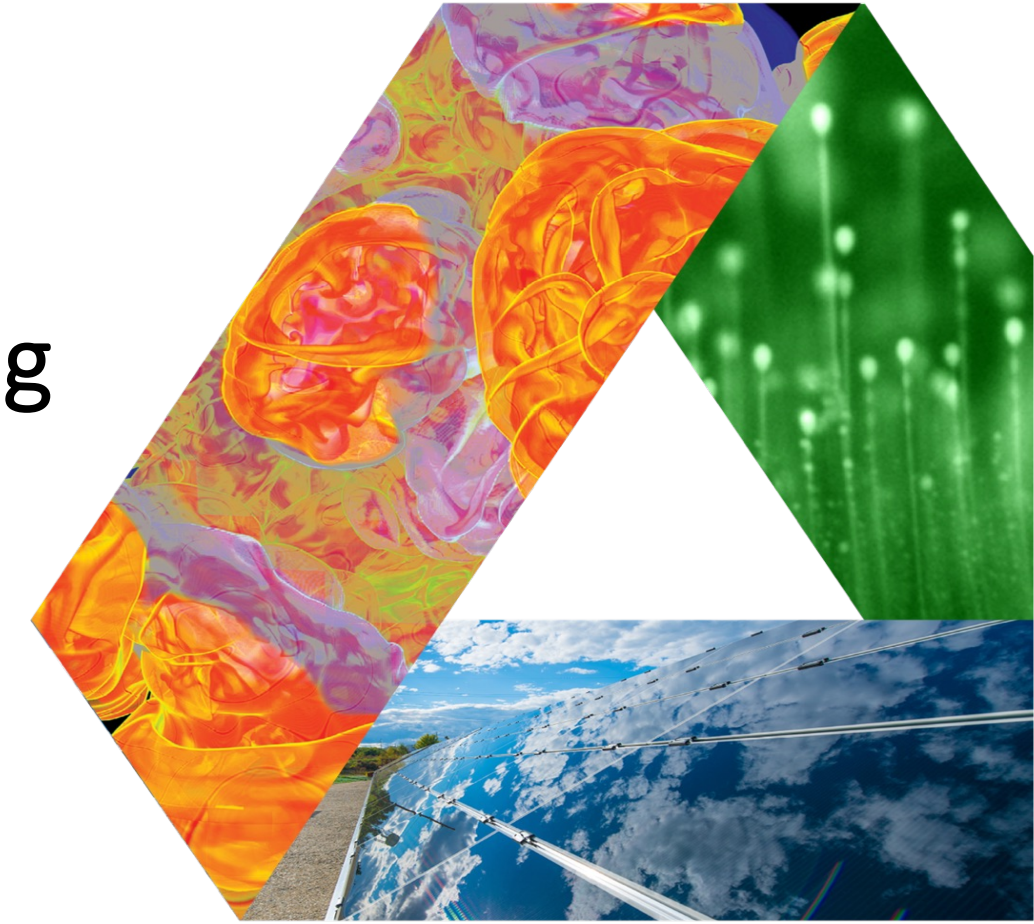
Why High Performance Computing Platforms Cannot be Eliminated



Anshu Dubey
Mathematics and Computer Science Division
Argonne National Laboratory

A Brief History of Application Simulations

Many things have changed, two have remained constant
skepticism, prediction of demise

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In the beginning -- theoreticians and experimentalists

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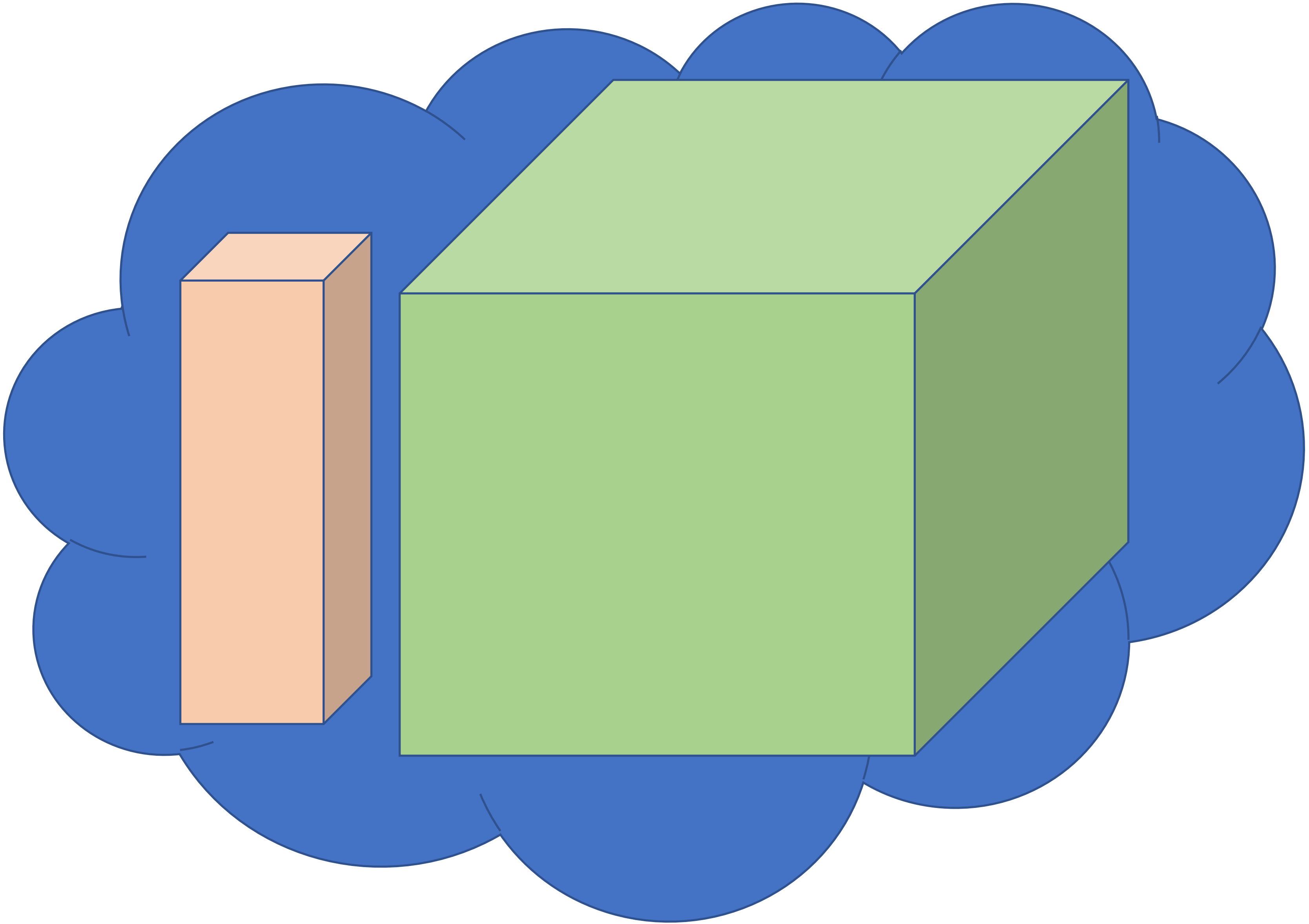
We, the applications people understand the plight of HPC centers

