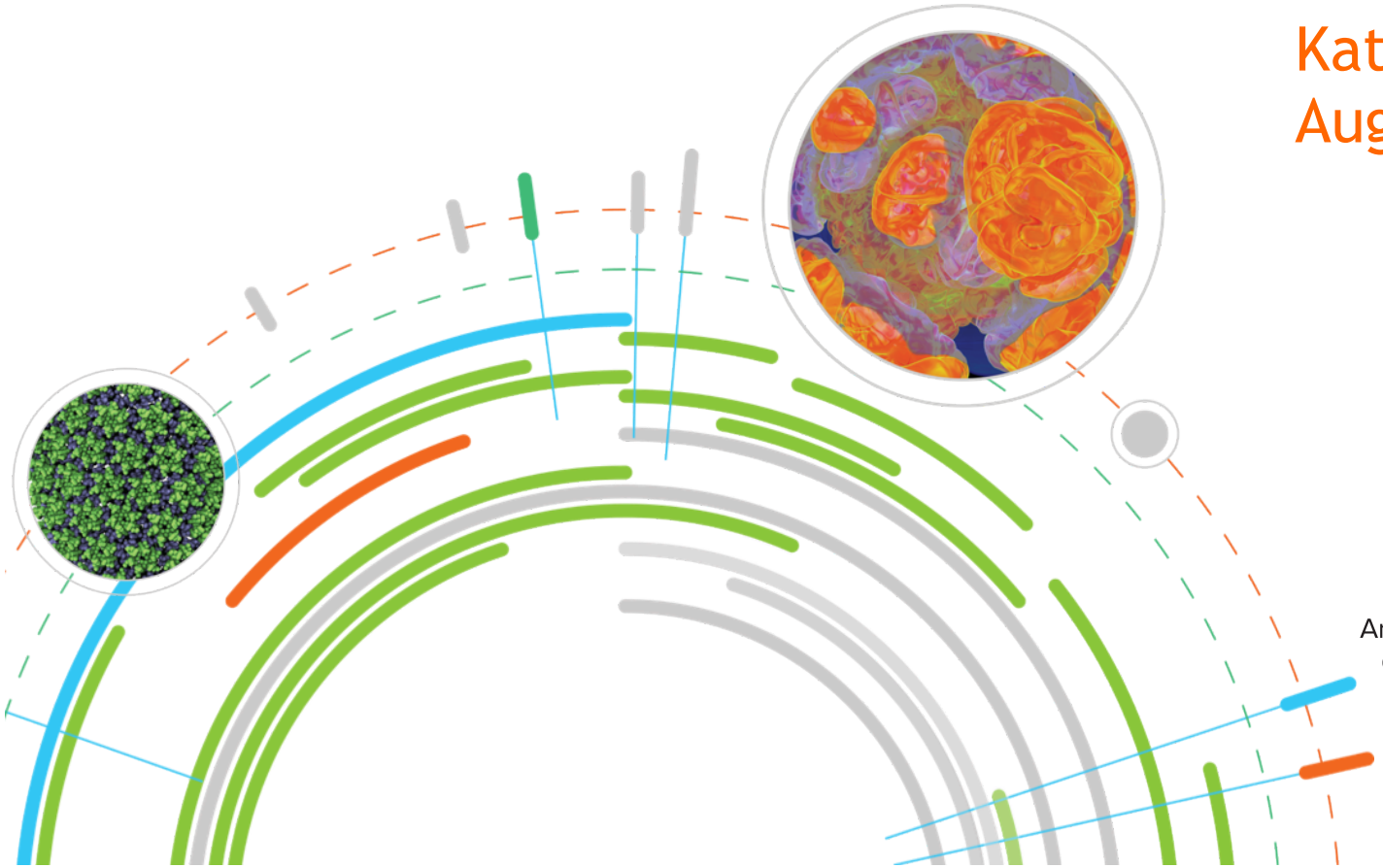
Why are the biggest supercomputers so challenging?

