Accelerating Scientific Discovery: The Need for Platforms

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Workshop on Opportunities for Accelerating Scientific Discovery: Realizing the Potential of Advanced and Automated Workflows
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Argonne NATIONAL LABORATORY

THE UNIVERSITY OF CHICAGO

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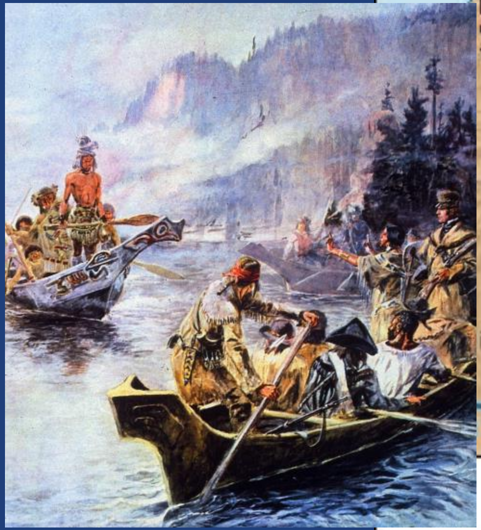
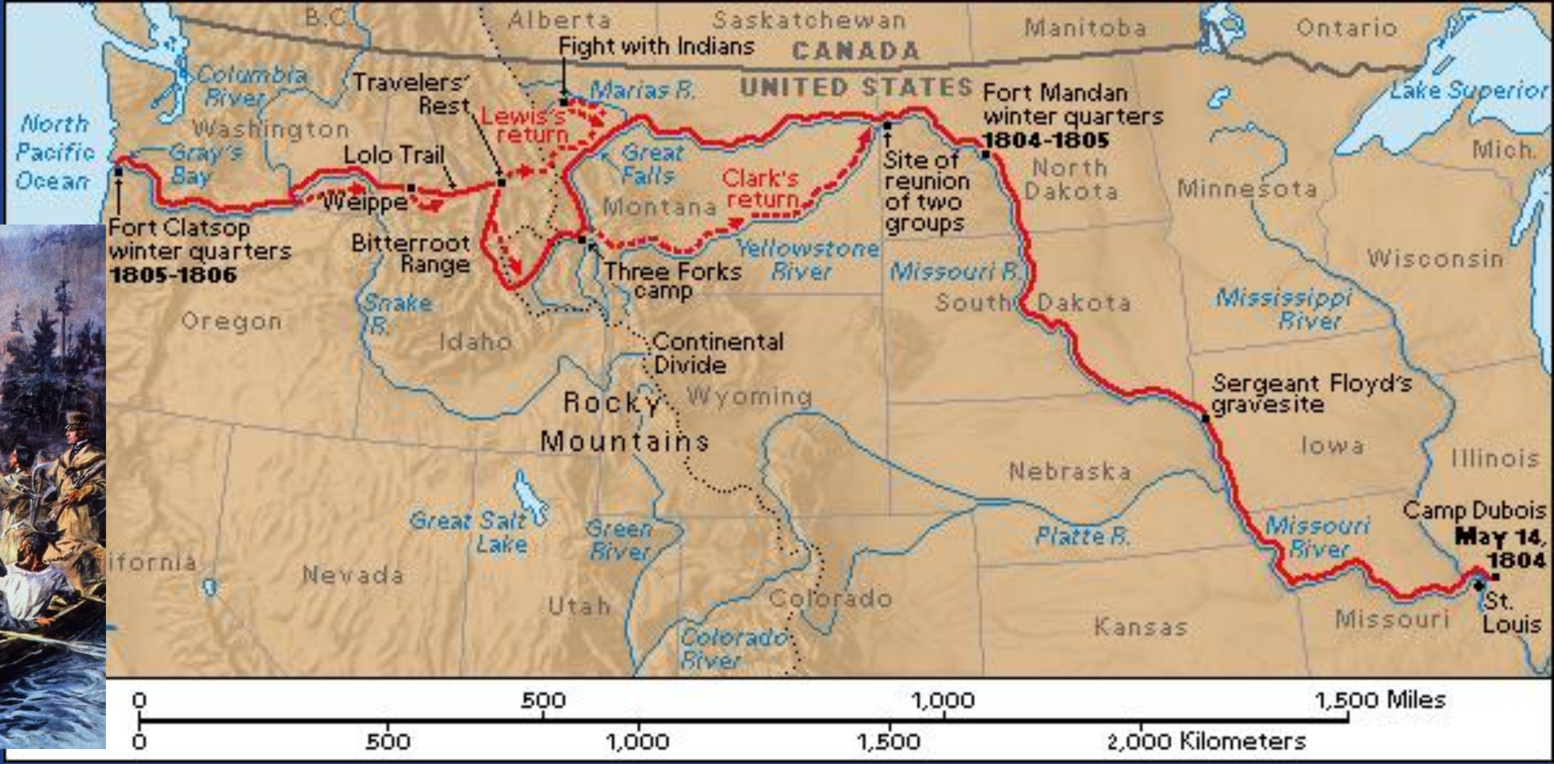
Lewis and Clark Expedition, 1804