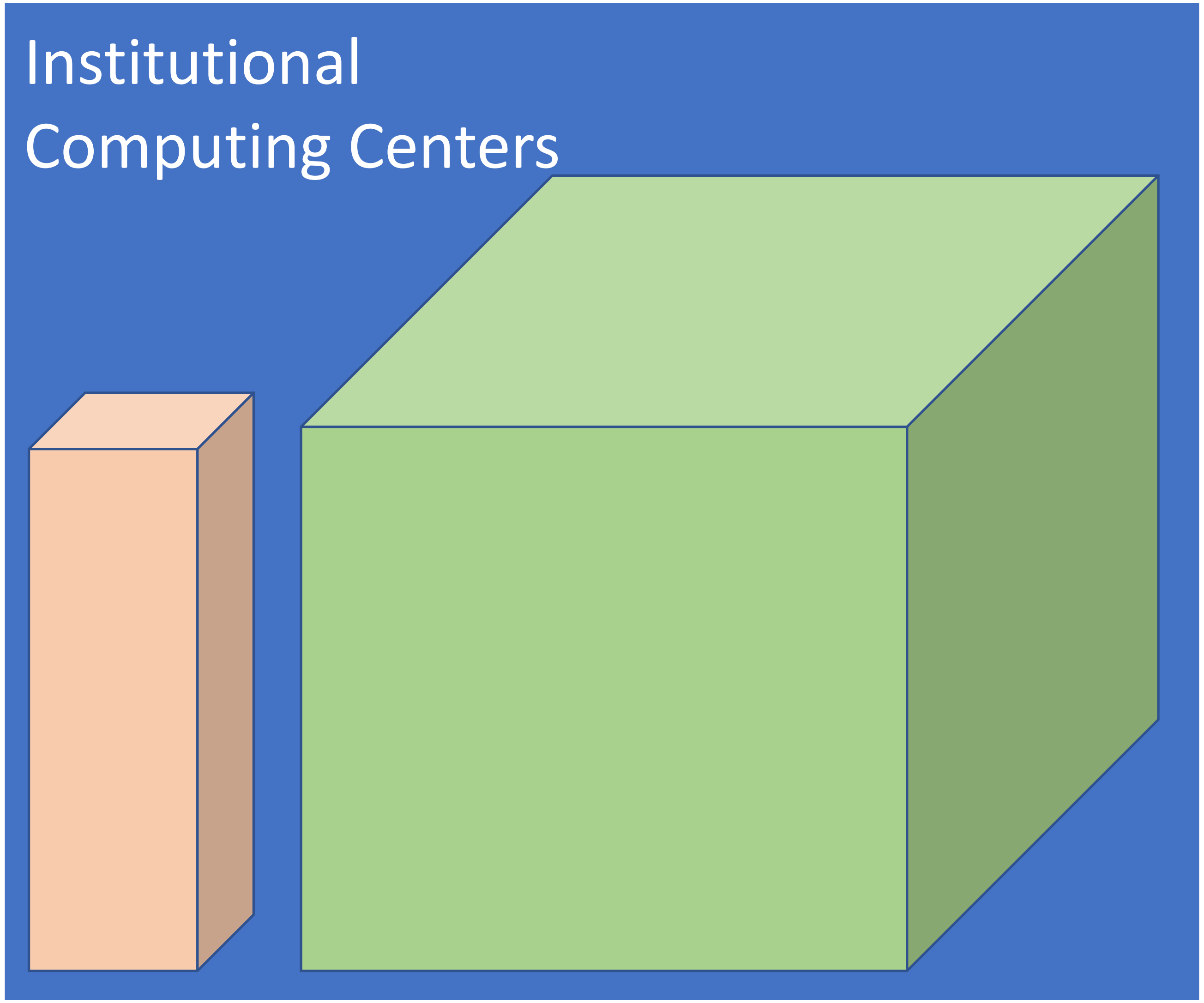
Arguments and counter arguments for HPC in Cloud

Argument -- Democratization of HPC



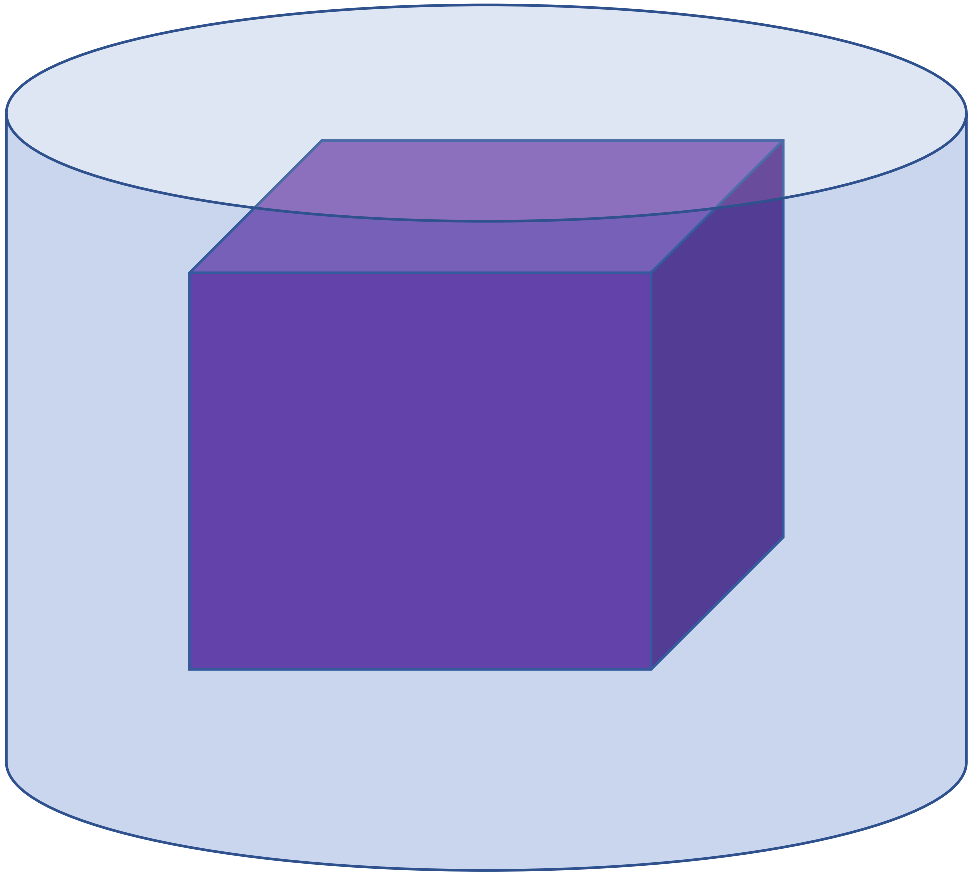
- Anyone can use
- Small/medium/large jobs
  - On demand
  - No dedicated sys-admins

Counter Argument – Cost effectiveness



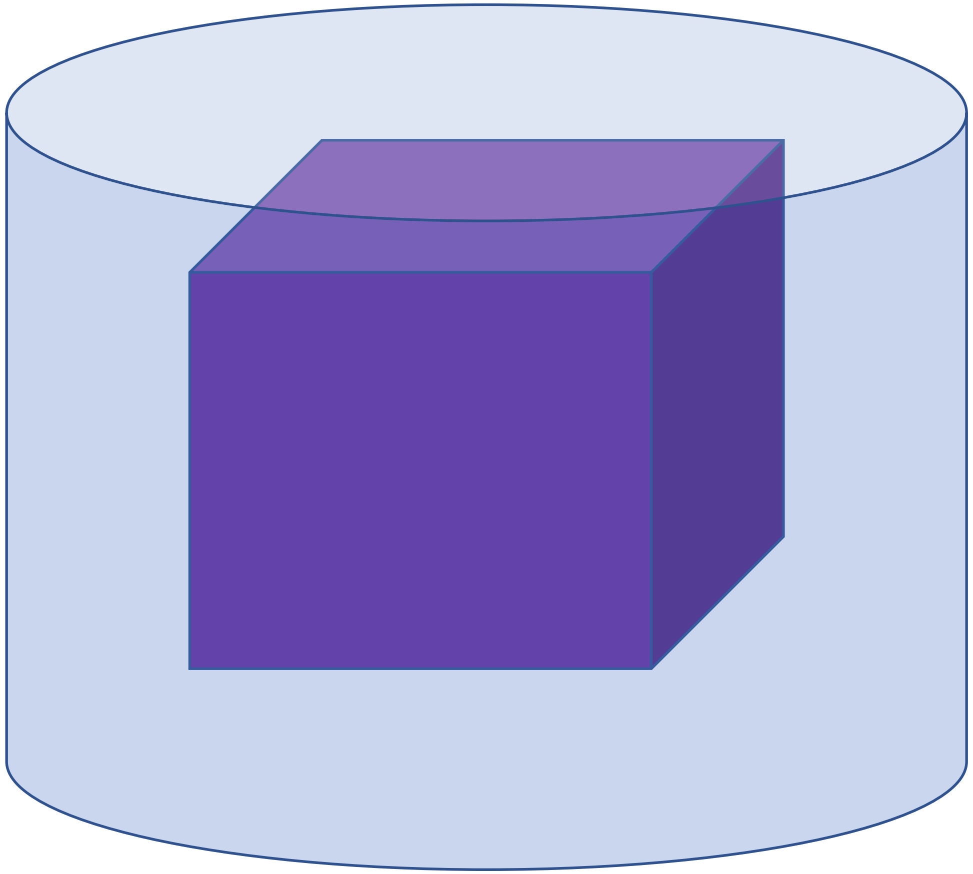
- Critical mass of users
- Fully subscribed resources
- Dedicated sys-admins still more cost effective
- Development platforms
- Testing platforms

Argument – Containers have Changed the Game



- They are getting better
- Easier to use
- More reproducible

Counter Argument – I am yet to be convinced



- Still slow down execution
- Definitely slow down build
- Terrible for development

If you need to get a platform to do your development, may as well do production on it