Balancing Software Engineering

Katherine Riley
August 14, 2013



Argonne **Leadership Computing** Facility

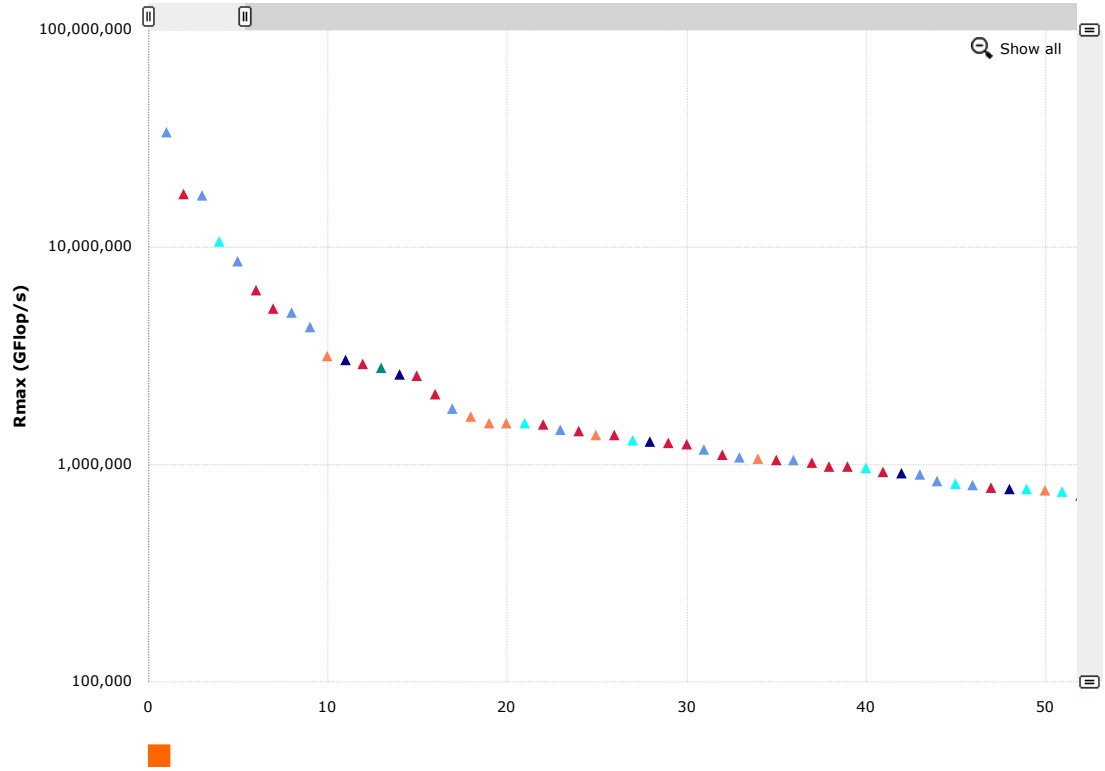
Argonne NATIONAL LABORATORY

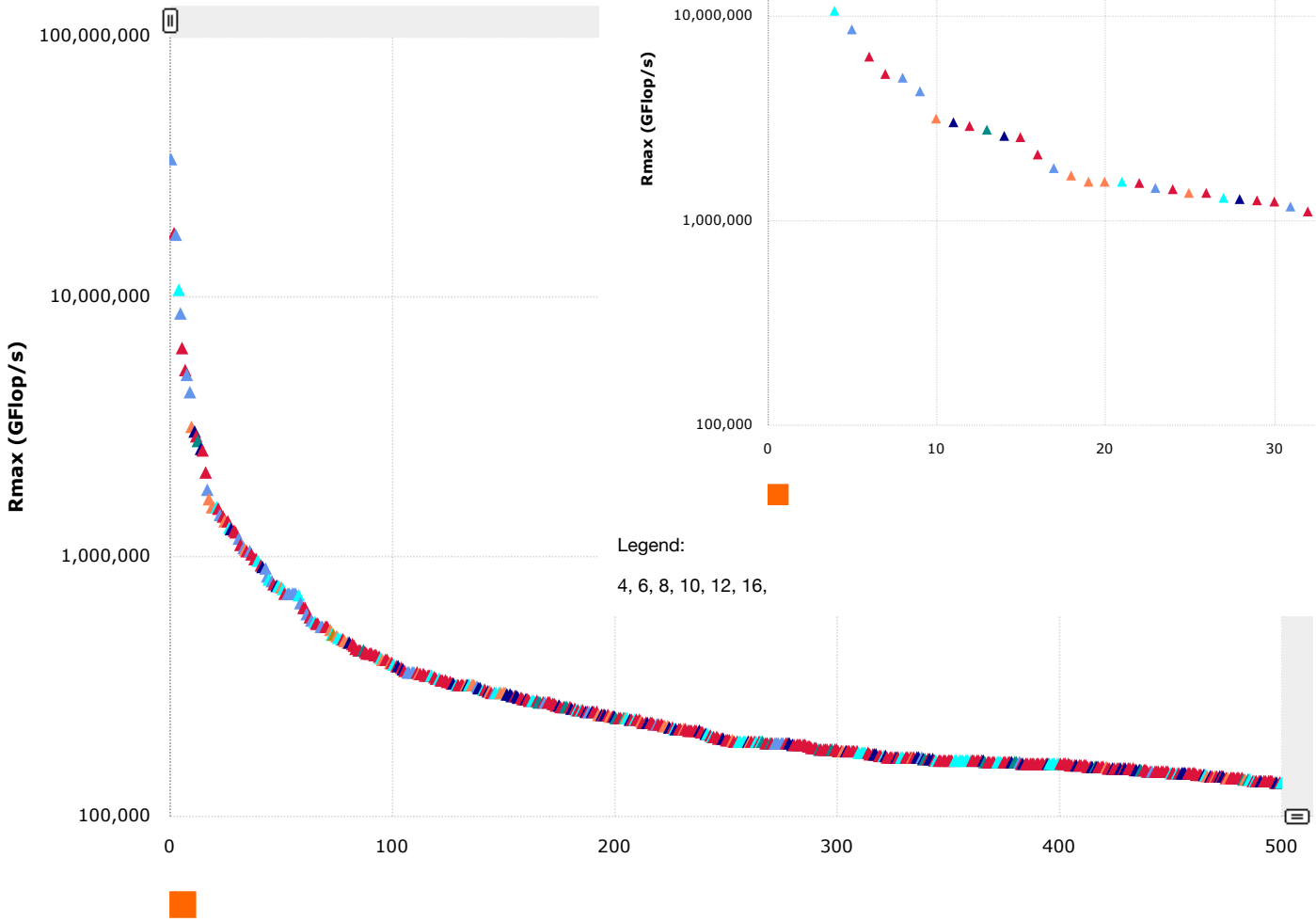
Define a supercomputer

"A supercomputer is a computer at the frontline of contemporary processing capacity – particularly speed of calculation which can happen at speeds of nanoseconds" - Wikipedia

- But not all supercomputers are as 'frontline' as others
- This makes the ecosystem … challenging.

Top 500 Comment





Legend:

4, 6, 8, 10, 12, 16,

Legend:

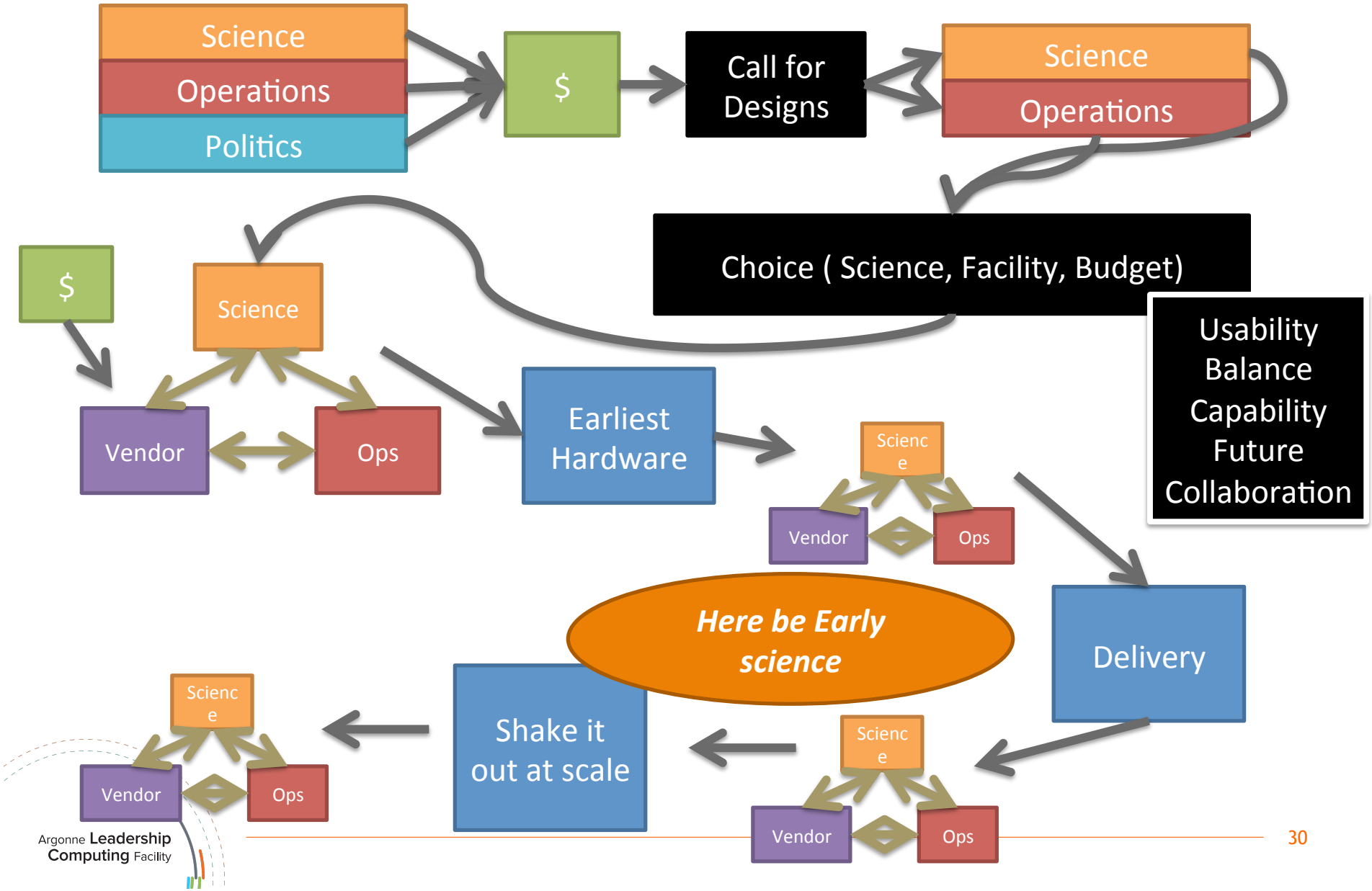
4, 6, 8, 10, 12, 16,

Top few vs Top 500

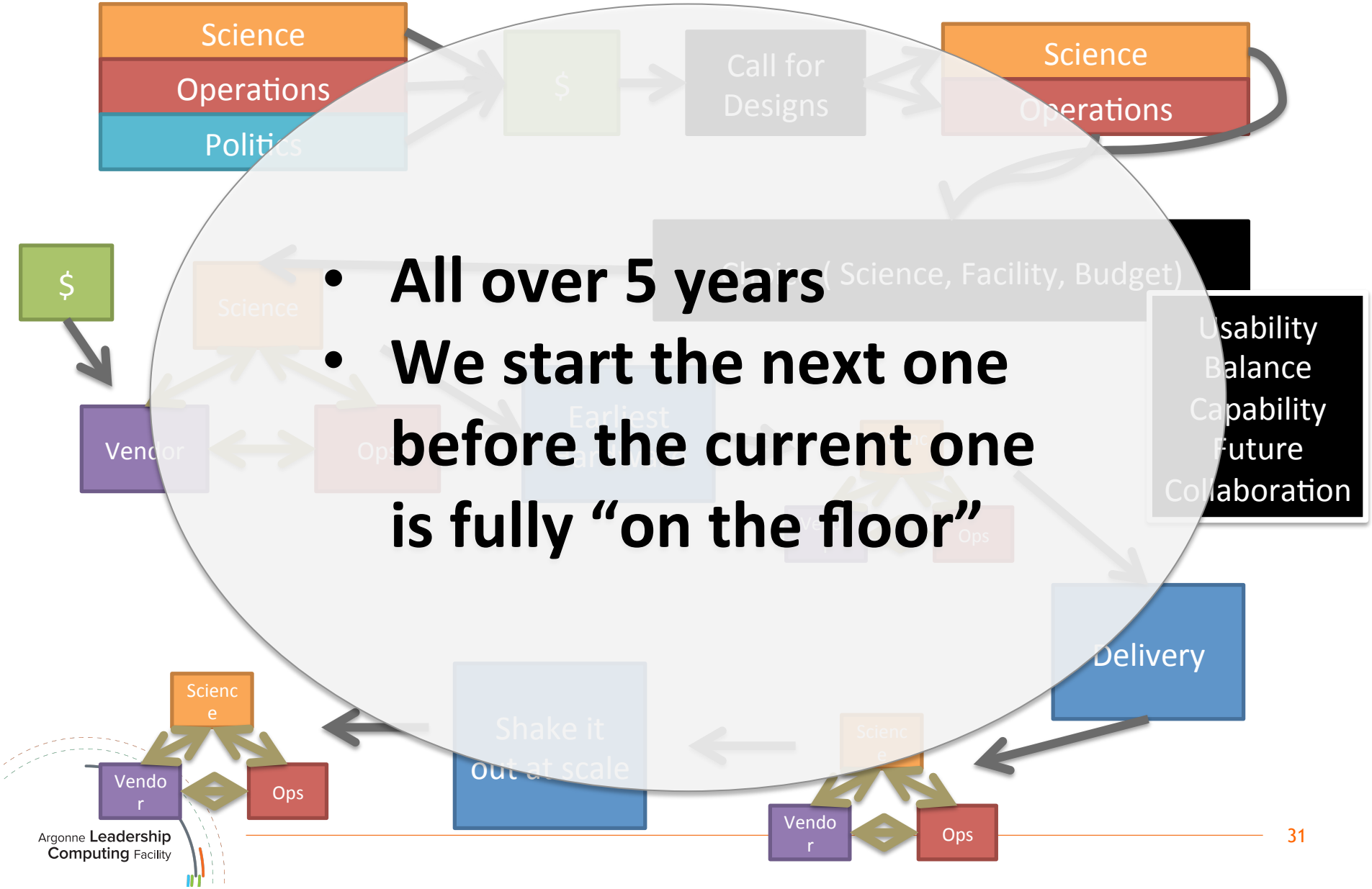
- There are not many huge supercomputers
- The biggest supercomputers are bleeding edge
  - Hardware is sort of hardened in install
  - Software is flushed out over the first year or two
  - What I consider normal, many might consider HOSTILE

- Why is That?
  - Reputation
  - Move science forward
    - Machines are targeted to a small number of users
  - Help steer technology

How is a big DOE supercomputer purchased?



