BNL Site Report

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Scientific Data and Computing Center (SDCC)

- Support for various programs:
    - RHIC, LHC ATLAS, BER ARM, LSST, DUNE, LQCD,RIKEN, BES, Center for Functional Nanomaterials(CFN), National Synchrotron Light Source(NSLS) II, National Nuclear Data Center, Simons Foundation,…

- ~2000 users from >20 projects

- Staff
    - 36 full-time regular members
    - 3 current openings

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Covid-19 Researches at BNL

Resource Providers

		total ▼
—	University of Chicago	1.25 Mil
—	Brookhaven National Laboratory	1.23 Mil
—	Massachusetts Institute of Technology	624.85 K
—	University of Nebraska	425.17 K
—	Fermi National Accelerator Laboratory	196.39 K
—	University of California San Diego	192.79 K
—	University of Wisconsin	55.13 K
—	University of Wisconsin Milwaukee	51.57 K
—	California Institute of Technology	35.28 K
—	University of Mississippi	33.91 K
—	University of Michigan	32.83 K
—	Universidade Estadual Paulista	27.46 K

Computational project details

⊕ PDBQT Docking Study

⊕ Molecules Docking Study

⊕ Search and Mining System for COVID-19-related Literature via Natural Language Processing

⊕ Natural Language Processing: Neural-network-based language model

⊕ Natural Language Processing: Keyword searching

⊕ Neural Fingerprint Method for Chemical Compound Characterization

⊕ Simplified Molecular-Input Line-Entry System (SMILES) Searching

⊕ Drug and Vaccine AI/ML Toolkit

⊕ Neural Fingerprint Method

⊕ ExaLearn Exascale Computing Project COVID-19 Response

⊕ KBase (Predictive Biology)

(https://gracc.opensciencegrid.org/dashboard/db/covid-19-research?orgId=1)

• Most of current BNL SDCC computing resource usage for covid-19 from Open Science Grid (Most resources provided until recently)
• Other BNL participation in covid-19 projects can be found in
https://www.bnl.gov/science/COVID-working-group.php#projects

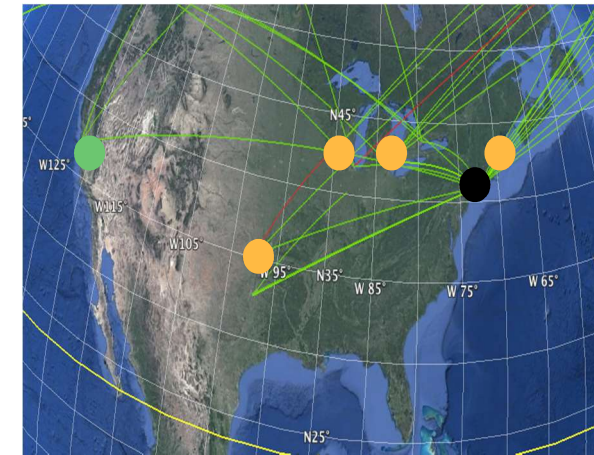# SDCC support for HEP experiments

- **The RHIC Tier 0**
  - Store and process data from RHIC experiments
  - Provide analysis means for 1'200 users
  - Long term data preservation
  - Simulation resources for future programs (sPHENIX & EIC)
- **The US ATLAS Tier 1**
  - ~25% of ATLAS Tier 1 computing capacity worldwide
  - Store RAW data from LHC and from simulation
  - Distribute data to the 4 US Tier 2 sites + analysis site (SLAC)
  - **Analysis center for US physicists**
    - From 41 institutes (incl. 4 Nat. Labs)
    - 600 physicists, 190 PhDs
- **A Belle II data center outside Japan**
  - **Initial operations began on Oct. 2017**
  - **Data taking began in Fall 2018**

