Achieving production-level use of HEP software at the Argonne Leadership Computing Facility

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Mira - Leadership-class Supercomputer at Argonne
Why use Mira for HEP?

- The HEP community is a leader in deploying grid computing
  - ~3 billion core hours delivered by grid each year
- Run II will demand a significant increase in computing resources
- Supercomputers will be an essential platform
  - to expand the computing resources available
  - to absorb spikes in computing demand
  - to produce events for complex processes not currently possible on the grid
- We are adapting legacy HEP codes to run on today’s (and tomorrow’s) supercomputers
Applications running on Mira

- Over the past two years, we have adapted several HEP codes to run on Mira
  - Alpgen
  - Sherpa
  - Pythia
  - MCFM
  - Geant4

- But which codes can we run in parallel on Mira?
  - Event generation codes are a good choice
- How to integrate with PanDA?
Adapting Alpgen to run on Mira

- Mostly straightforward compilation
- Use MPI ranks to determine random seeds
- Use MPI to distribute input data (configuration + grids + pdf)
- Decomposed execution into serial and parallel portions

1. integration
   x86 cluster

2. event generation
   Mira

3. unweighting
   x86 cluster
Adapting Alpgen to run on Mira

- Mostly straightforward compilation
- Use MPI ranks to determine random seeds
- Use MPI to distribute input data (configuration + grids + pdf)
- Decomposed execution into serial and parallel portions
- Coupled event generation and unweighting in single Mira job
Adapting Alpgen to run on Mira

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- Decomposed execution into serial and parallel portions
- Combined event generation+unweighting+aggregation
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Mira status page showing Alpgen running on the entire machine (1.5M processes)

For more details on adapting Alpgen for Mira, see Taylor Childers’ CHEP2015 talk
Simulation of LHC events on a million threads (#536)
How to integrate with PanDA?
How to integrate with PanDA?

- A job management service, Argo, runs within ANL–HEP domain to control job execution
  - Stores Athena job description
  - Submits integration job to x86 cluster
  - Submits event generation + unweighting job to Mira
  - Converts to pool files
  - Sends files to the grid
- Python/Django-based, backed with MySQL (or other databases)
How to integrate with PanDA?

- A job execution service, Balsam, prepares and runs jobs on target resources
  - Subscribes to job message queue
  - Stages in job input
  - Submits job to schedulers (Condor, Cobalt, Torque)
- Monitors running job
  - Stages job output to specified destination
  - Sends completion message to message queue
- Python/Django-based, backed with MySQL (or other databases)
Integration with PanDA

- PanDA
  - Argo
    - message queues
      - Balsam
        - integration
          - x86 cluster
        - event generation
        - unweighting
        - MPI-IO aggregation
      - Mira
        - compute node ramdisk
          - 1
          - 2
          - 3
          - 4
Progress using 50M hour ALCC award

HadronSim
Machine: MIRA
Allocation: 50,000,000
Usage: 34,234,852.67 (68.5%)
2014-07-01 to 2015-04-12

On track to use full allocation

16K+ nodes
8K+ nodes
<8K nodes
Next in Queue

- Working with PanDA team to build pilot job runner
- Integrate Sherpa
  - Sherpa has long been running on Mira, and has run through Argo
  - Scales to ~512 nodes; running as 256-node subjobs within larger jobs
  - Working (with Stefan Hoeche) to scale event generation to larger sizes
- Consider integrating Pythia
  - Pythia has long been running on Mira, and has run through Argo
  - Large memory footprint (2GB) initially restricted execution to 4 cores per node
  - Use LHAPDF6 to reduce memory footprint to 200MB: 64 cores per node now possible (LHAPDF5 reserves space for large uninitialized memory that bloats executable size)
Mira - Allocation Process

- How do projects get allocations on Mira?
  - Through a competitive proposal process operated by the U.S. Department of Energy
  - Open to projects worldwide
  - 5B hours awarded at Argonne in 2015
- INCITE program: 60%
  - Granted at DOE level
  - Largest, most strategic and most mature projects
- ASCR Leadership Computing Challenge (ALCC) program: 30%
  - Granted at DOE level
  - For projects vectored toward INCITE proposals
- Director’s Discretionary: 10%
  - Small startup allocations granted by ALCF director
Summary

- We are running Alpgen on the 49,152 nodes on Mira, the 10PFLOPs supercomputer at Argonne
- Using Argo and Balsam, we have used 34 million core hours on Mira (16 million more hours remaining this year)
  - Produced tens of millions of Alpgen events
  - Producing high multiplicity events (w/z+5, w/z+6) that can't be generated on the grid today
  - ANL/HEP is now the primary Alpgen event generation site for ATLAS
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