Months of preparation
18 months one way
Expert guides
Much discovery
Mortality, bugs, …





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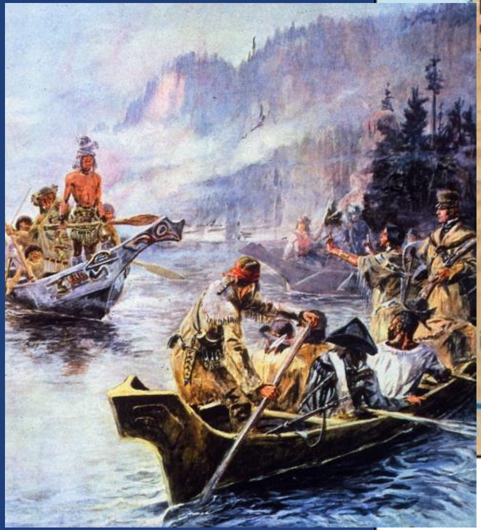
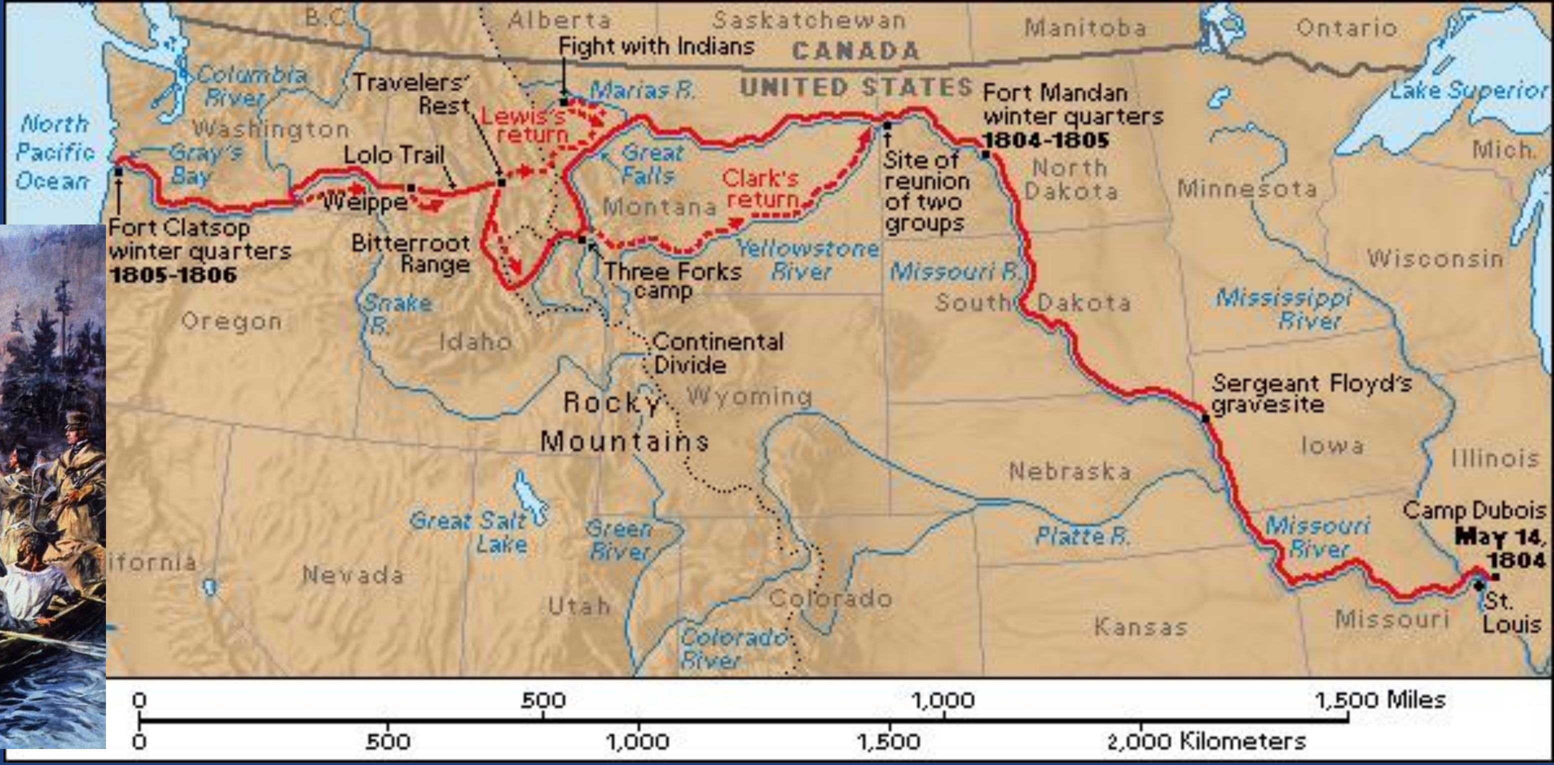
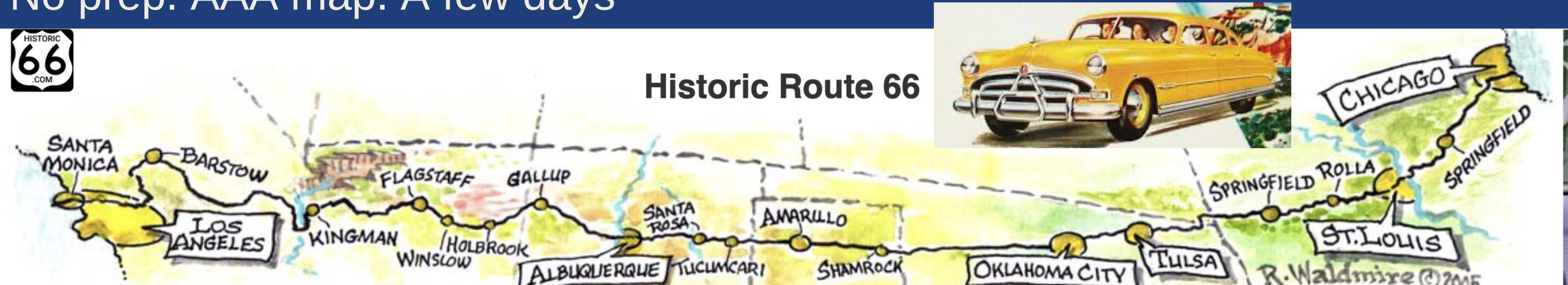