24/7 availability

SDCC Resources Summary

- 90+k CPU cores — 4 PFlops
  - 4 HPC Institutional Clusters (GPU, KNL, Skylake,ML)
- 688 GPUs
  - K80, P100, V100
- ~80 PB of disk storage
  - Central and distributed storage systems
- 165+ PB of tape storage
  - Largest HPSS tape library in the US, 3rd worldwide
- 2x100 Gbps connection to ESnet
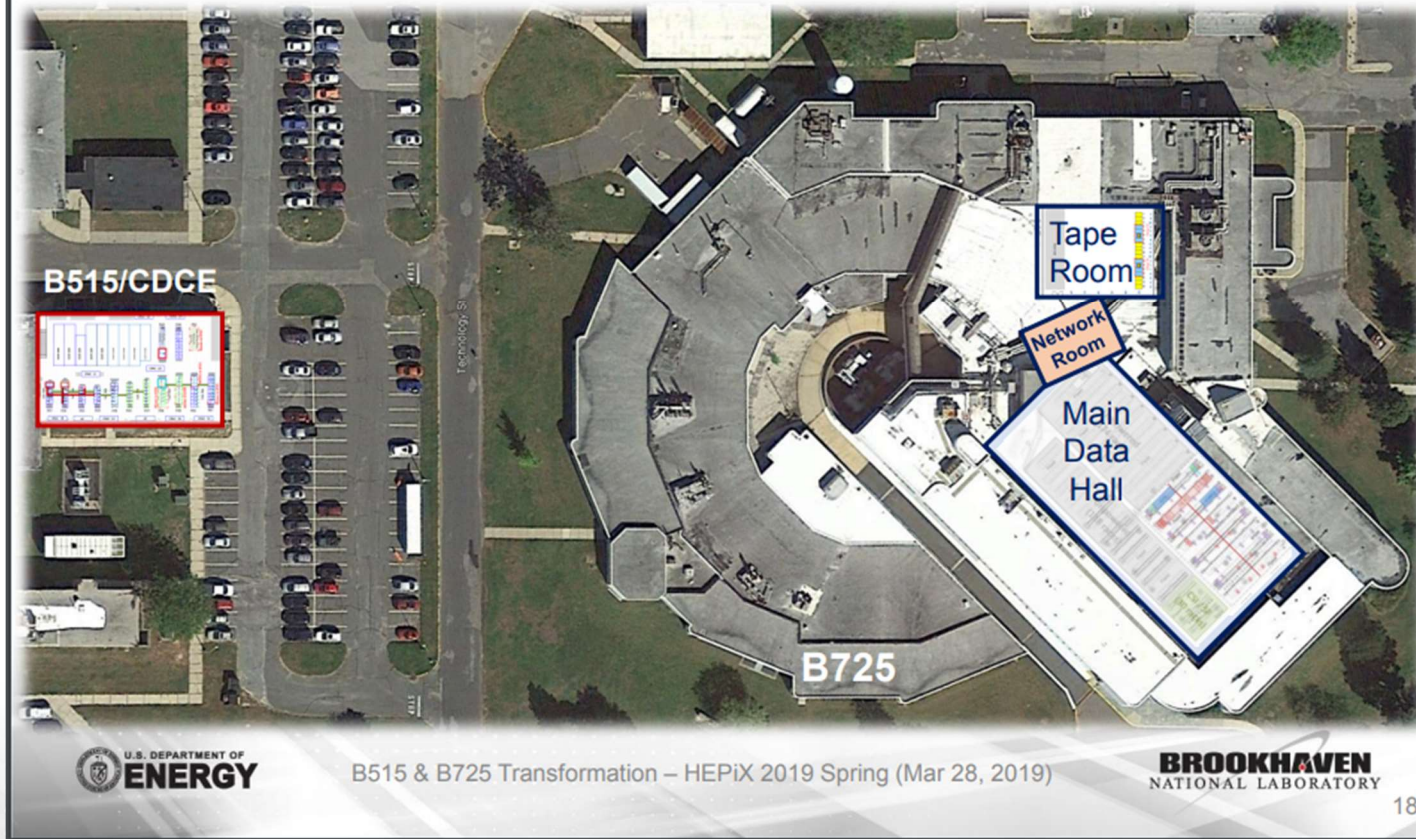 - 100Gbps redundancy
  - Onsite ESNet support

