Issues Raised by Extreme Heterogeneity in Analytics

ASCR Extreme Heterogeneity Workshop

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Data: Product or Source?

Modeling/simulation: Solution to equations produces data.

Navier-Stokes momentum equation (convective form)

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u} + \frac{1}{3} \nu \nabla (\nabla \cdot \mathbf{u}) + \mathbf{g}.
\]

Data Analytics: From data, derive a model, model parms, quantitative information.
Heterogeneity in Use Cases, Data Sources

• Distributed collection of multi-modal sensors, produce curated data products (e.g., ARM/PNNL)
• Science user facility, individual experiments that produce data (e.g., ALS/LBNL, LCLS/SLAC, APS/ANL, SNS/ORNL, ...)
  • Near-instrument processing
  • At-HPC center processing
  • Complex, multistage data-centric processing needs
  • Data lifecycle concerns
• Traditional computational science, simulation and modeling
  • Scale: Individual PI/project team, community-wide efforts
  • Data lifecycle concerns
• Lots of others:
  • Precision, personalized medicine
  • Cybersecurity, facilities operations
Heterogeneity in the Way Data is Used

- Datasets that are input to a method or aggregation
  - Hypothesis testing, discovery
- Collections that promote and facilitate scientific advances
  - Produced, shared by a community (e.g., AR, CMIP, SDSS, ...)
- For training
  - Curated collections of labelled data for training supervised ML
- For optimization
  - Tune, optimize experiments
- For inference and prediction

- Note #1: the close symbiotic relationship (synergy) between data and compute
- Note #2: software and parameters are also “data”

Industry view (probably biased). More info: t.co/pXhCFOFvUz t.co/40ykMOLvNr. We need a similar diagram for science uses of data.
Heterogeneity in Methods and Software Environment (Partial View)
Analytics: Performance and Portability

• **Individual methods:**
  - Statistical/quantitative analysis, feature detection, learning, inference, visualization, ...
  - Portable node-level parallelism, hybrid parallelism
  - Write once, run everywhere
    - X86, GPU, FPGA, TPU, NM, ...

• **Potential paths:**
  - Traditional BSP design pattern:
    - MPI+X: where X provides for portable node-level parallelism
      - OpenMP 4.5: offload code onto accelerators (from FSD)
  - Alternate design pattern:
    - UDF in “hosted” environment or runtime system
      - Spark, TECA/DAGR, Legion, etc.
    - Traditional HPC vs. ”Big Data” software stack

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<th>EH Trends</th>
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Analytics: Performance and Portability

• **Aggregations of methods:**
  • A sequence of individual methods
  • Data model and data movement issues
  • Resource marshaling and provisioning issues
  • Heterogeneous components:
    • OTS segmentation -> custom feature detection -> TensorFlow inference

• **Potential paths:**
  • Traditional workflow: Kepler, Tigris, etc.
  • Wide area (data movement): Globus, etc.
  • Analytics “environments”:
    • TensorFlow [, Caffe, PyTorch, ...], Jupyter, ...
    • UDF-based (TECA/DAGR, ArrayUDF, Spark, ...)

• Note: these could be considered “workflow” issues, which Ewa will discuss next

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Analytics: Reproducibility and Repeatability

• Desired outcome:
  • Yourself and others can reliably reproduce results of a computation

• What are the components?
  • Data, code, system environment (h/w, s/w)
    • Source code for methods: C++, Python, ...
    • Environment: compiler, O/S, software environment (TensorFlow, PyTorch, MPI, VisIt, ...)
    • DNN network topology, CART topology, etc.
    • Problem configuration: processing steps, ordering, parameters (layer weights, etc.), ...

• Why is it important?
  • Integrity of scientific results
  • Basis for comparison of new methods: is the new method any better?
  • Preservation of knowledge

• How are we going to do this?
Closing Thoughts

• How to achieve performance and portability: 5, 10, 20 yrs?
  • Researcher/developer viewpoint
  • Scientist/consumer viewpoint

• Do we need abstractions for memory and storage hierarchy?
  • E.g., language-level constructs in CUDA

• Or do we let the language/compiler/environment take are of this?
  • PGAS memory model
  • Spark data/memory management

• Diversity in resources, policies and its impact on deployment, operations

• Tradeoffs between wanting to facilitate innovation, research and having a stable, predictable, maintainable ecosystem

• What can we “count on” being there for us in 5, 10, 20 yrs out?

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