Harvester: non-HEP experiments

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pandawms.org update

- PanDA Server has been upgraded to a latest version
- Database has been updated with tables necessary for support of Harvester
- Some queries originally written for Oracle were ported to MySQL
- job submission works correctly, correct communication with Harvester (jobs fetching, status update)
- tested for compatibility with plain old pilot launcher (tested with LQCD jobs on BNL Institutional Cluster)

nEDM challenge fragment

| Pavlo Svirin / 16 | | | | | | | | | | | |
|--|----------------|--|----|--------|----------|--|-----------|-----------|--|-----------------------|-----|
| Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 | | Svirin / | 16 | #json# | starting | | 0:0:00:52 | 0:1:34:34 | | ANALY_ORNL_Titan_nEDM | 986 |
| Pavio Svirin / Isst 16 | | Job name: b1e117a6-4f70-42c9-af8c-967e552191fc #0 | | | | | | | | | |
| Svirin | | Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 | | | | | | | | | |
| Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Pavlo Svirin / Isst | Attempt 0 9774 | Svirin / | 16 | #json# | failed | | 0:1:08:55 | 0:0:02:32 | | ANALY_ORNL_Titan_nEDM | 986 |
| Pavlo Svirin / Isst | | Job name: 7330e63c-a838-4dba-aa6a-9ca65a799d28 #0 | | | | | | | | | |
| Svirin / Isst 16 | | Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 | | | | | | | | | |
| Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Pavlo Svirin / 16 #json# running 2018-02-25 23:47 0:1:32:43 0:0:02:43 02-26 01:20 ANALY_ORNL_Titan_nEDM 986 Job name: 64ec0ad1-5197-41c9-bd39-d9a09c9828bc #0 Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Pavlo Svirin / 2 #json# finished 2018-02-25 22:57 0:0:30:56 0:0:02:31 02-25 23:40 ANALY_ORNL_Titan_nEDM 987 Job name: 6ac84a9f-d3bf-4a97-af9a-ad653e8157ae #0 | | Svirin / | 16 | #json# | holding | | 0:1:25:34 | 0:0:02:42 | | ANALY_ORNL_Titan_nEDM | 986 |
| 9775 Attempt 0 Pavlo Svirin / Isst | | Job name: beb0e06e-b866-4e7e-8006-b33d5c76f4c0 #0 | | | | | | | | | |
| 9775 Attempt 0 Svirin / lsst 16 #json# running 2018-02-25 23:47 0:1:32:43 0:0:02:43 02-26 01:20 ANALY_ORNL_Titan_nEDM 986 Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Pavlo Svirin / lsst Pavlo Svirin / lsst Pavlo Svirin / lsst Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Job name: 6ac84a9f-d3bf-4a97-af9a-ad653e8157ae #0 | | Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 | | | | | | | | | |
| Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 Pavlo Svirin / Isst | Attempt 0 9767 | Svirin / | 16 | #json# | running | | 0:1:32:43 | 0:0:02:43 | | ANALY_ORNL_Titan_nEDM | 986 |
| 9767 Attempt 0 Pavlo Svirin / lsst 2 #json# finished 2018-02-25 22:57 0:0:30:56 0:0:02:31 02-25 23:40 ANALY_ORNL_Titan_nEDM 987 Job name: 6ac84a9f-d3bf-4a97-af9a-ad653e8157ae #0 | | Job name: 64ec0ad1-5197-41c9-bd39-d9a09c9828bc #0 | | | | | | | | | |
| 9767 Attempt 0 Svirin / Isst 2 #json# finished | | Datasets: Out: panda.destDB.81206256-4e2a-45b8-b263-29eba4c25118 | | | | | | | | | |
| Job name: 6ac64a91-G3b1-4a97-al9a-ad653e8157ae #U | | Svirin / | 2 | #json# | finished | | 0:0:30:56 | 0:0:02:31 | | ANALY_ORNL_Titan_nEDM | 987 |
| Datasets: Out: panda.destDB.1cb268b2-a748-4f2b-a204-30e85a0950d6 | | Job name: 6ac84a9f-d3bf-4a97-af9a-ad653e8157ae #0 | | | | | | | | | |
| | | | | | | | | | | | |

Installation script for Harvester

 It takes ~2 mins to deploy and provide a simple configuration for Harvester with one PanDA queue:

./install-harvester.sh -d ~/harvesters -h TJLab -q ANALY-TJLAB-LQCD -b torque -p /tmp/proxy -c /etc/grid-security/certificates

