Managing Computational Experiments

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Better Scientific Software tutorial @ NOAA Global Systems Laboratory

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- **The requested citation the overall tutorial is:** David E. Bernholdt, Anshu Dubey, and Patricia A. Grubel, Better Scientific Software tutorial, in NOAA Global Systems Laboratory, Boulder, Colorado, 2023. DOI: 10.6084/m9.figshare.23796606.
- Individual modules may be cited as *Speaker, Module Title*, in *Tutorial Title*, …

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Running simulations for science discovery is more of a craft and less of science. More than any other aspect of computational science it relies on experience and acquired wisdom that helps one develop a nose for fruitful possibilities.

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  - Operating them is also very expensive
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In the 2005 simulation mentioned earlier, out of 5 teams, ours was the only team that had success in getting a good science outcome

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How do you plan

- Focused verification of the target simulation on the target platform
  - Over and above regular testing
  - Emphasis on understanding solver validity regime

- Pathfinder runs to get a good estimate of needed resources
  - Cost benefit analysis of fidelity vs reaching science goals in allocated resources

How do you plan

- Develop helpful diagnostics
  - Low overhead ways of confirming the health of the run
    - Are conserved quantities conserved?
    - Has any quantity become unphysical?

- Develop hierarchy of analysis
  - Full analysis of runs is not feasible in flight
  - Intermediate level analysis can give further insight into health of the simulation

Story of one simulation campaign

- Theory of Type Ia supernova explosion – 2006/2007
  - Evidence from observations:
    - Light curve powered by Ni56 decay
    - Evidence of medium weight elements, but in much smaller quantities
  - Implied transition from deflagration to detonation
- A 2D exploratory run had given a tantalizing answer to how?
  - To confirm a full 3D run was needed at good enough resolution
  - It would be the largest run of its kind at the time – totally uncharted territory
  - Until then 3D runs had been octants relying on symmetry
    - The 2D run had shown that symmetry had to be avoided

Preparation Steps

- Step 1 – develop a test that represents the most complex physics interactions
- Challenges:
  - Features take a long time to develop
  - Want to ensure that at least one refinement step occurs during the test
  - IO too slow to restart from a large checkpoint at late stage of the run
    - Also test would need a large chunk of the machine
- Use physics understanding to create initial conditions that would quickly develop comparable complexity

Preparation Steps

- Step 2 – Use the new test to characterize the performance behavior of the target platform
- Motivation:
  - Standard performance studies could not give crucial information
  - AMR refinement patterns make each application different
  - Interoperability and trade-off opportunities needed to explored in a closely resembling simulation behavior
- Full fidelity 2D runs, and a set of runs of the new test provided enough information to extrapolate and estimate needed CPU hours

Preparation Steps

- Step 3 – Look for trade-offs and optimization opportunities
- Motivation:
  - Initial CPU estimates too high to complete the runs within allocations
  - Exploration of any parameter space needs to minimize individual run times
- Many opportunities were found, documented in reference below.
  - Identify redundant refinement and get rid of it
  - Coarsen computations for some physics
  - Move some computations to post-processing
- **All optimizations were based on scientific and numerical intuitions**

Dubey A, Calder AC, Daley C, et al. Pragmatic optimizations for better scientific utilization of large supercomputers. The International Journal of High Performance Computing Applications. 2013;27(3):360-373. doi:10.1177/1094342012464404

Preparation Steps

- Step 4 – Prepare diagnostics and quick analysis mechanism
- Examples-- diagnostics
  - Conservation of mass, momentum energy
  - Changes in dt recorded in the logfiles
  - Spikes in variable values
- Examples – quick analysis
  - Quick visualization of random 2D slices
  - Inspection of critical quantities in 1D

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Lab notebook artifacts

- every run registers all configurations and runtime parameters in a logfile.
- logfiles are cumulative
- dedicate space for storing all results in a preconfigured directory structure
- scripts to move output from scratch to the dedicated space

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- A successful campaign
  - But not without hitches
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- A successful campaign
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- Optimization related runs were not given the same level of care
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- For the paper the referee asked for details from optimizations
  - We did not have them
  - Fortunately the referee was satisfied with reasoning and other supporting evidence we produced

Summary and Takeaways

- Good science with computation is a craft -- training is needed in how to do it
- Machines are expensive to build and expensive to run
  - They provide opportunity for great work
  - Care is needed to ensure that the outcome meets expectations
- Reproducible results are a necessity, not a luxury
  - There is no credible science without provenance

"a parameter combination that induces erroneous results is easily selected"
- https://doi.org/10.1063/1.476021

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