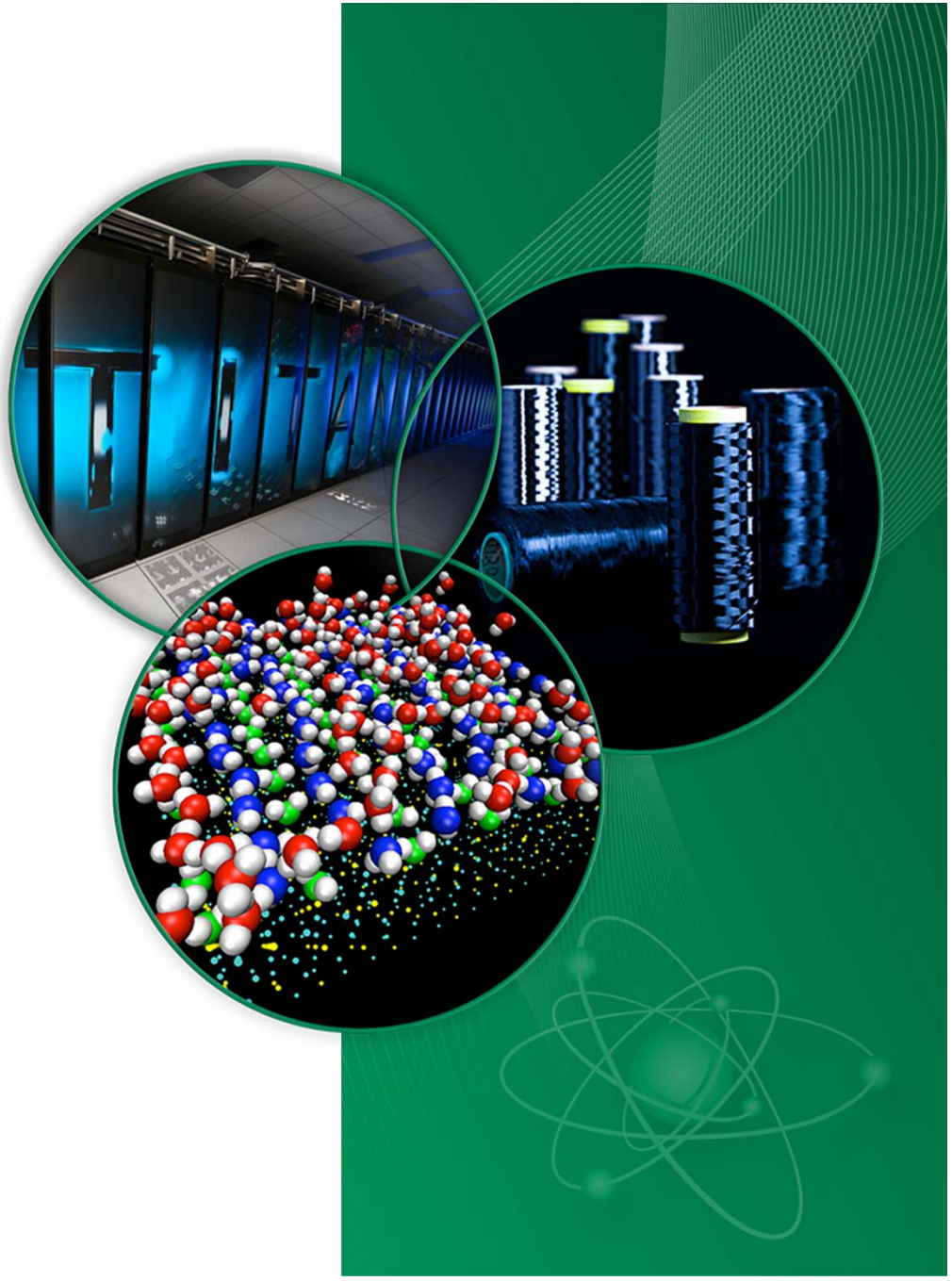
Software as Instrumentation for Computational Research