- Uses latest Harvester from "OLCF_validation" branch
- Uses updated saga_monitor and saga_submitter modules
- Some manual intervention still needed to "submitter" section to tune queue/projectname/etc.
- In case of installation on machine without access to superuser:
 - Steps described how to compile a personal installation for python 2.7.14, pip, virtualenv, sqlite3, curl 7.58.0

panda_harvester.cfg template

```
[master]
                                                [pandacon]
uname = ${USERNAME}
                                                nConnections = 5
gname = ${GROUPNAME}
                                                timeout = 180
loggername = harvester
harvester_id=${HARVESTERID}
                                                ca_cert = ${PATH_TO_CERTIFICATES}
                                                cert_file = ${PATH_TO_PROXY}
                                                key_file = ${PATH_TO_PROXY}
[db]
                                                pandaURL = http://pandawms.org:25080/
database_filename = ${BASE_DIR}/var/
harvester/test.db
                                                server/panda
verbose = False
                                                pandaURLSSL = https://pandawms.org:25443/
nConnections = 5
                                                server/panda
# database engine : sqlite or mariadb
                                                pandaURLProxy = http://pandawms.org:25080/
                                                server/panda
engine = sqlite
# user name
                                                verbose = True
user = harvester
# password
                                                [qconf]
password = harvester@olcf
                                                configFile = ${BASE_DIR}/etc/panda/
                                                EC2_queueconfig.json
# schema
schema = HARVESTER
                                                queueList =
                                                     ${QUEUENAME}
```

Queueconfig template

```
"${QUEUENAME}": {
     "prodSourceLabel":"user",
     "nQueueLimitJob":5,
     "nQueueLimitWorker":5,
     "walltimeLimit": 10,
     "maxWorkers":5,
     "mapType":"OneToOne",
    "preparator":{
          "name": "RseDirectPreparator",
          "module": "pandaharvester.harvesterpreparator.rse_direct_preparator",
          "basePath": "${TOP_DIR}/harvester-preparator"
     "submitter":{
          "name": "SAGAYAMLSubmitter",
          "module": "pandaharvester.harvestersubmitter.saga_yaml_submitter",
          "nCorePerNode": 16,
          "adaptor": "${BATCH_SYSTEM}://localhost",
          "localqueue": "debug",
          "projectname": "Iqcd17q1"
     }, .....
```

Harvester file hierarchy

```
|-- /home/user_home/harvesters
  |-- harvester-messenger
  |-- harvester-preparator
  |-- harvester-worker-maker
  |-- harvester-TJLab
     -- bin
     I-- etc
     |-- include
     |-- lib
     |-- lib64 -> lib
     -- share
     |-- start_harvester.sh
     |-- stop_harvester.sh
     |-- clean_logs.sh
     `-- var
       -- harvester
         `-- test.db
       `-- log
         `-- panda
```

Job descriptions in YAML

- we introduced job description in Yet Another Markup Language (YAML), so users don't have any need to do Python programming
- LQCD and LSST expressed interest in this format

```
seqname: Test_Seq_LQCD
jobs:
    J0B1:
        walltime: "20:00:00"
        nodes: "8000"
        command: |+
          export PMI NO FORK=1
          export CRAY_CUDA_MPS=1
          cd $PBS_0_WORKDIR
          conf_num=0
          for i in \{0...31\}; do
           aprun -n 12 -N 1 ./wrapper1.sh \
                 $((i*12+conf_num*396)) &
           sleep 2s
          done
    J0B2:
sequence:
 J0B1 : J0B2
```

User environment

- Simple user environment developed, independent from experiment
- No programming needed to control or define jobs
- Offers basic job control: pansub, panstat, pankill, panretry
 - Also includes a tool to spawn multiple jobs from template