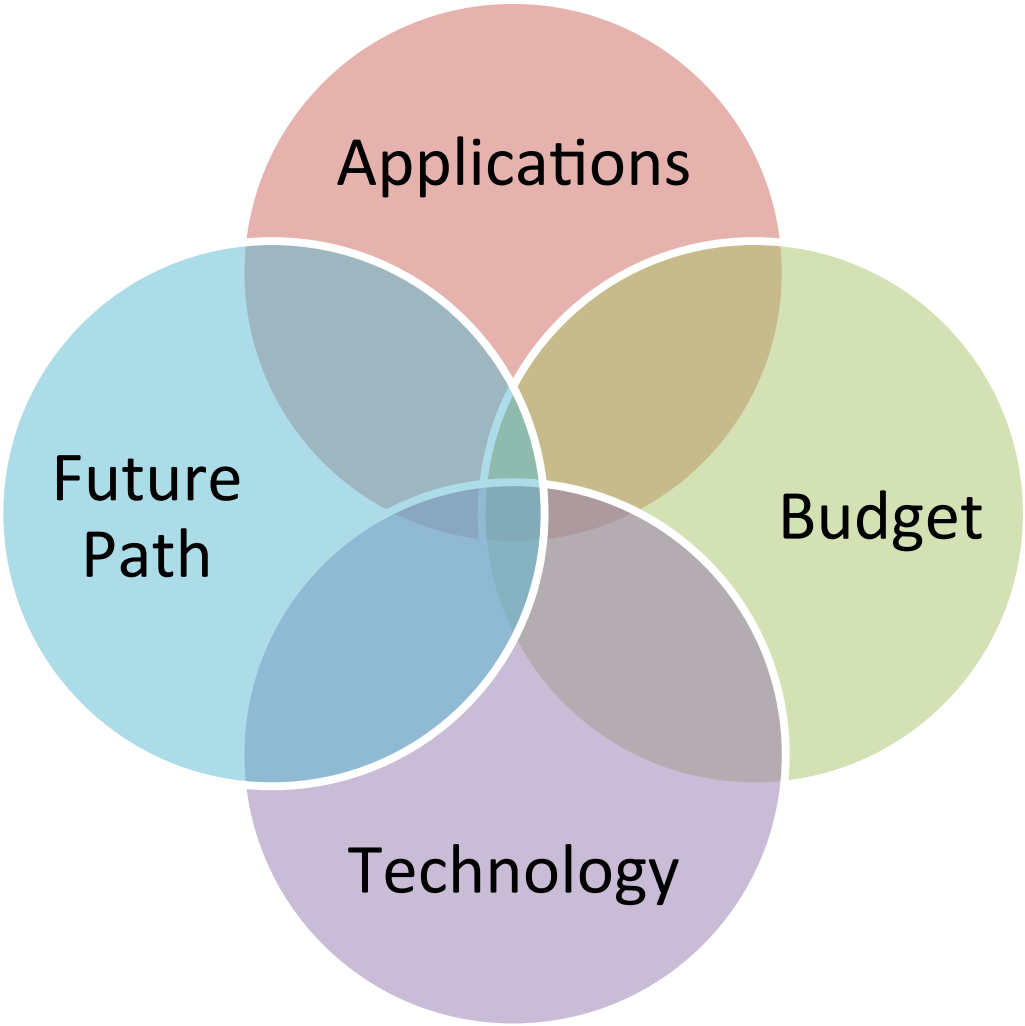
How is a big DOE supercomputer purchased?



- **All over 5 years**
- **We start the next one before the current one is fully "on the floor"**

