Structural Bioinformatics Training Workshop & Hackathon 2018

mmtfPyspark

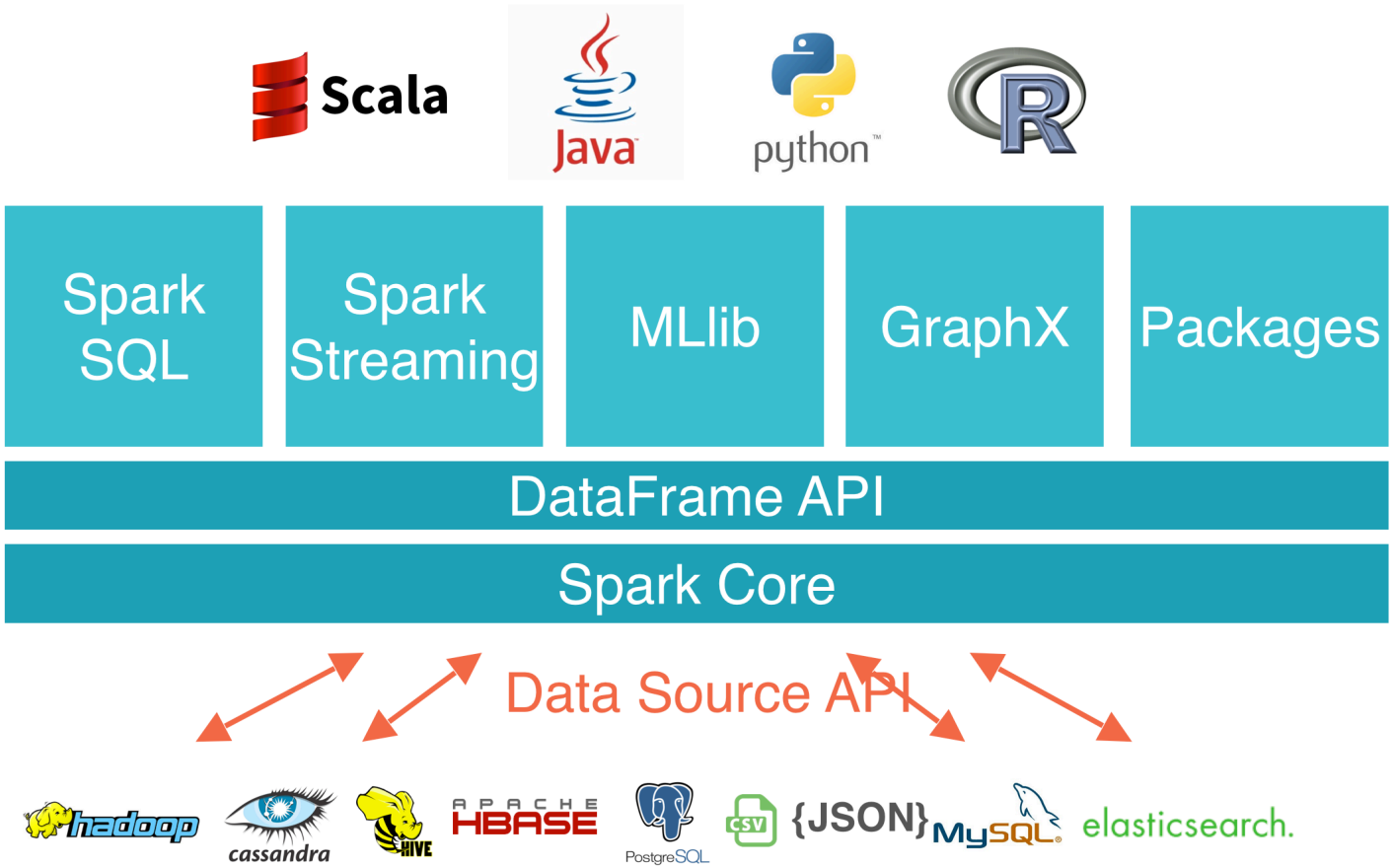
Peter Rose
Structural Bioinformatics Laboratory
San Diego Supercomputer Center
UC San Diego

SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Spark Ecosystem

Apache Spark is a fast and general engine for large-scale data processing



What is mmtfPyspark?