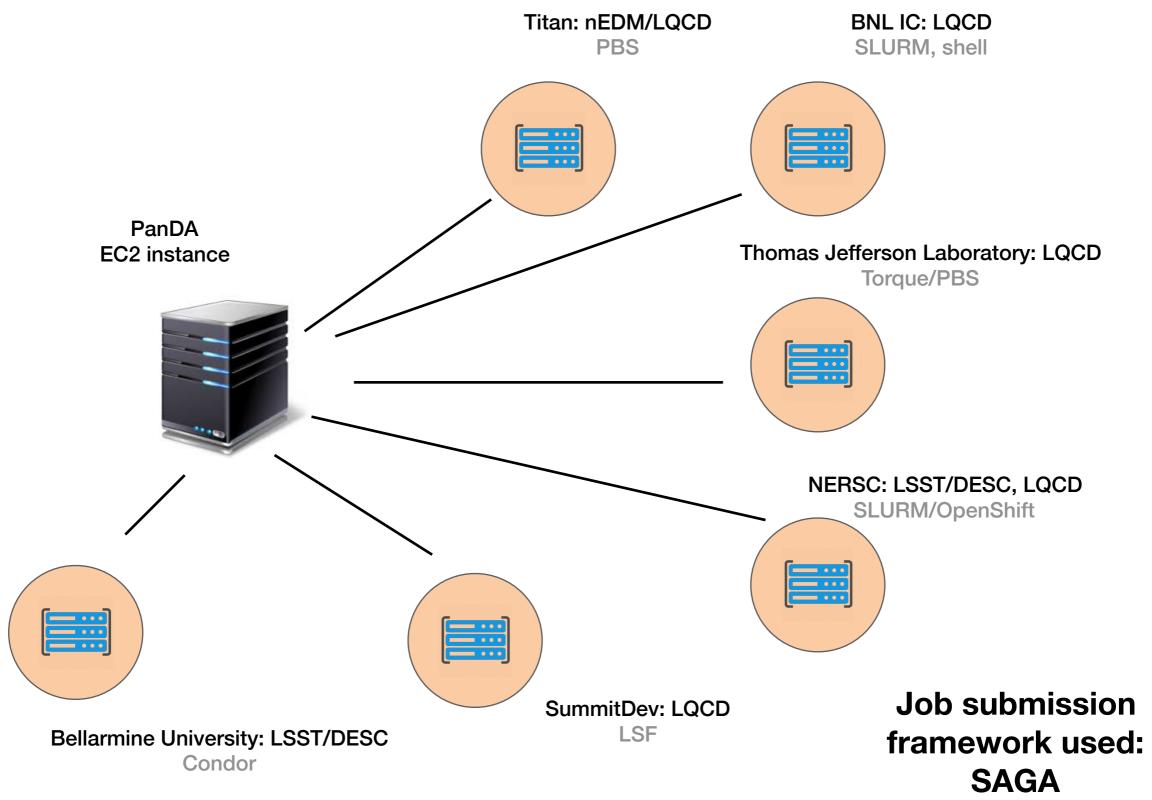
User environment

```
2. mc [pavlosvirin@130-199-21-196.dhcp.bnl.gov]:~/dev/panda-submission2/tmp (bash)
 X ...las/u/psvirin (ssh) • #1 X ...virin@lxplus016:~ • #2 X ...mission2/tmp (bash) #3 X ...~ (sshconnector) • #4 X ...6_553/Run1 (ssh) • #5
(panda-submission2) bash-4.4$
(panda-submission2) bash-4.4$ ../bin/panstat 10064 10069 10063 9997 10048
 10064: finished (staged): {"nodes": 1, "command": "rm -rf /hpcgpfs01/work/lqcd/thermoG/rlarsen/charm_runs/conf_l
4812f21b6825m00161m0436/14812f21b6825m00161m0436_553\n\n", "name": "jobR1", "walltime": "00:30:00"}
 10069: finished (staged): {"nodes": 1, "command": "/hpcgpfs01/work/lqcd/thermoG/rlarsen/charm_runs/Nt12_rasmus_c
harm/run_dens14812f21b6825m00161m0436_553.sh\n# extracting dataset\nmkdir /hpcgpfs01/work/lgcd/thermoG/rlarsen/c
harm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\ntar_xf_/hpcgpfs01/work/lgcd/thermoG/rlarse
n/Cori_conf/conf_archive_14812f21b6825m00161m0436_s418_s673_c1050_c3010_m02y18/_s553.tar -C /hpcgpfs01/work/lqcd
thermoG/rlarsen/charm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\ncd_/hpcgpfs01/work/lgcd/
 thermoG/rlarsen/charm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\nmv__s553/* .\n\n\n\n", "n
 ame": "job1", "walltime": "00:30:00"}
 10063: failed (staged): {"nodes": 1, "command": "/hpcgpfs01/work/lqcd/thermoG/rlarsen/charm_runs/Nt12_rasmus_cha
 m/run_dens14812f21b6825m00161m0436_553.sh\n# extracting dataset\nmkdir /hpcgpfs01/work/lqcd/thermoG/rlarsen/ch
 rm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\ntar xf /hpcgpfs01/work/lqcd/thermoG/rlarsen/
Cori_conf/conf_archive_14812f21b6825m00161m0436_s418_s673_c1050_c3010_m02y18/_553.tar -C /hpcgpfs01/work/lqcd/thermoG/rlarsen/charm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\ncd /hpcgpfs01/work/lqcd/thermoG/rlarsen/charm_runs/conf_14812f21b6825m00161m0436/14812f21b6825m00161m0436_553\nmv _s553/* .\n\n\n\n", "name
 ': "job1", "walltime": "00:30:00"}
9997: cancelled (NULL): {"nodes": 1, "command": "#SBATCH -p long\n#SBATCH --time=15:00:00\n#SBATCH -A thermog\n#
SBATCH --nodes=1\n#SBATCH --gos=normal\n#SBATCH --gres=gpu:4\n#SBATCH -J charmb6825nt122\n\ncd /hpcgpfs01/work/l
gcd/thermoG/rlarsen/charm_runs/Nt12_charm_b6825/dens14812f21b6825m00161m0436_549/Run1/Set3\n\nmodule load gcc/5.
3.0\nmodule load mvapich2\n\nsrun gpu_dens do_arg dens_arg 10 trlan_arg\n\n", "name": "job3", "walltime": "15:00
:00"}
10048: starting (prepared): {"nodes": 1, "command": "#SBATCH -p long\n#SBATCH --time=12:00:00\n#SBATCH -A thermo
g\n#SBATCH --nodes=1\n#SBATCH --gos=normal\n#SBATCH --gres=gpu:2\n#SBATCH -C pascal\n#SBATCH -J charmb6825nt122\
n\ncd /hpcgpfs01/work/lgcd/thermoG/rlarsen/charm_runs/Nt12_charm_b6825/dens14812f21b6825m00161m0436_553/Run1/Set
1\n\nmodule load gcc/5.3.0\nmodule load mvapich2\n\nsrun gpu_dens do_arg dens_arg 10 trlan_arg\n\n", "name": "jo
b1", "walltime": "12:00:00"}
(panda-submission2) bash-4.4$
```