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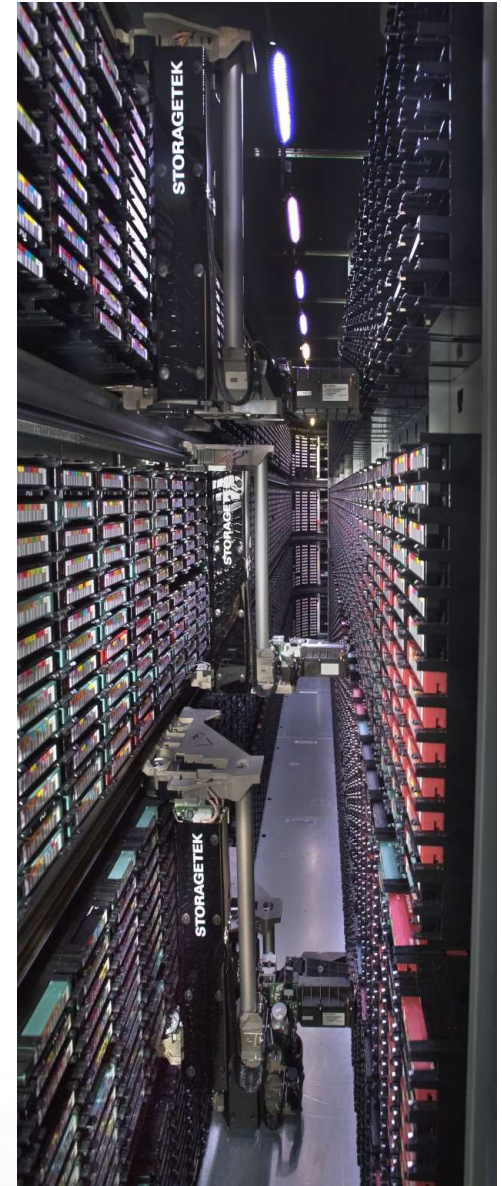
BNL Data Center (CFR)

- Existing data center is full

- Construction of new data center
    - Began last May,
    - Demolition phase close to finish …halted.
    - Was expect to be online On Feb 2021, but could be delayed…

- Approximately 3x times more floor space and electrical power with room to expand if needed

- Higher PUE (power utilization efficiency) – mandated by DOE

- Any new LQCD-accessible systems post-2021 would be housed in the new data center

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New BNL Data Center (CFR)

Proposed solution: Constructing the new datacenter in B725 in FY19-21, migrating all spinning disk storage and compute to it in FY21-23; leaving the B515 datacenter reduced to just one area (CDCE) as a tape storage room

B515/CDCE

Tape Room

Network Room

Main Data Hall

B725

B515 & B725 Transformation – HEPiX 2019 Spring (Mar 28, 2019)

SDCC support for HPC

- Institutional Clusters

1. CPU-GPU cluster (aka "Annie") with 216 compute nodes (36 physical core Xeon Broadwell and 2 GPUs each: K80 & P100) inter-connected with dual-rail Infiniband EDR

2. KNL cluster (aka "Frances") with 144 nodes (64 cores each) interconnected with dual-rail Intel OPA

3. Skylake cluster: 64 nodes (36 physical cores each) with single-rail Infiniband EDR

4. Machine Learning Cluster: 5 EDR connected nodes, each have 8 Nvlink connected V100 GPU

5. Start In production since January 2017

    - >300 registered users

MoUs (describing level of resources and services) organized with each user community

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Monitoring

- Several tools available
  - Graphical interface here (**authentication required**)
    - https://monitoring.sdcc.bnl.gov/pub/grafana/
  - Accounting information
    - https://monitoring.sdcc.bnl.gov/pub/allocation
    - <mark>LQCD only</mark>
      - https://monitoring.sdcc.bnl.gov/pub/allocation/lqcd.html
      - After loading module lqcd, Command line "lquota" for same information

Accounting https://monitoring.sdcc.bnl.gov/pub/allocation/lqcd.html

BNL SDCC LQCD Projects Usage Sumary

Institutional Cluster

(Sky Core Hours)