- A framework for interactive analysis and mining of 3D macromolecular structures
- Powered by MMTF (MacroMolecular Transmission Format), a compact data format that facilitates efficient network transfer and high-performance parsing and processing of 3D structures
- Built on Apache Spark, a framework for distributed, parallel in-memory processing
- Uses Spark-SQL for queries and Spark-Mllib for machine learning
- Available with Java and Python API

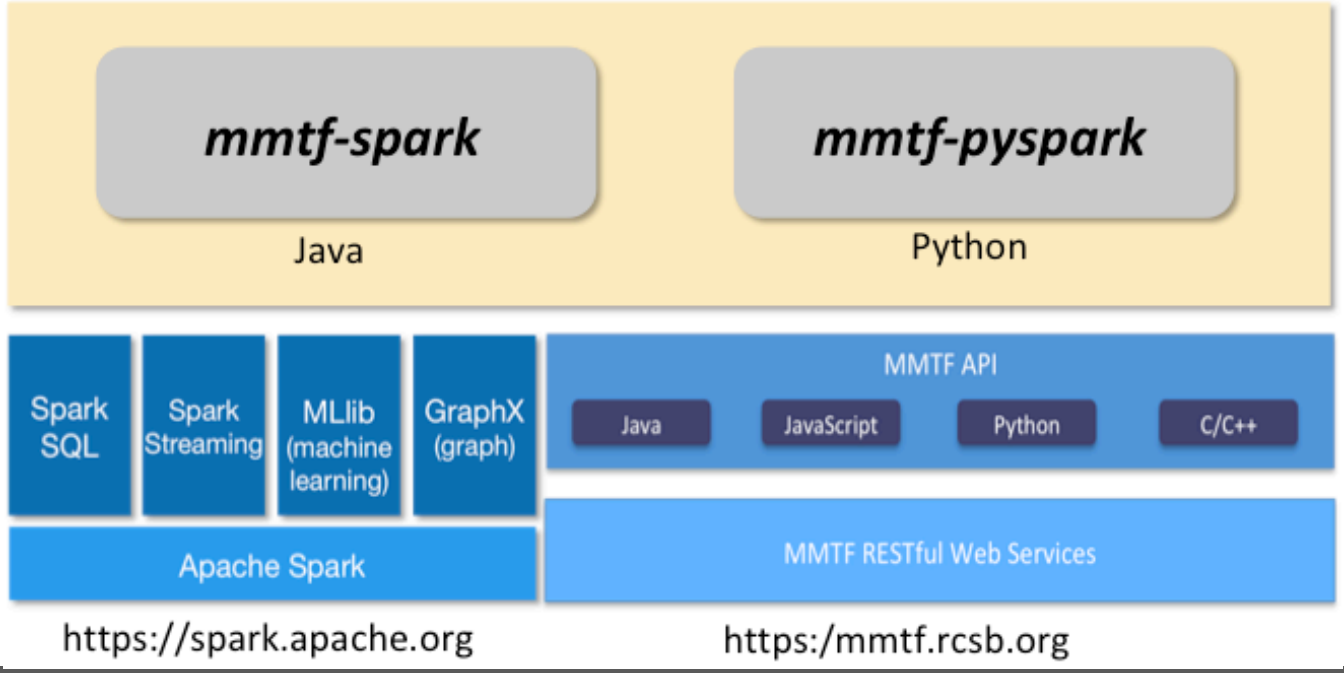
MMTF-Spark

mmtf-spark (Java)

- High performance processing
- Suitable for large-scale calculations
- Integration with other libraries, e.g., BioJava

mmtf-pyspark (Python)

- Interactive scripting
- 2D and 3D visualization
- ML/DL tool ecosystem
- Sharable data analysis in Jupyter Notebooks



MMTF Data Sources

- **Download single MMTF files using web services**
  - Analyze 10s – 100 PDB entries
  - https://mmtf.rcsb.org/v1.0/full/4HHB.mmtf.gz

- **Download MMTF Hadoop Sequence files**
  - Analyze 1000s or all PDB entries
  - https://mmtf.rcsb.org/v1.0/hadoopfiles/full.tar
  - https://mmtf.rcsb.org/v1.0/hadoopfiles/reduced.tar

- **Info about downloading**
  - https://mmtf.rcsb.org/download.html

Hadoop "Sequence" Files

- **A flat file of binary key/value pairs**
- **Used by Big Data Frameworks (Hadoop, Spark)**
  - File systems need few big files for efficient processing
- **Files are splittable**
  - Can be processed in parallel
- **Often consists of a directory of Sequence files**
- **See** https://wiki.apache.org/hadoop/SequenceFile