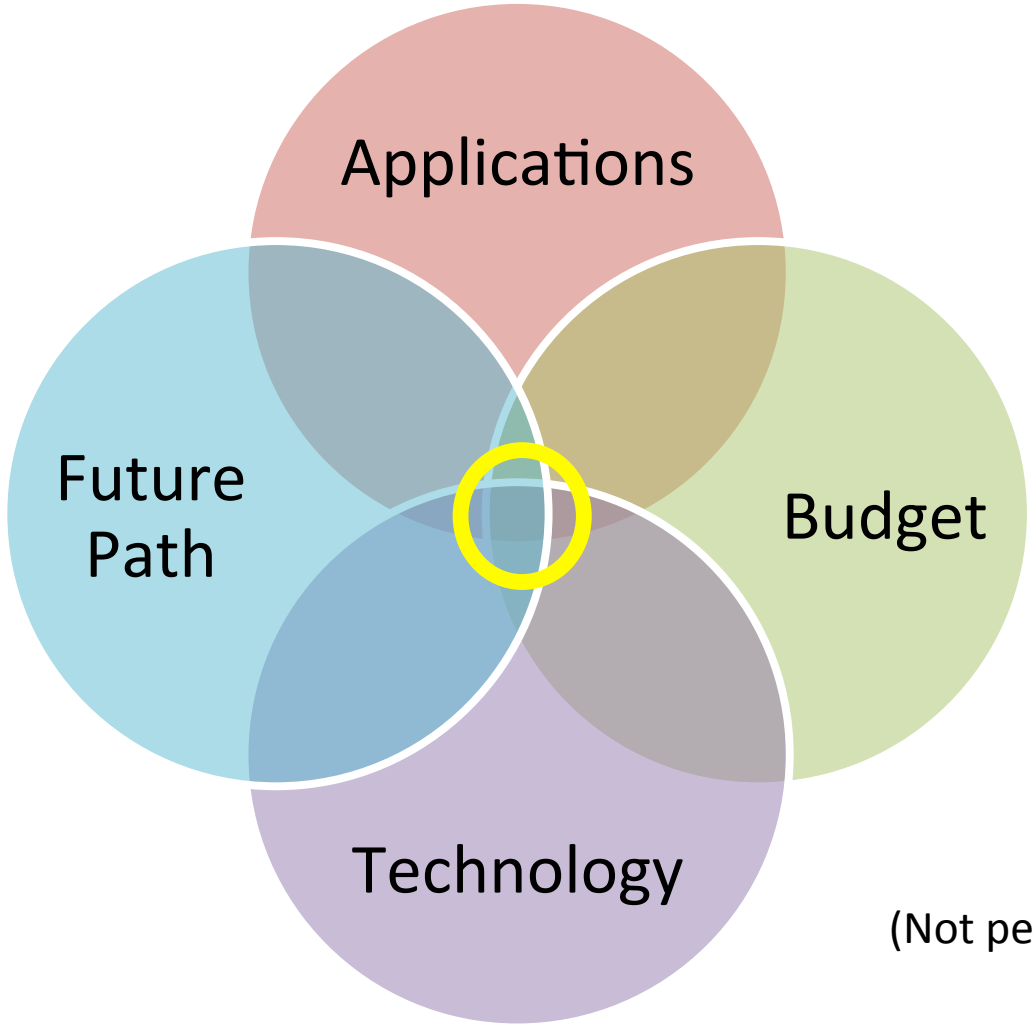
Collaboration does not yield perfection

- Even with all these iterations with the vendor, the machine will not be perfect



Collaboration does not yield perfection

- Even with all these iterations with the vendor, the machine will not be perfect



(Not perfectly weighted)

What this means for your SW ecosystem?

- Bleeding edge systems are their own fun
- The system is available for production REALLY near to it's first construction
  - Early science buffers this, but not completely
  - It takes time to move software to a new architecture at a new scale
  - Even earliest access won't really resolve this
  - Vendor does not have a significant leg up
- As SW on a machine stabilizes, the machine reaches end of life

- The available software will be bare bones
- Complicated requirements can slow you down
- Facilities tries very very hard to expand that as fast as possible

Why Engineering Principles are Crucial

- Testing of your software is crucial
  - You might have a better process than library developers & vendors
  - Defense against other people's bugs
- Versioning
- Abstraction of functionality
  - To address the speed of change
  - Help debug problems
  - Help with performance
- Document to help us help you
- Running on the biggest systems is a competitive advantage
  - Own all of your code. Even libraries.

- Let the compiler do the work with limits
- Use high level languages with care

Questions