



Numerical Reproducibility Challenge



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Experimental or Scientific Reproducibility

- *Foundational assumption of the Scientific Method*
- Essential goal
 - Requires practices, organizational & others, that go beyond purely technical ones.
- Doug James, Nancy Wilkins-Diehr, Victoria Stodden, Dirk Colbry, and Carlos Rosales (Principal Editors). Standing Together for Reproducibility in Large-Scale Computing: Report on Reproducibility@XSEDE. July 2014.

Numerical Reproducibility

- *Foundational assumption in Computational Science*
- Computing is the “Third Leg of Science”
Ken Wilson, 1987
- Obtain *same* results on different machines

Predictable Hardware

- Operational assumptions
- IEEE floating point standard (IEEE 754-2008)
- Single core, single threaded
- ...
- Numerical reproducibility “straight-forward”

Unpredictable execution order

- Out of order execution
- Multicore architectures
- Special purpose accelerators
- Intel Xeon Phi & Intel Xeon Knights Landing
- FPGAs
- Unreliable systems

Workshops:

- ICERM, Brown U., 2012 & 2014
- SC13 workshop

Solution Approaches

Better algorithms

- Extended precision
- Numerically stable algorithms
- Uncertainty quantification

Computational measurements

- Associate uncertainties with results
- **Stochastic algorithms**
- **Ensemble runs**

NRE2015: Numerical Reproducibility at Exascale

- SC15 workshop
- Friday, Nov. 20, 2015; Austin, TX
- Co-organizers
 - Michael Mascagni & Walid Keyrouz
- Plenary speakers
 - Mike Heroux (Sandia)
 - David Bailey (UC Davis)