MMTF Hadoop Sequence Files

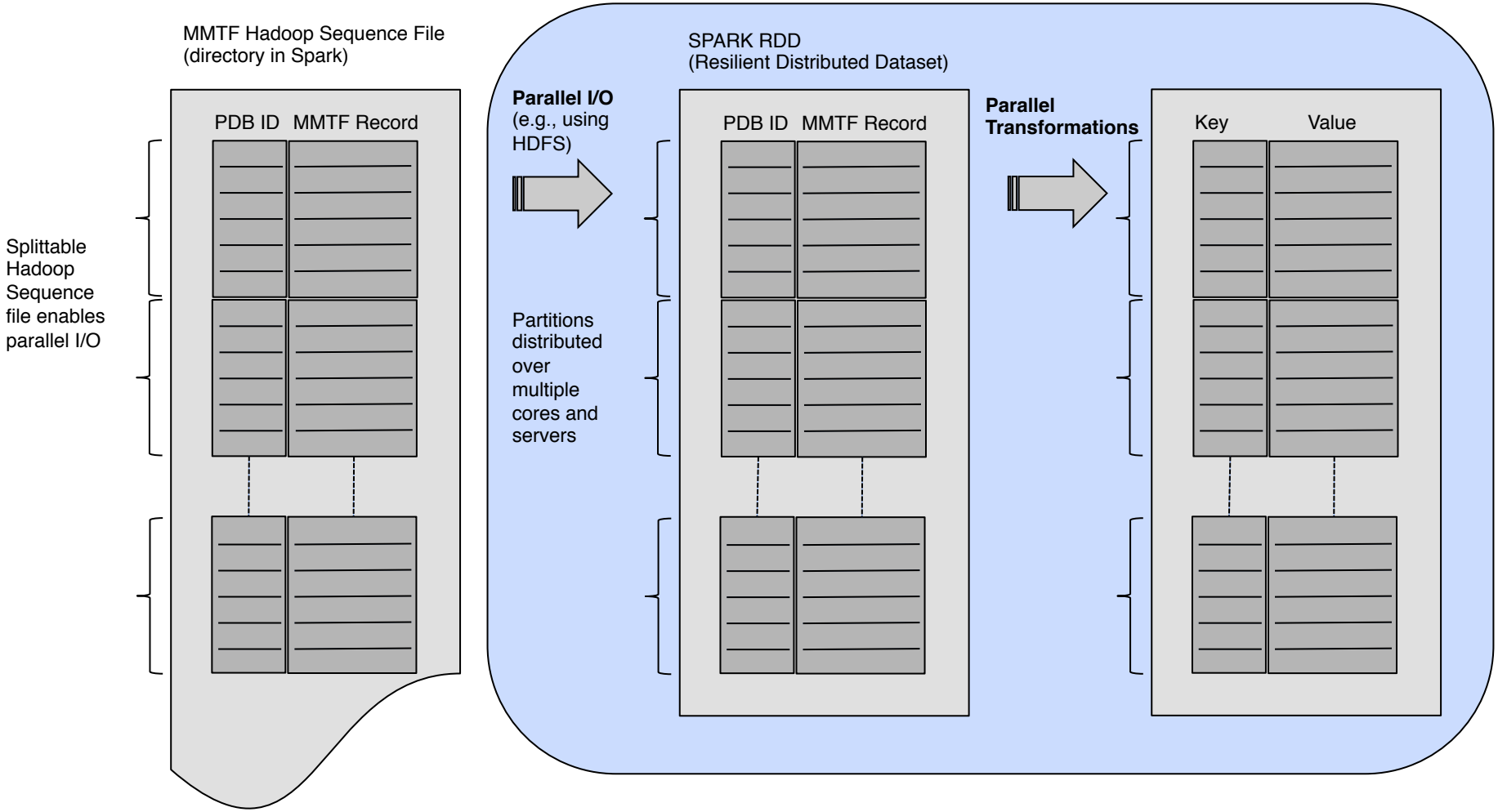
- **Two representations**
  - **full**
    - all atoms
    - full data precision
  - **reduced**
    - polymers
      - polypeptides: C-alpha
      - polynucleotides: P
      - 1st model only (e.g., NMR)
      - no alternative locations
      - except polysaccharides
        - » all atom
    - non-polymers
      - all atoms
    - water
      - excluded
    - Reduced precision (0.1): coordinates, temperature-factor, occupancy