updated: 2020-03-31 00:03:25

	Cluster	Account	Start Date	End Date	Allocation	Usage	Usage(%)	
	Annie-IC	lqcd-19-20	2019-07-01	2020-06-30	6,728,385	4,783,845	71.10%	
	Project	Original SPC Allocation	Adjustment	Adjusted SPC Allocation	Usage	Progress(%)	Remain	30Day Usage	30Day BurnRate
1	stagmug-2-19-20	1,034,714	425,017	1,459,731	1,609,524	110.26%	0	473,015	32.40%
2	semibdff-19-20	691,747	273,454	965,201	857,264	88.82%	107,937	120,253	12.46%
3	nucstructclover-19-20	842,885	170,303	1,013,188	740,004	73.04%	273,185	125,144	12.35%
4	axialgpu-19-20	697,560	296,936	994,496	676,647	68.04%	317,849	1,299	0.13%
5	sextet-19-20	546,422	156,075	702,497	604,166	86.00%	98,330	49,126	6.99%
6	class-c-19-20	10,765	0	10,765	615	5.72%	10,149	0	0.00%
7	qgpd-19-20	1,499,742	0	1,499,742	295,625	19.71%	1,204,117	295,625	19.71%
8	UnAllocated:	-1,510,507	1,593,273	82,766	0	0.00%	0	0	0.00%

Skylake Cluster

(Sky Core Hours)

updated: 2020-03-31 00:03:25

	Cluster	Account	Start Date	End Date	Allocation	Usage	Usage(%)	
	Skylake	lqcd-sky-19-20	2019-07-01	2020-06-30	17,278,272	11,118,173	64.35%	
	Project	Original SPC Allocation	Adjustment	Adjusted SPC Allocation	Usage	Progress(%)	Remain	30Day Usage	30Day BurnRate
1	semibdff-sky-19-20	4,500,000	2,414,093	6,914,093	5,208,518	75.33%	1,705,575	407,806	5.90%
2	stagmug-2-sky-19-20	5,000,000	(2,731,934)	2,268,066	2,417,375	106.58%	0	731,201	32.24%
3	etap-sky-19-20	1,500,000	300,000	1,800,000	625,947	34.77%	1,174,053	53,883	2.99%
4	qgpd-sky-19-20	5,000,000	17,841	5,017,841	2,862,086	57.04%	2,155,755	367,215	7.32%
5	class-c-sky-19-20	8,333	0	8,333	4,247	50.97%	4,086	0	0.00%
6	UnAllocated:	1,491,667	(221,728)	1,269,939	0	0.00%	0	0	0.00%

KNL Cluster

(Sky Core Hours)

updated: 2020-03-31 00:03:09

	Cluster	Account	Start Date	End Date	Allocation	Usage	Usage(%)	
	Frances-KNL	lqcd-knl-19-20	2019-07-01	2020-06-30	11,133,023	9,796,792	88.00%	
	Project	Original SPC Allocation	Adjustment	Adjusted SPC Allocation	Usage	Progress(%)	Remain	30Day Usage	30Day BurnRate
1	qcdqedta-knl-19-20	6,756,000	164,205	6,920,205	7,142,674	103.21%	0	478	0.01%
2	posnpr-knl-19-20	1,689,000	328,417	2,017,417	1,376,230	68.22%	641,186	137,502	6.82%
3	ndbeta-knl-19-20	1,970,500	(492,622)	1,477,878	1,251,523	84.68%	226,355	978,515	66.21%
4	class-c-knl-19-20	28,150	0	28,150	26,365	93.66%	1,785	0	0.00%
5	UnAllocated:	-928,950	1,618,323	689,373	0	0.00%	0	0	0.00%