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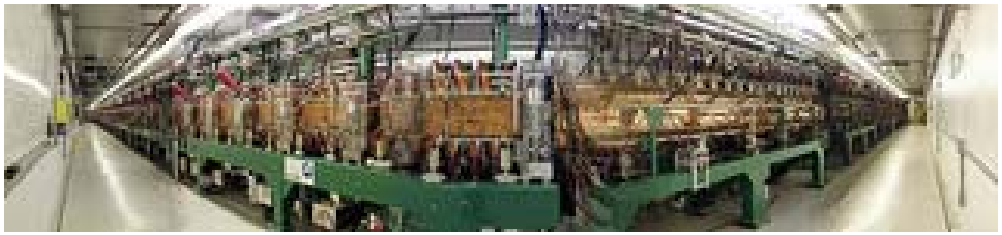
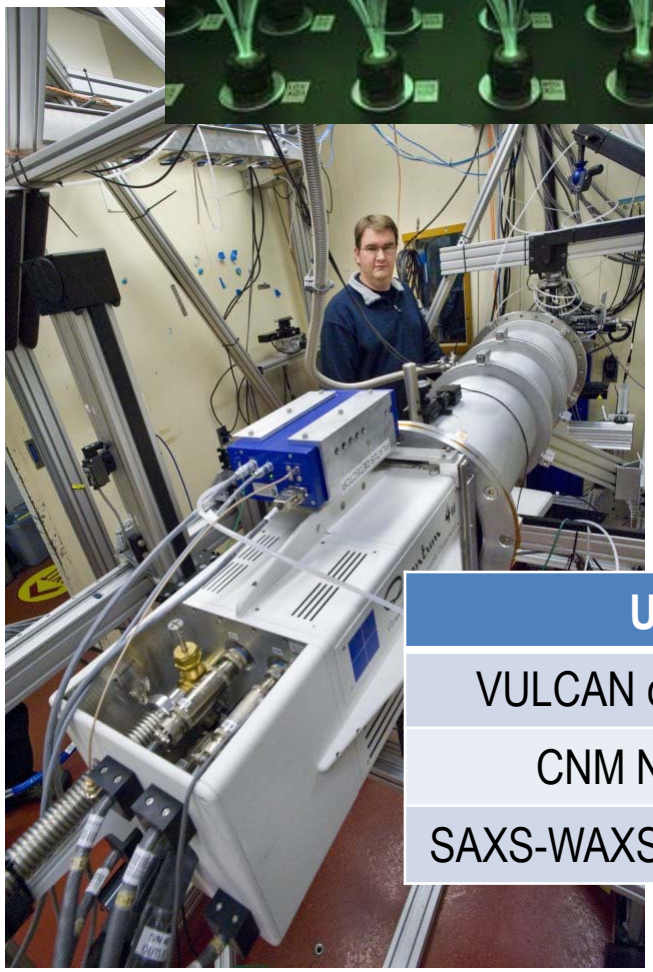
What Do These Things Have in Common?



DOE User Facilities	
SNS	OLCF
ALCF	APS
ALS	NERSC

How Far Does the Analogy Extend?



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User Facility Instrumentation	
VULCAN diffractometer @ SNS	? @ OLCF
CNM Nanoprobe @ APS	? @ ALCF
SAXS-WAXS x-ray scattering @ ALS	? @ NERSC

Characteristics of Instrumentation Projects

Experimental

- Complex, long-term R&D activity
- Developed and maintained by teams of researchers
  - Users & developers partly overlap
- Serve community
  - Users require support
- Entire lifecycle managed as a single project
- Focus on development and support of instrument
  - Users do science

Computational

- Complex, long-term R&D activity
- Developed and maintained by teams of researchers
  - Users & developers partly overlap
- Serve group(s), community
  - Users require support
- Lifecycle spans multiple projects
- Focus on science
  - Software (instrument) is a by-product
  - Support is not even mentioned

Note: Not all computational science applications reach the level of "instrumentation"

Some Questions to Ponder…

- Will the current science-first funding model take computational science where it needs to go in the future?
- Should large-scale scientific software be treated more like experimental instruments
  - By funding agencies?
  - By developers?
- How do we institute necessary changes?
  - New funding model necessary? Sufficient?
  - Change thinking of grant proposal reviewers? How?
- Are research leaders prepared to follow changes in the funding model?
  - Are they too entrenched in the science-first mode?
- Are current reward systems adequate/appropriate?
  - What changes are needed?
  - How to institute them?