Job templates

```
variables:
  nodes: "1"
  walltime: "00:30:00"
  om: "[0.3:0.5:0.1]"
  seed: "[1:3]"
  rafts: "['01', '02', '03', '10', '11', '12']"
command: I+
  #!/bin/bash -I
  #SBATCH --partition debug
  #SBATCH --image=docker:slosar/desc_lss:v0.21
  #SBATCH --nodes {{nodes}}
  #SBATCH --time={{walltime}}
  #SBATCH --job-name=CoLoRe_test_{{seed}}_{{om}}
  #SBATCH -C haswell
  #SBATCH --volume="/global/cscratch1/sd/psvirin/run_one_test:/predir;/global/cscratch1/sd/psvirin/
run_one_test/test0-{{seed}}}:/rundir"
  export OMP_NUM_THREADS=64
  gen_config {{seed}} {{om}}}
  srun -n {{nodes}} -c 64 shifter /home/lss/CoLoRe/runCoLoRe /rundir/param_files/param_colore_.cfg
```

Map of non-ATLAS Harvesters



JEDI

- JEDI components installed on <u>pandavm.cern.ch</u> instance
- Configuration was done with assistance from Ruslan Mashinistov and Alexander Novikov
- JEDI takes task description and spawns jobs into PanDA Server, jobs reach "activated" status
 - testing for the whole JEDI's workflow functionality not done yet
- JEDI also installed on <u>pandawms.org</u>, required python 2.7 and the latest version of MariaDB

JEDI

IN/L: a comma-concatenated list of input file names (there is also IN but it is deprecated)

OUTPUTn: n is 0 or a positive integer. The output file name in the job for n-th output dataset

TRN_OUTPUTn: a comma-concatenated list of premerged file names which are merged to produce OUTPUTn

SN: a unique serial number in each output stream

SN/P: 6 digts SN padded with leading zeros

RNDMSEED: a unique random seed

MAXEVENTS: the total number of events for the job

SKIPEVENTS: the number of events to be skipped before

starting processing

FIRSTEVENT: the first event number of the job

SURL: URL of input sandbox

- JEDI seems to be too oriented on LHC even-based experiments
 - for example, LSST does not have events
 - what if LSST runs a simulation "N rafts * M sensors * X parameters per sensor?"

Next-generation pandawms.org

- Current pandawms.org runs Scientific Linux 6.4
- A new virtual machine with CentOS 7.4 already created and configured in Amazon Cloud
- Database already configured and data transferred from old pandawms.org
- PanDA Server and PanDA Monitor will be run in Docker containers developed by Ruslan, can be possible to run production version of PanDA Server together with an experimental one
- Transfer of domain names expected after we complete LQCD production campaign (mid-May)

Summary

- 4 instances of Harvester configured and ready to use for non-ATLAS experiment
- An installer has been developed which will allow a fast installation for people not involved in Harvester development
- Harvester tested with nEDM, LQCD, LSST, also testing performed with Next Generation Executer (NGE)
- Production runs started with payloads from BNL LQCD team, expecting to finish this run next week

Next steps

- Finish Harvester testing with the first LQCD production at BNL
- Support TJLab team instance into production mode
- Finish testing client tools and provide user documentation
- Test Harvester with Summit