Accounting https://monitoring.sdcc.bnl.gov/pub/grafana/
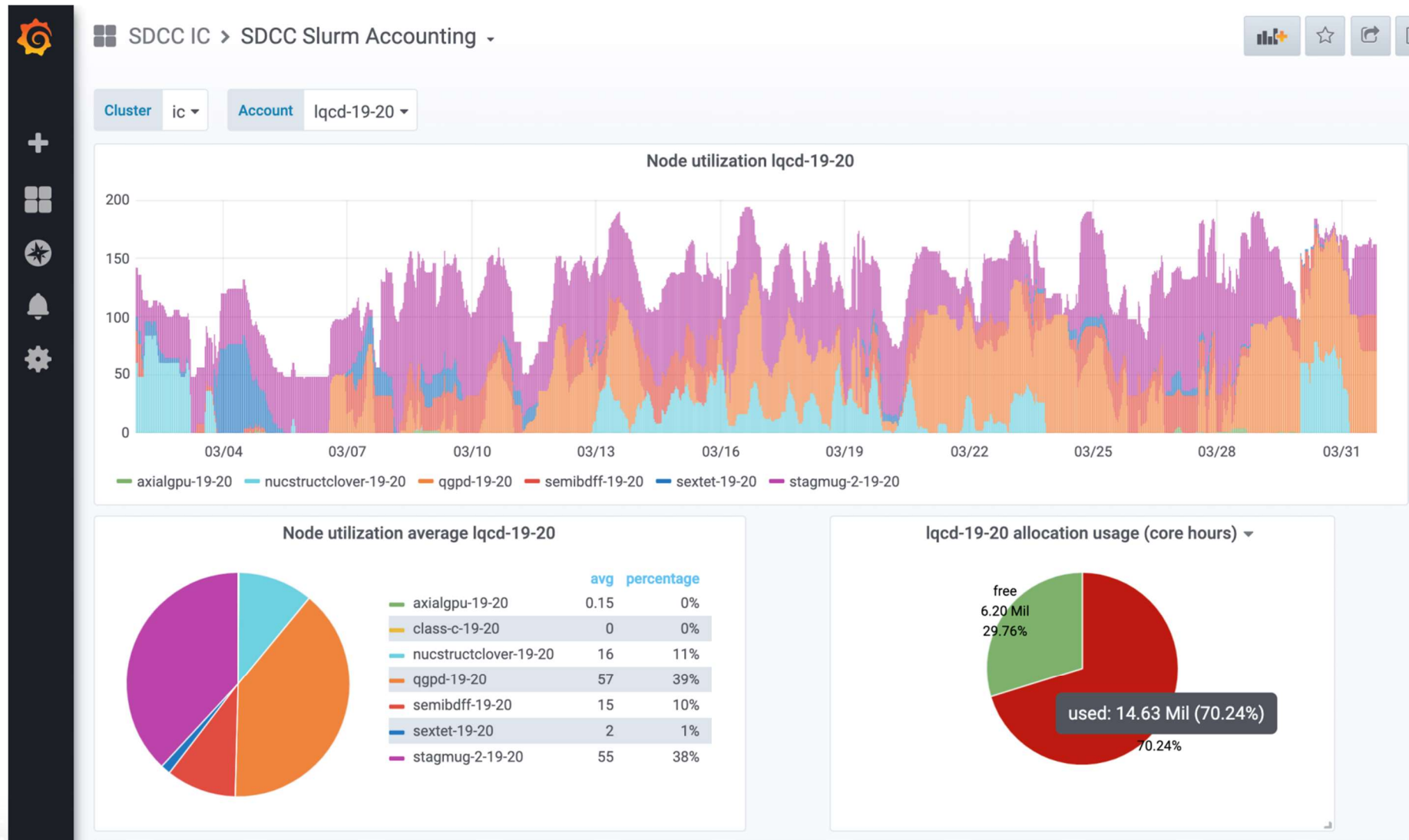
LQCD Access to SDCC Resources

- Current resources allocated
  - 578k node-hour allocation on CPU-GPU cluster
  - 309k node-hour allocation on KNL cluster
  - 480k node-hour allocation on Skylake cluster
  - 600 TB of GPFS storage
  - 600 TB of Tape Storage service (134TB used so far)
- Usage policy
  - SDCC does not decrement underused allocations as a function of time, but unused allocations are increasingly "at risk" as we approach end of year when resource contention can become an issue.
  - Opportunistic lower priority usage after allocation used up, when cluster have available resource.