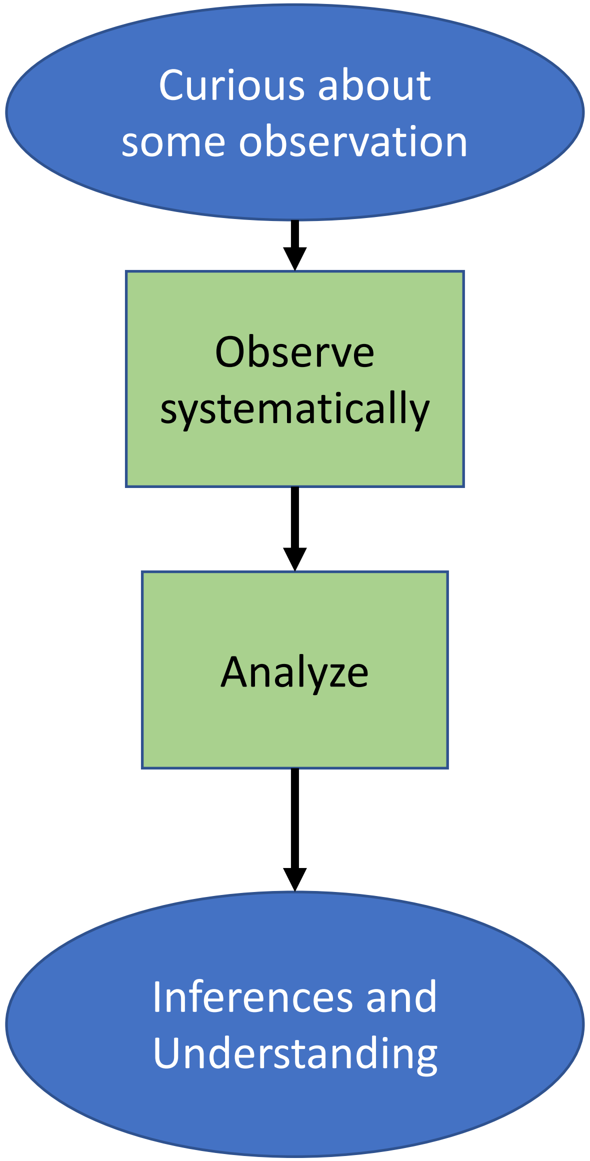
Argument – Cloud can serve HPC needs

- May be a large enough fraction, but all ….?

A long counter argument

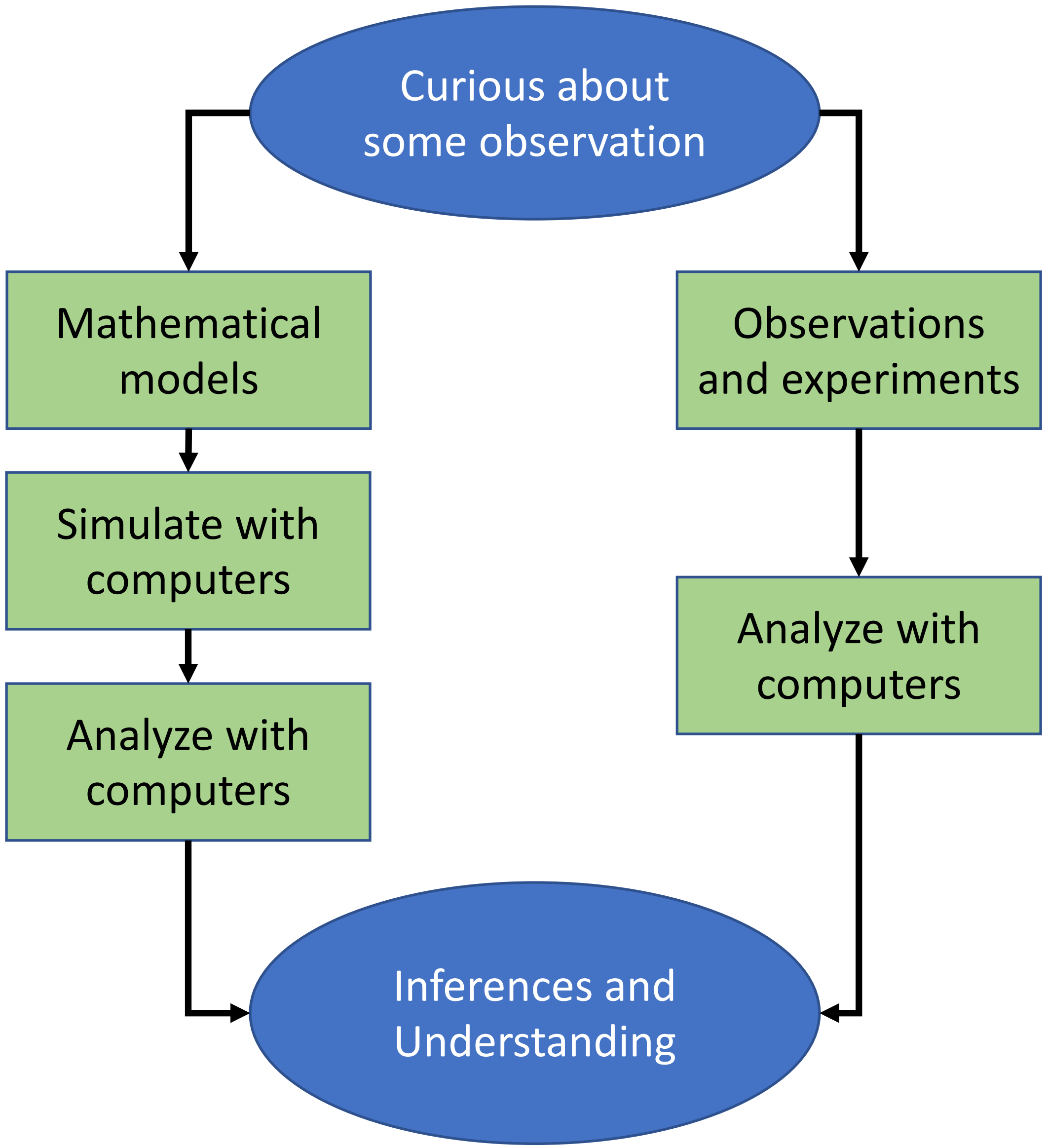
Understanding Our World

- Human beings are curious
- Have always wanted to understand how things around them work
- Many approaches have been used in the past



Understanding Our World

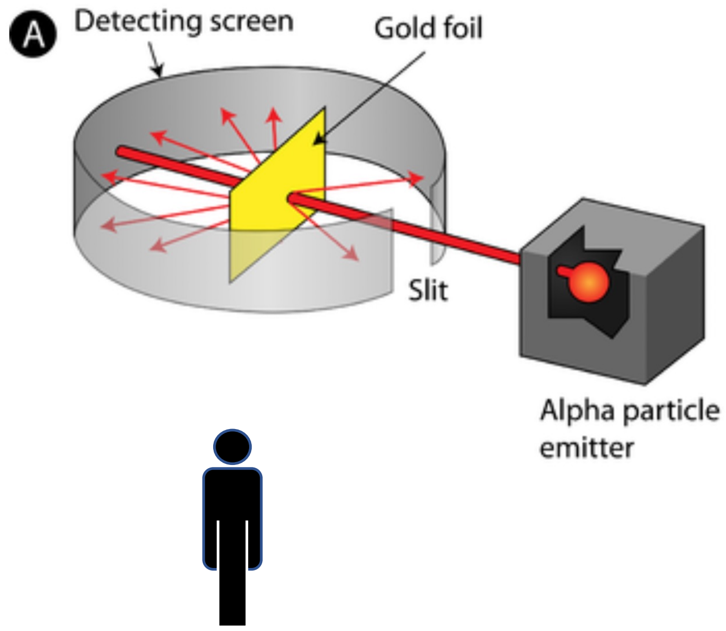
- Human beings are curious
- Have always wanted to understand how things around them work
- Many approaches have been used in the past
- New approaches continue to be developed
- And they get more complex



Atomic Physics Experiments

Rutherford Experiment

Figure from
https://courses.lumenlearning.com/cheminter/chapter/rutherfords-atomic-model/