Route 66, 20th Century

No prep. AAA map. A few days

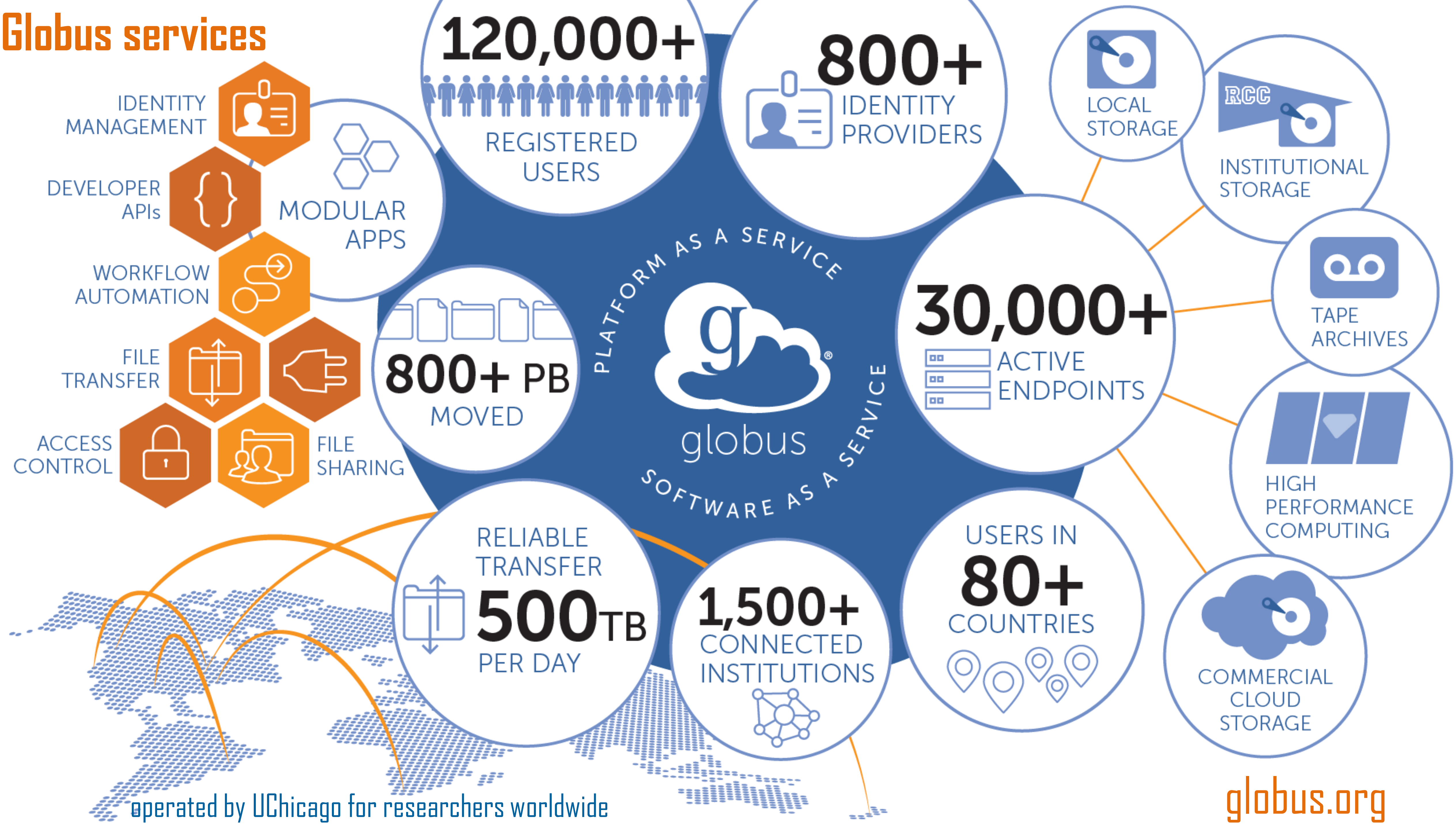


Route 66 crosses IL, MO, KS, OK, TX, NM, AZ and CA

https://www.historic66.com

Higgs discovery “only possible because of the **extraordinary achievements** of … **grid computing**”—Rolf Heuer, CERN DG

Globus services



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Takeaway lessons