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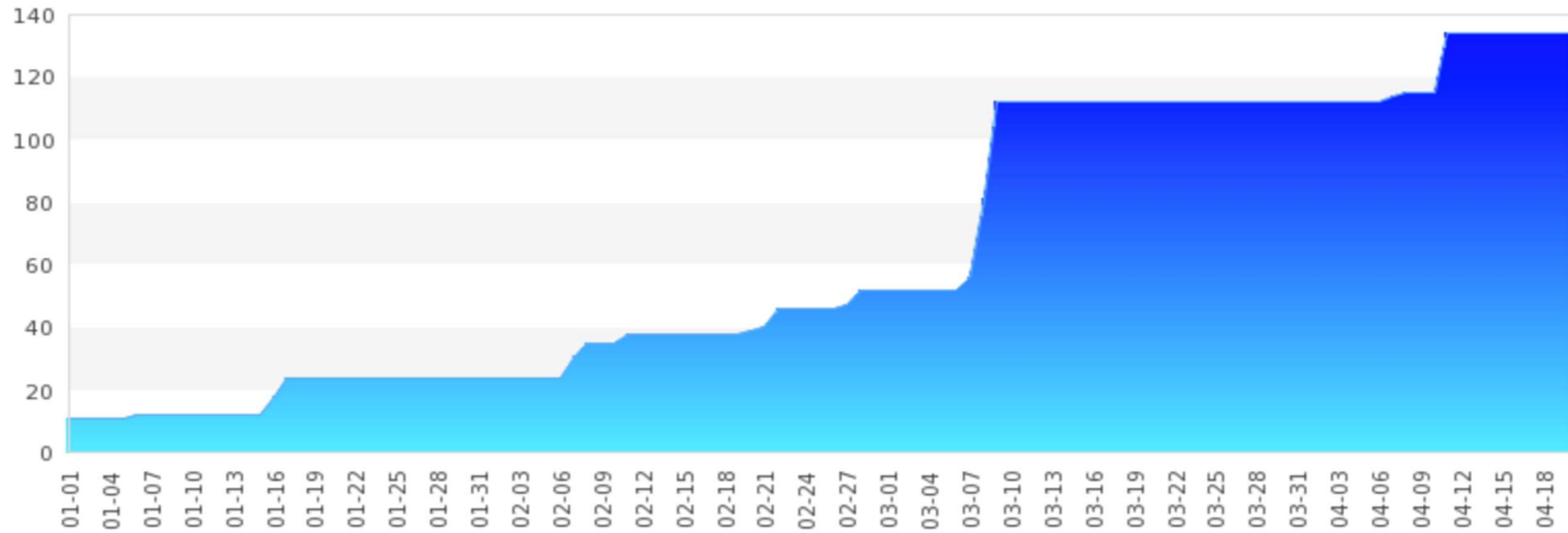
USQCD data growth at BNL(134TB as of 4/20)

User Support

- Facility website is www.sdcc.bnl.gov .
  - New accounts
    - Instructions on website
    - Usually ~24 hours to process after verification
  - User support requests
    - SDCC policy is to respond within 3 business days. Majority is resolved within this period
    - In the July 1, 2018 to June 30, 2019, 200 tickets were submitted to ticket queues (majority from LQCD users) and 91% were resolved within 3 business days

- Bi-weekly meetings between facility staff and program/experimental Liaisons
  - Agenda on https://indico.bnl.gov/category/169/
  - Remote access via BlueJeans—Minutes of meeting posted for those who cannot join in person or remotely

Recent Developments

- Globus endpoint @ the SDCC
    - Fast point-to-point data transfer mechanism
    - Available on Institutional Clusters (Endpoint 'SDCC')
    - https://www.racf.bnl.gov/experiments/sdcc/institutional-cluster/storage

- Tape archival services available for LQCD
    - All hardware installed and tested. Initially 600 TB of tape storage with room to grow
    - Interface mechanism and documentation (including a Data Management Plan) available in early May 2019.
    - Information on USQCD webpage (https://www.usqcd.org/bnl/tape-archive.html)
    - Deletion or renaming creates dead space. Will count against USQCD.

- BNLBox service operational since December 2019 – file sharing and archiving (like CERNBox) between SDCC users
    - www.racf.bnl.gov/docs/services/cloud-storage/using-cloud-storage

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Federated User Management

- SDCC moving towards accepting selected federated identity provider (IDP) for user management
    - First step towards Single Sign-On (SSO) with Multi-Factor Authentication (MFA)
    - InCommon and OneID– used at many universities and labs
    - SDCC establishing IDP under InCommon (independent from BNL Active Directory IDP)
    - Some issues still unresolved
        - Trust levels
        - Resources available to BNL users vs. non-BNL users
    - Some applications already enabled (Jupyter, Indico and Invenio)
    - Potentially beneficial to LQCD users at BNL—SDCC account can be used to authenticate to external organizations
    - Evolving cyber-security policy to accommodate federated access to BNL resources

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Questions?