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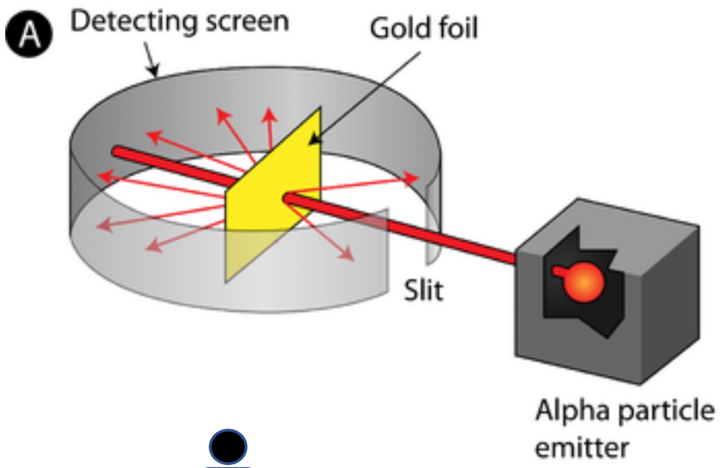
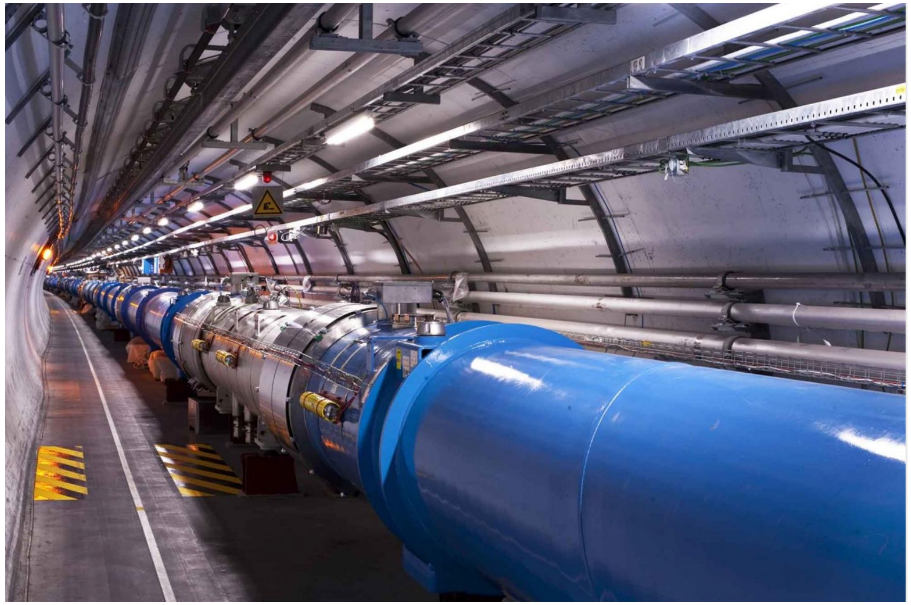
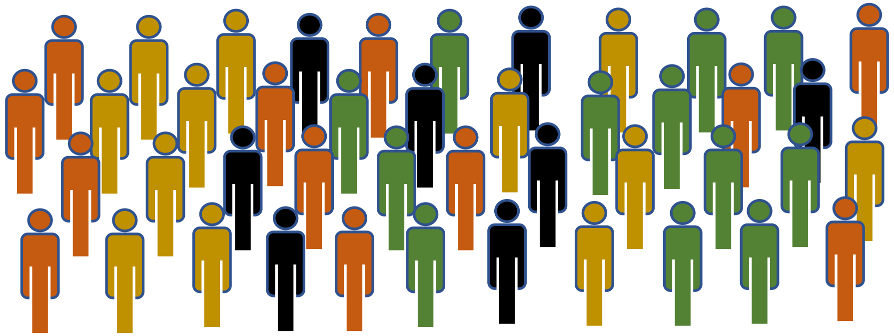
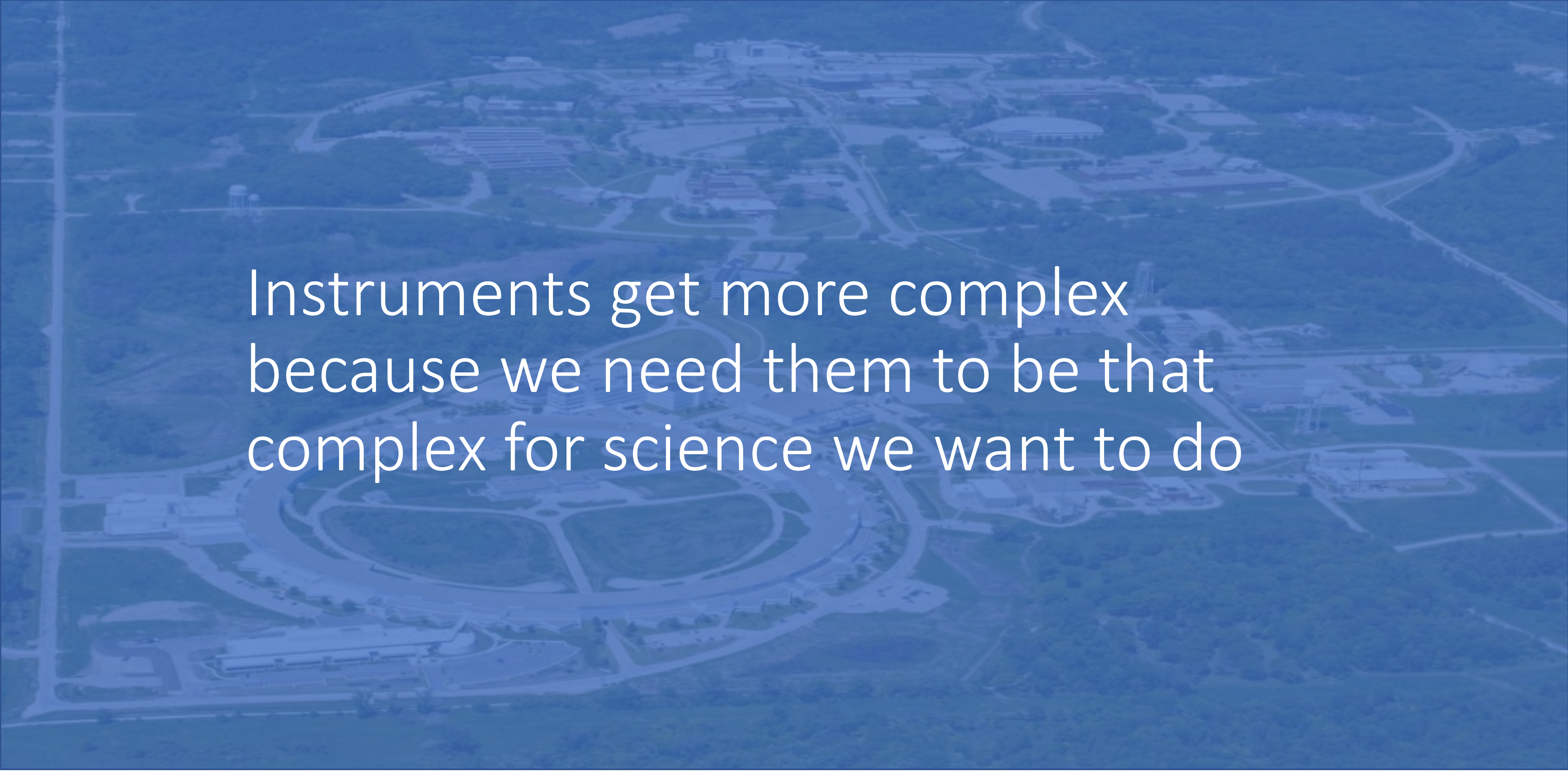


Large Hadron Collider

Figure from https://home.cern/resources/faqs/facts-and-figures-about-lhc



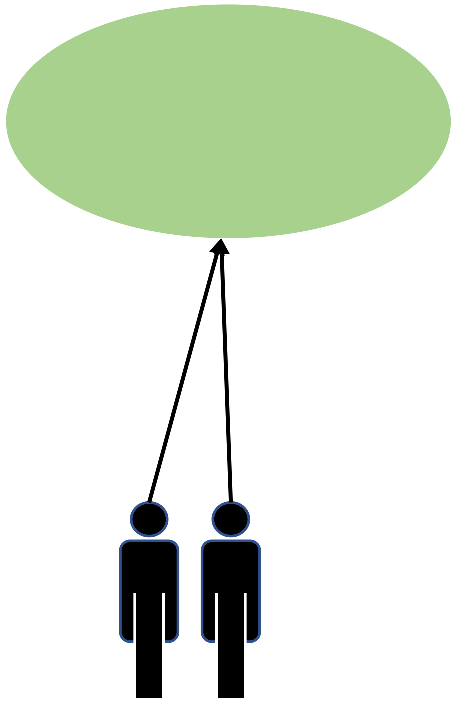




Instruments get more complex because we need them to be that complex for science we want to do