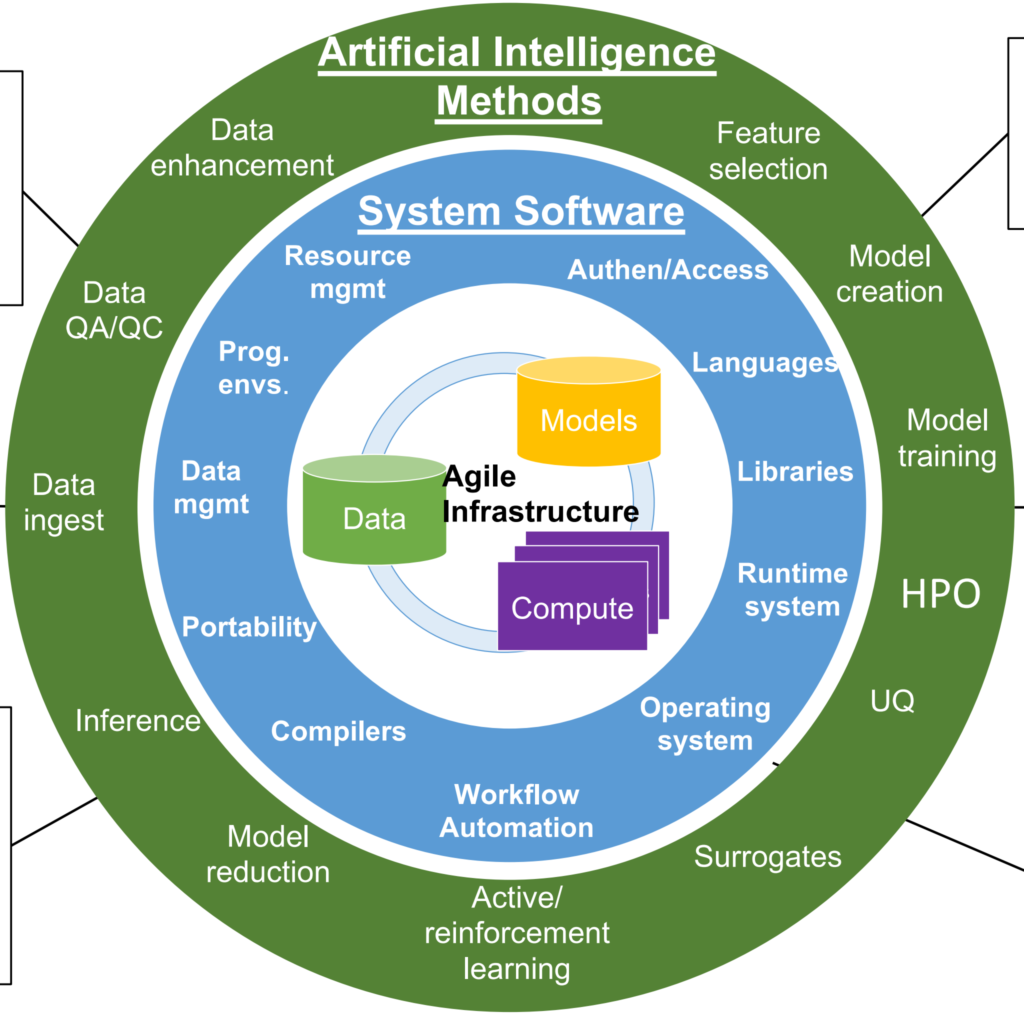
- **The power of platforms**
- **The power (but also the cost) of quality**
- **The power of combining public cloud & science resources**
- **The need for sustainability so that projects can build with confidence**
- **Subscriptions as a sustainability model that works**
- **The need to address the economies of scale**