Computational Experiments

Exploratory models simplified with many approximations



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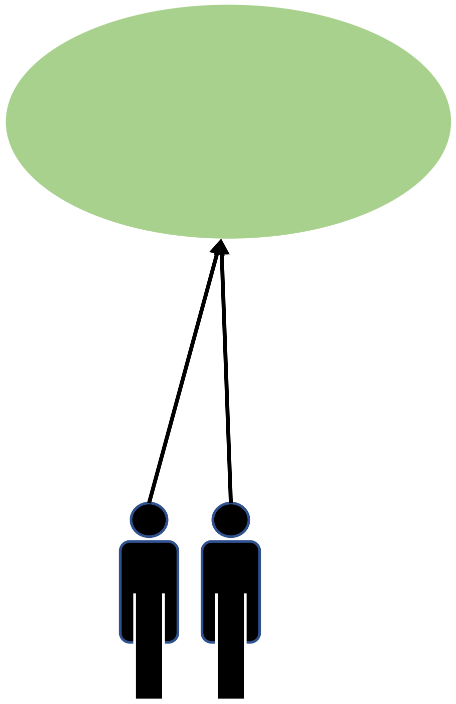
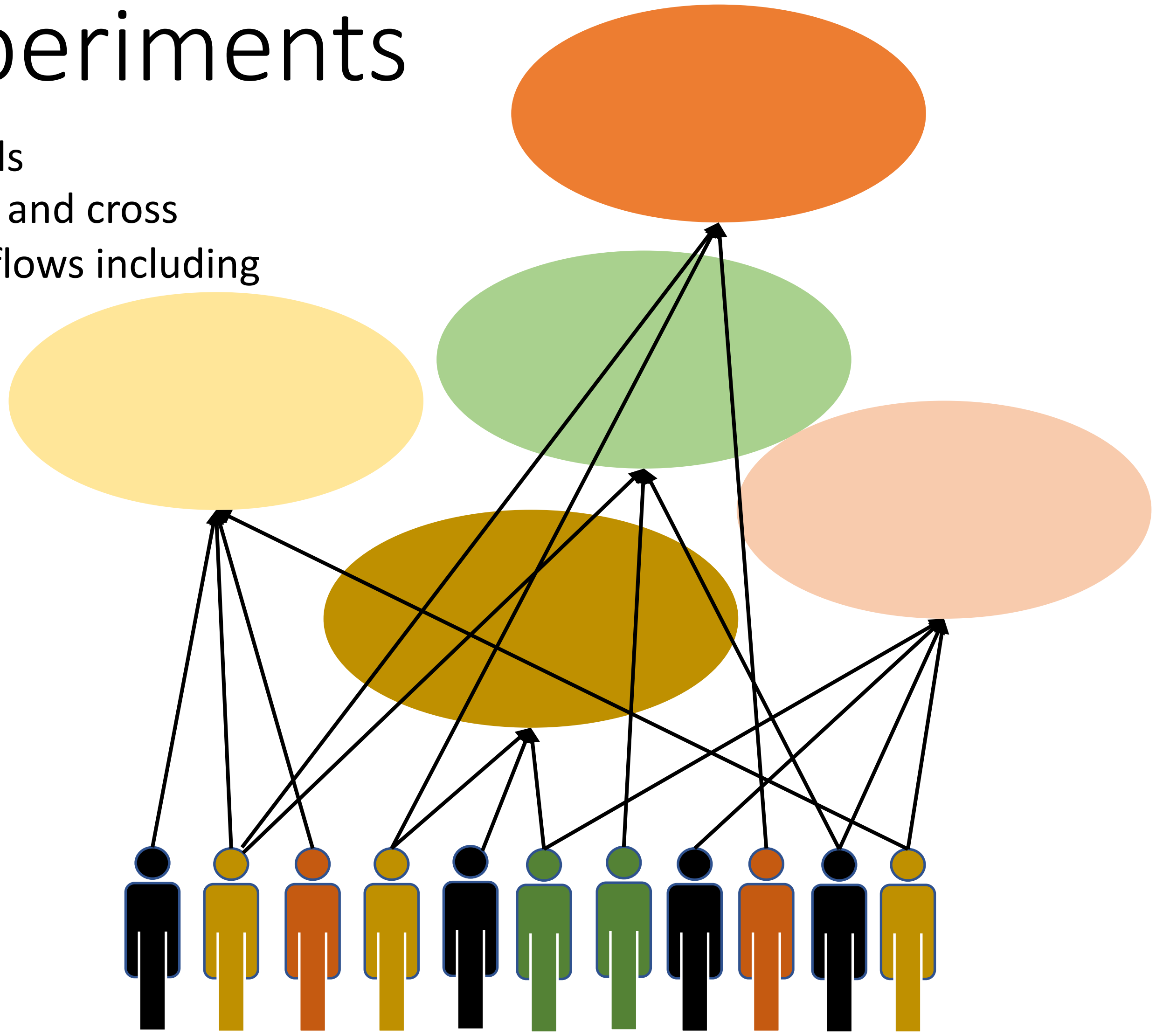
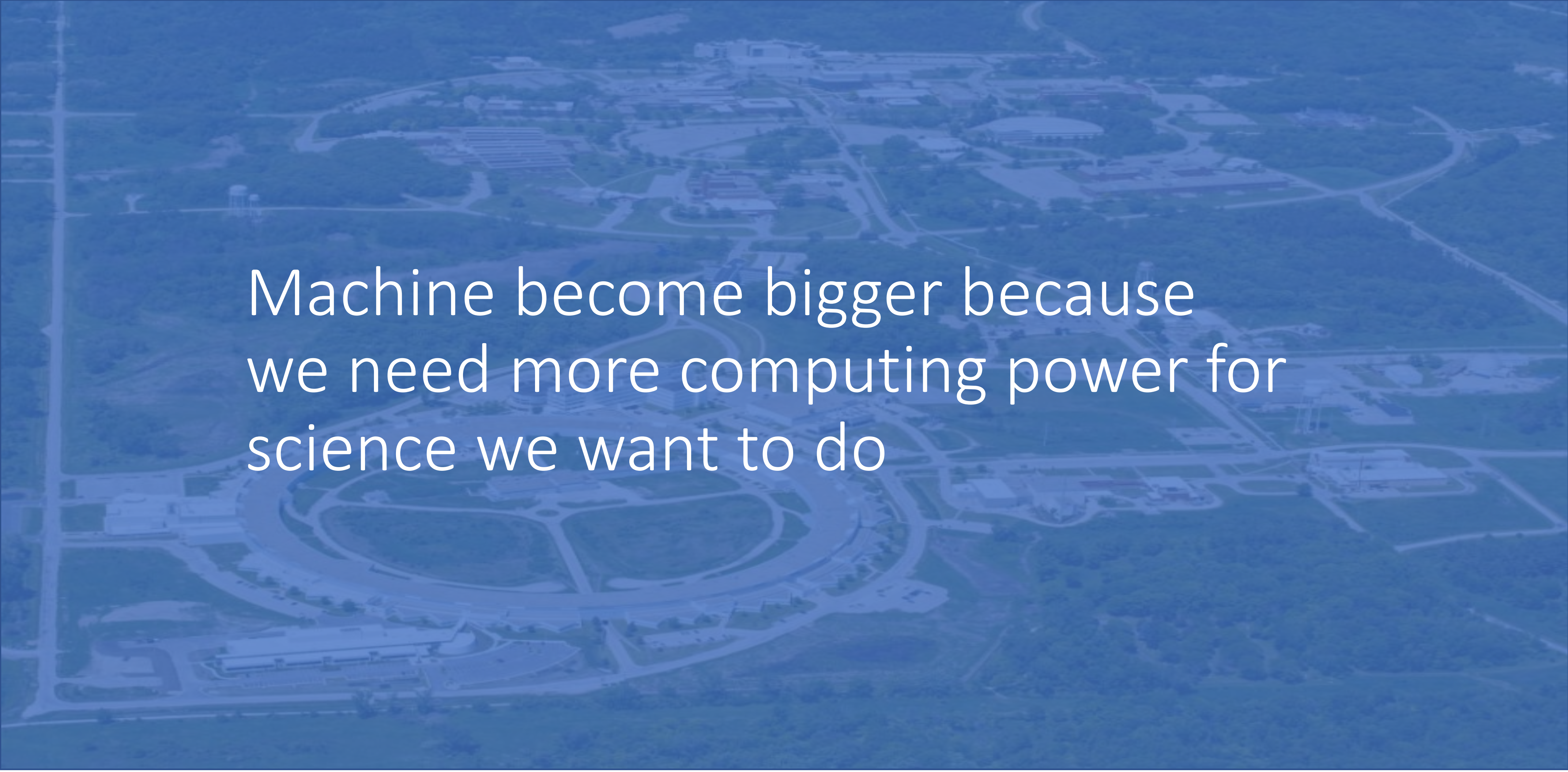
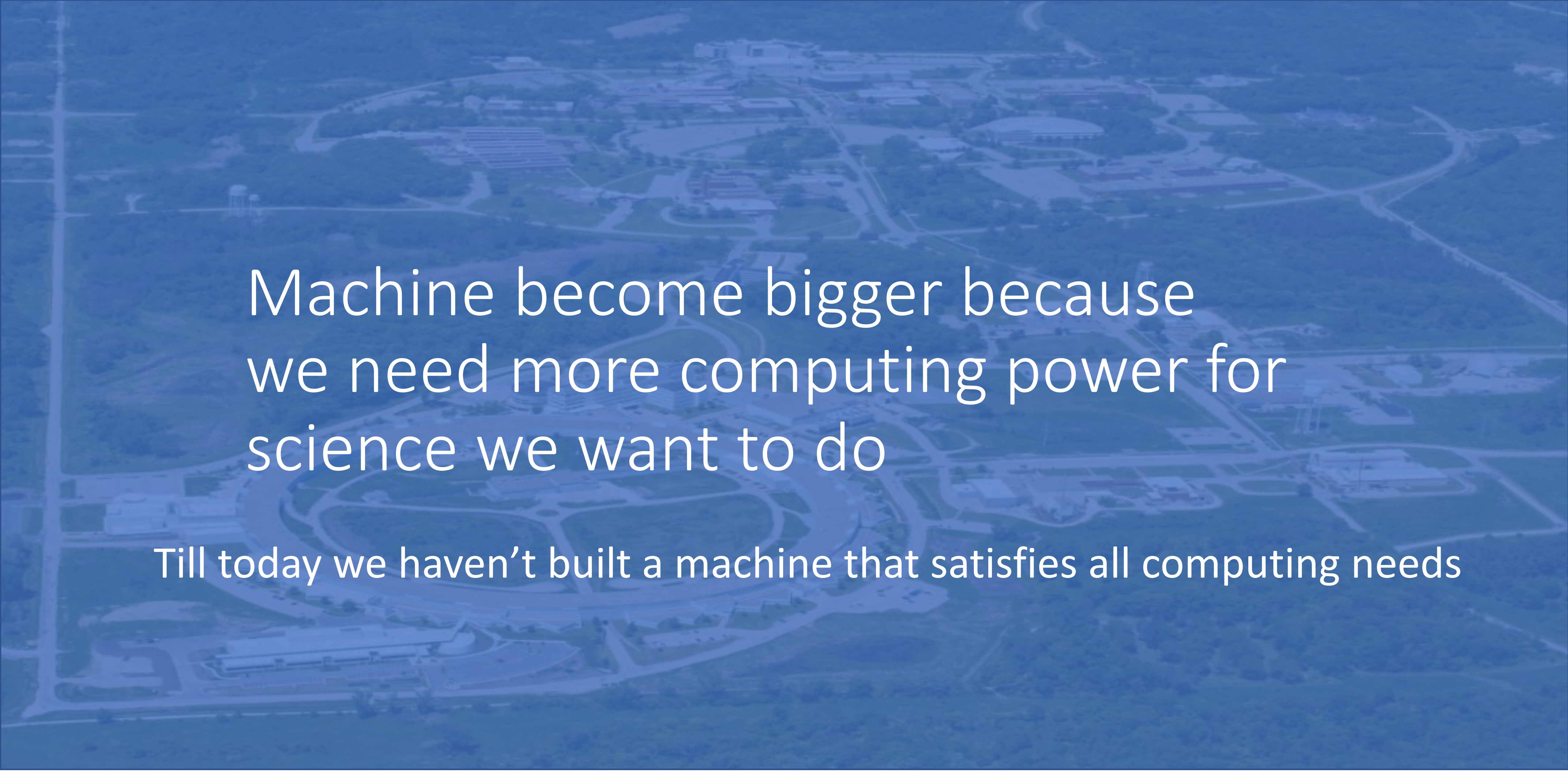


Multiphysics models with higher fidelity and cross coupling and workflows including AI/ML





Machine become bigger because we need more computing power for science we want to do



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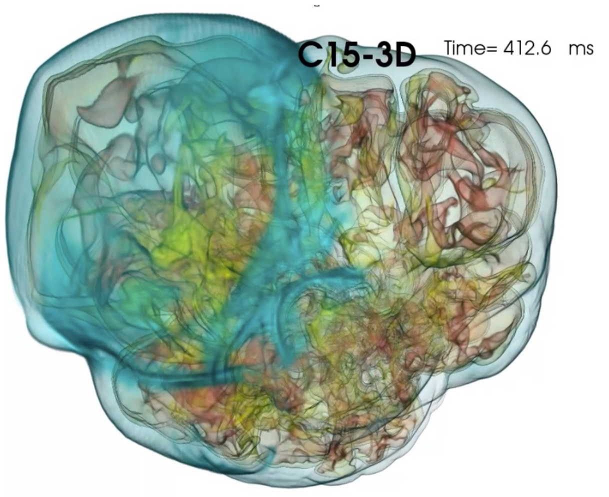
Till today we haven’t built a machine that satisfies all computing needs

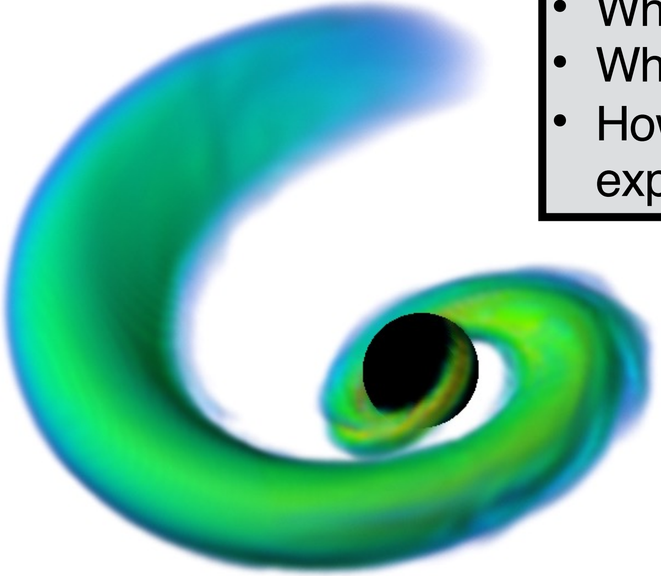
Machine become bigger because we need more computing power for science we want to do

Till today we haven’t built a machine that satisfies all computing needs
Or perhaps we always get ideas about how we can use more computing power for more insight ….

One Example -- Stellar explosions - cosmic laboratories of physics



core collapse
supernova simulations



- What is the cosmic origin of the elements?
- What are the sources of gravitational waves?
- What is the nature of matter at extreme densities?
- How can we use stellar explosions to map out the expansion of the Universe (dark energy)?

neutron star mergers

Plus related phenomena:
Thermonuclear (Type Ia) supernovae
X-ray bursts (neutron star eruptions)
Gamma-ray bursts
Magnetar powered supernovae
Black hole formation + accretion

A Brief History of Supernovae Simulations

- 1960s-1970s: Simple, one-dimensional (1D) models that treated the explosion as a shockwave propagating through a spherically symmetric star.
- 1980s-1990s: More sophisticated two-dimensional (2D) simulations
  - More realistic physics, including multi-group neutrino transport and nuclear reactions
  - Able to reproduce explosion energy and the production of elements
- 2000s-2010s: Development of three-dimensional (3D) models
  - Complex fluid dynamics and turbulence
  - More accurate neutrino transport and nuclear reactions
  - insights into the role of rotation and magnetic fields
- 2010s-Present: Development of multi-messenger simulations
  - Model both the electromagnetic radiation and non-electromagnetic
  - New insights into the role of neutrinos in driving the explosion and have helped refine our understanding of the nucleosynthesis processes in supernovae.

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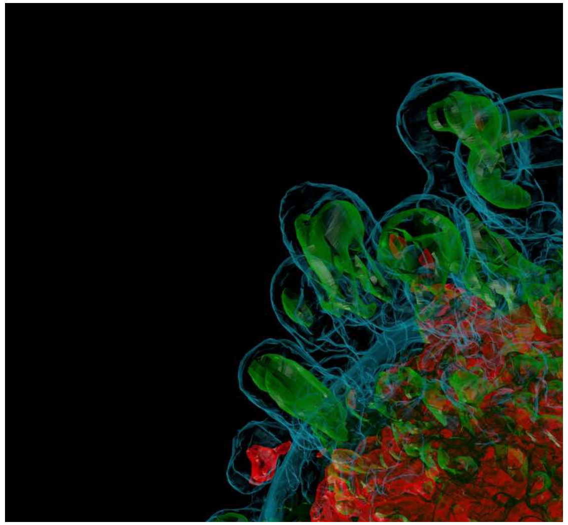
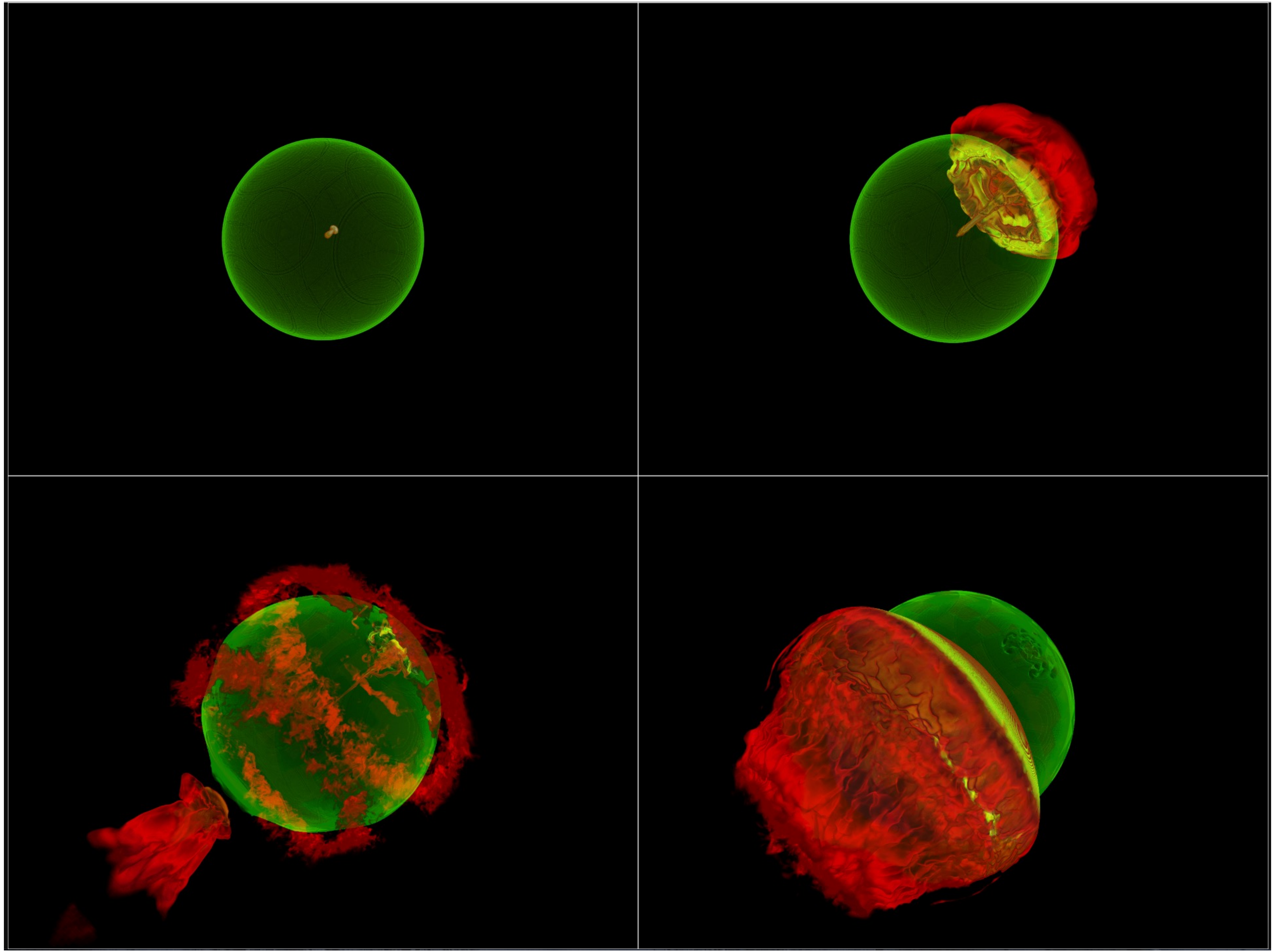
Courtesy of ChapGPT