New instrumentation and AI methods require new platform services

<u>Scientific instruments</u>
Major user facilities
Laboratories
Automated labs
…

<u>Sensors</u>
Environmental
Laboratories
Mobile
…

<u>Databases</u>
Reference data
Experimental data
Computed properties
Scientific literature
…



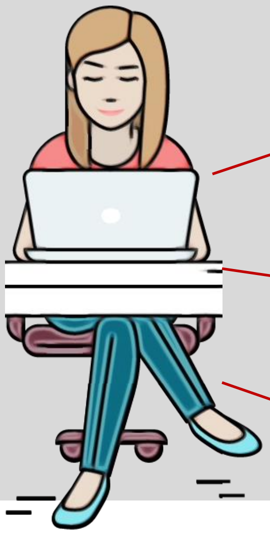
<u>Simulation codes</u>
Computational results
Function memoization
…

<u>Industry, academia</u>
New methods
Open source codes
AI accelerators
…

<u>Scientists, engineers</u>
Expert input
Goal setting
…

Model registry	DLHub
Flows	Automate
Write programs	Parsl
Cost map	SCRIMP
Function fabric	funcX
Data fabric	Data services
Trust fabric	Auth

Next steps: Automated discovery engines. E.g., for materials



Give me a **polymer dielectric** with dielectric constant >10, energy density > 30 J cm^{-3}, breakdown strength > 700 MV m^{-1}, efficiency > 95%

Give me a **solid-state electrolyte** with current density >10 mA cm^{-2}, high stability, low toxicity, moderate cost

Give me a **semiconductor** with bandgap suitable for photovoltaics

Composition, properties, synthesis pathway

Materials Analytics and Design Engine

Organism Designer

Physics Comprehension Sys.

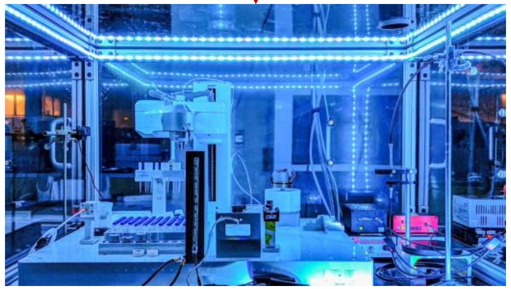
. . .

Self-driving laboratory

AI for scient. program.

Generalized inverter

. . .



- Incorporate state-of-the-art methods for simulating complex materials systems
- Learn continuously as new data are obtained from simulations, experiments, and the literature, transferring knowledge across materials systems

Our goal is to make all research data reliably, rapidly, and securely accessible, discoverable, and usable.

https://labs.globus.org

Relevant references

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