My History of Supernova Simulations





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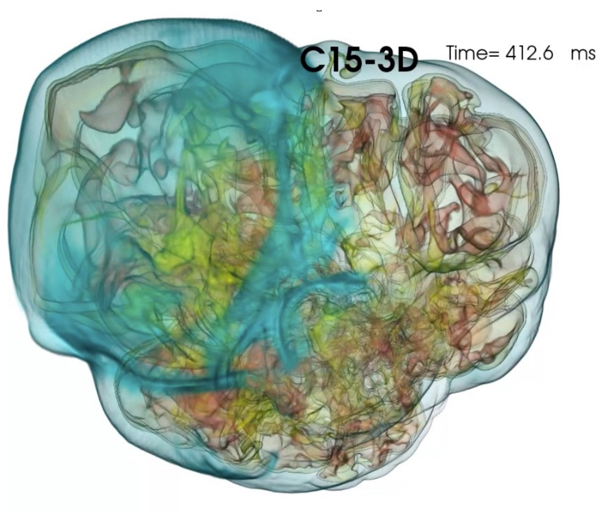

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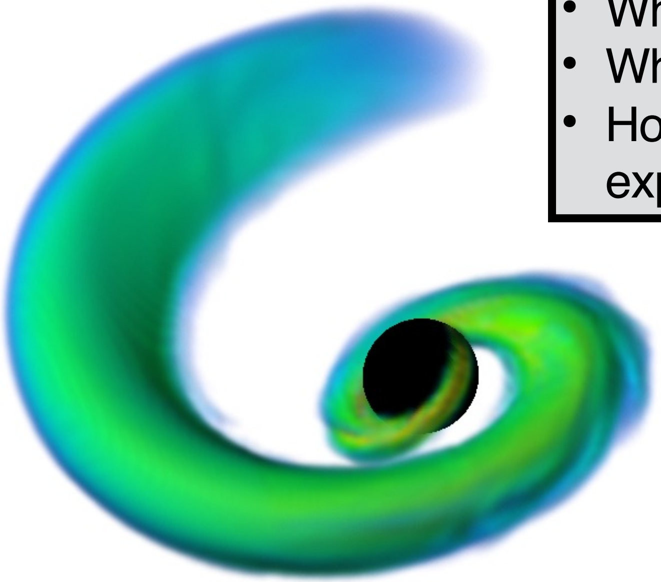

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Guide/enable science from experimental nuclear physics programs

- Determine key nuclei/reaction to study and provide astrophysical context

Provide reliable templates for gravitational wave/neutrino detectors

- Optimize science output from major experimental facilities

Interpret data from astronomical experiments

- Connect microscopic nuclear physics to macroscopic astrophysical phenomena

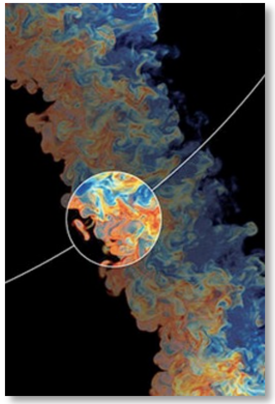
More examples -- The Exascale Computing Project

National security

Next-generation, **stockpile stewardship** codes

Reentry-vehicle-environment simulation

Multi-physics science simulations **of high-energy density physics** conditions



Energy security

Turbine **wind plant** efficiency

Design and commercialization of **SMR**s

Nuclear fission and fusion reactor **materials design**

Subsurface use for **carbon capture**, petroleum extraction, waste disposal

High-efficiency, low-emission **combustion engine** and gas turbine design

Scale up of **clean fossil fuel** combustion

Biofuel catalyst design

Economic security

Additive manufacturing of qualifiable metal parts

Reliable and efficient planning of the **power grid**

Seismic hazard risk assessment

Scientific discovery

Cosmological probe of the standard model of particle physics

Validate fundamental laws of nature

Plasma wakefield accelerator design

Light source-enabled **analysis of protein and molecular structure** and design

Find, predict, and control materials and properties

Predict and control **magnetically confined fusion plasmas**

Demystify **origin of chemical elements**

Earth system

Accurate regional impact assessments in **Earth system models**

Stress-resistant crop analysis and catalytic conversion of **biomass-derived alcohols**

Metagenomics for analysis of biogeochemical cycles, climate change, environmental remediation

Health care

Accelerate and translate **cancer research** (partnership with NIH)

What seems reasonable is technology that enables cloud-like interface for dedicated HPC resources

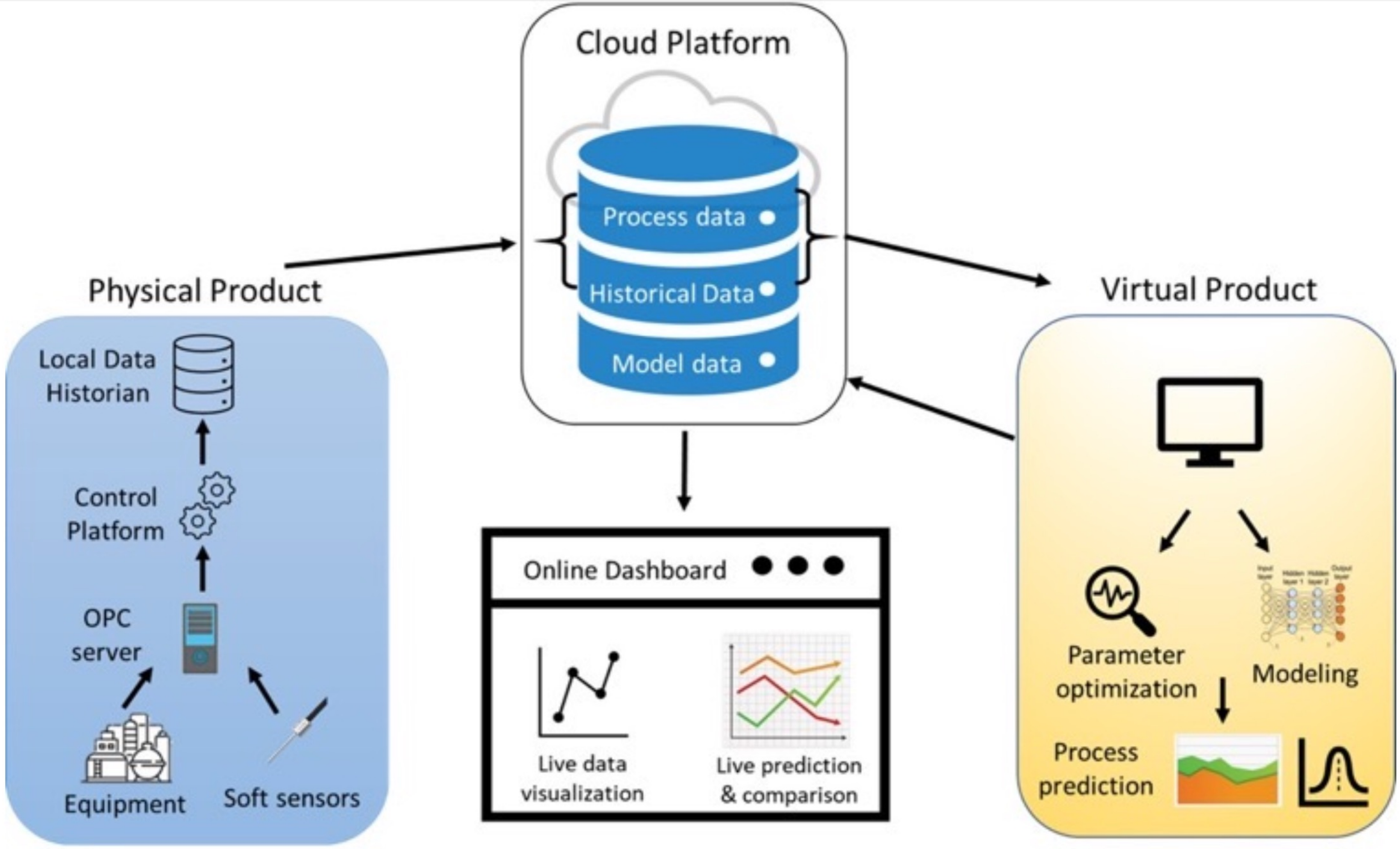
…. Presentation by Sadaf Alam, a few slides reproduced with permission …..

University of BRISTOL

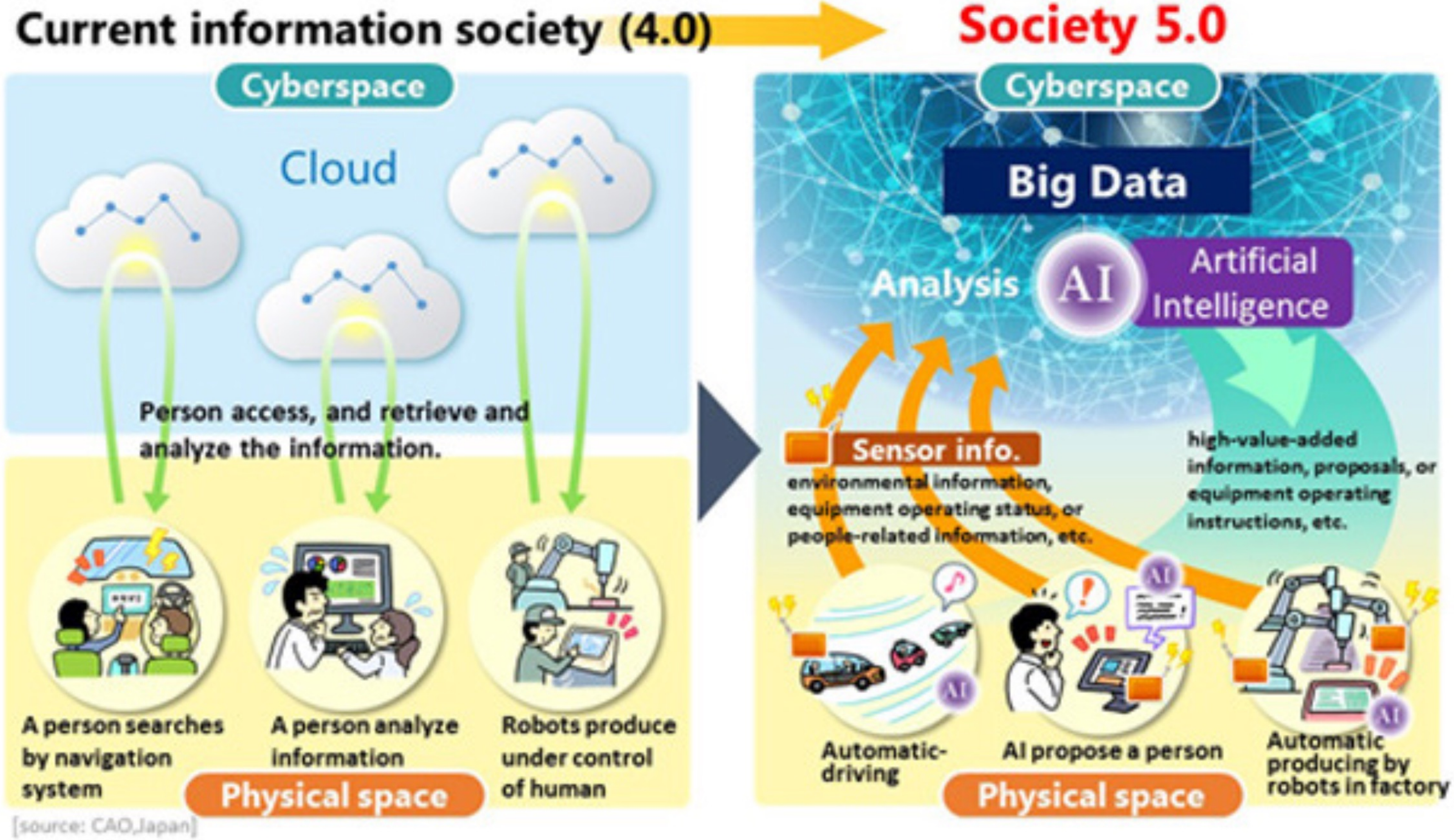
Co-designing Self-Service Digital Twin Workflows with DIY Cluster Toolbox and DRI Leasing Federation

Sadaf Alam

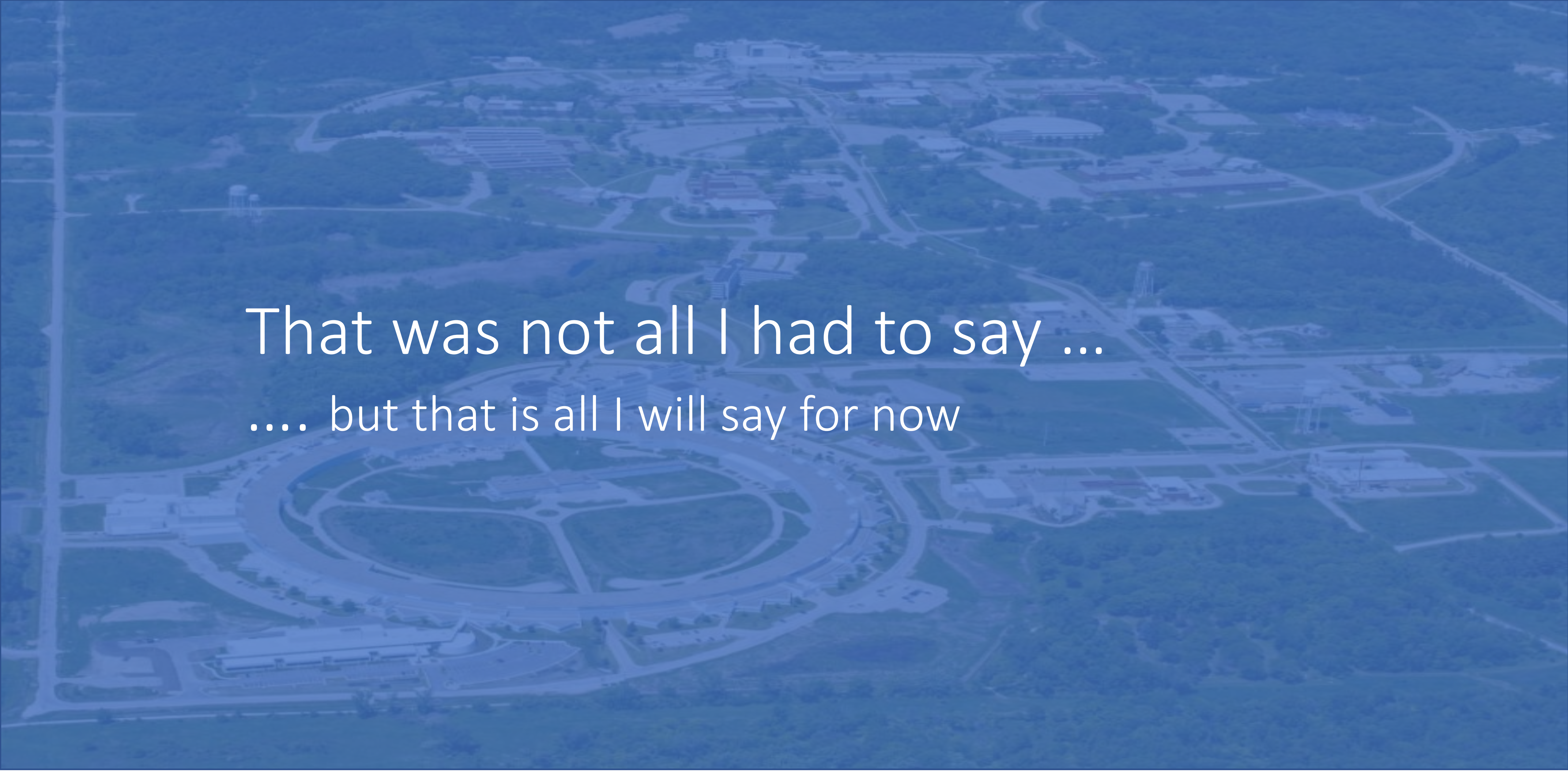
15th JLESC Workshop, March 21-23, 2023



https://encyclopedia.pub/entry/1915



https://www8.cao.go.jp/cstp/english/society5_0/index.html



That was not all I had to say …

…. but that is all I will say for now