- **Example: full directory structure**

Name	Date Modified	Size
_2017-06-06.txt	Jun 6, 2017, 5:02 PM	Zero bytes
_SUCCESS	Jun 2, 2017, 2:07 PM	Zero bytes
part-00000	Jun 2, 2017, 2:00 PM	9.8 MB
part-00001	Jun 2, 2017, 2:00 PM	13.9 MB
part-00002	Jun 2, 2017, 2:00 PM	33.3 MB
part-00003	Jun 2, 2017, 2:00 PM	33.4 MB

- **Timestamp file (release date)**
  - _yyyy-mm-dd.txt
- **Updated every Wed. ~00:00 UTC**
- **Multiple sequence files**
  - part-00000 …
- **Download**
  - https://mmtf.rcsb.org/download.html

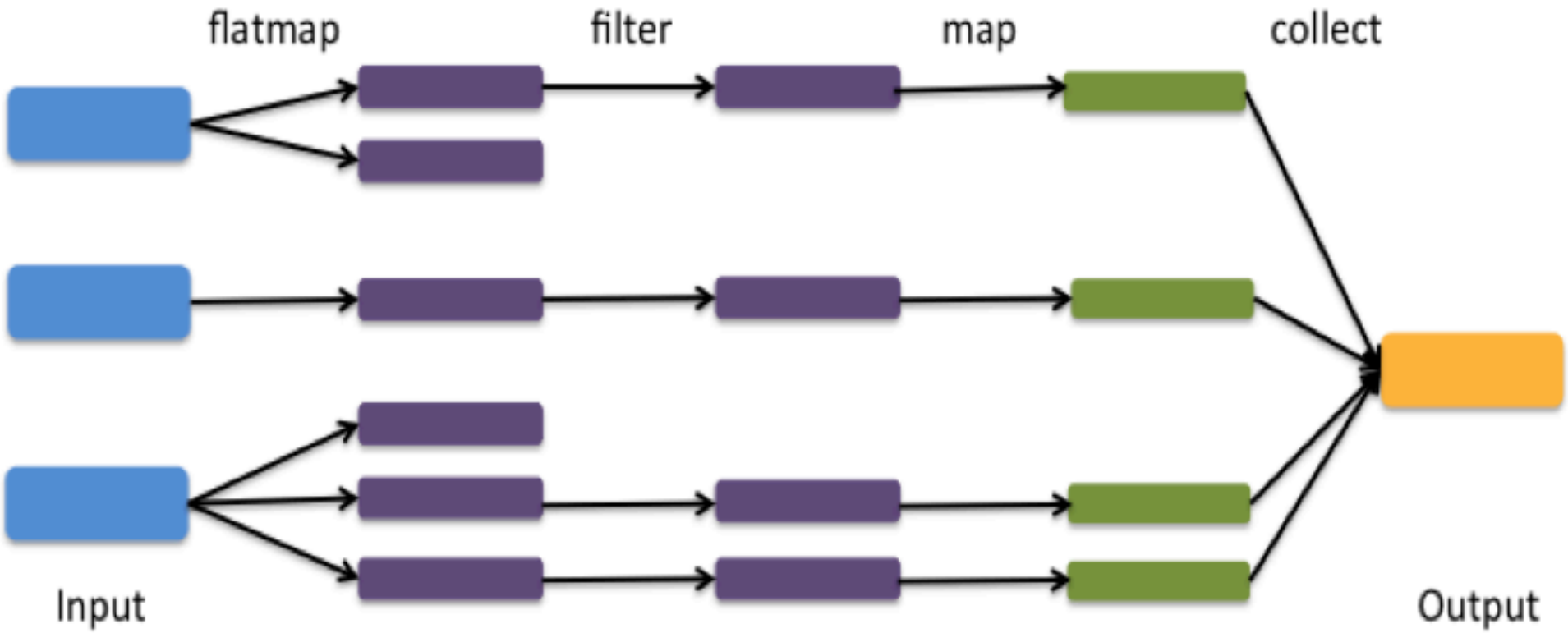
MMTF-Spark Data Pipeline



MMTF Hadoop Sequence Files for Workshop

- Sample MMTF Hadoop Sequence Files are included in the workshop repository
  - https://github.com/sbl-sdsc/mmtf-workshop-2018/tree/master/resources
- The sample files contain 9756 representative PDB structures
    - mmtf_full_sample
    - mmtf_reduced_sample

Example of a Spark Workflow



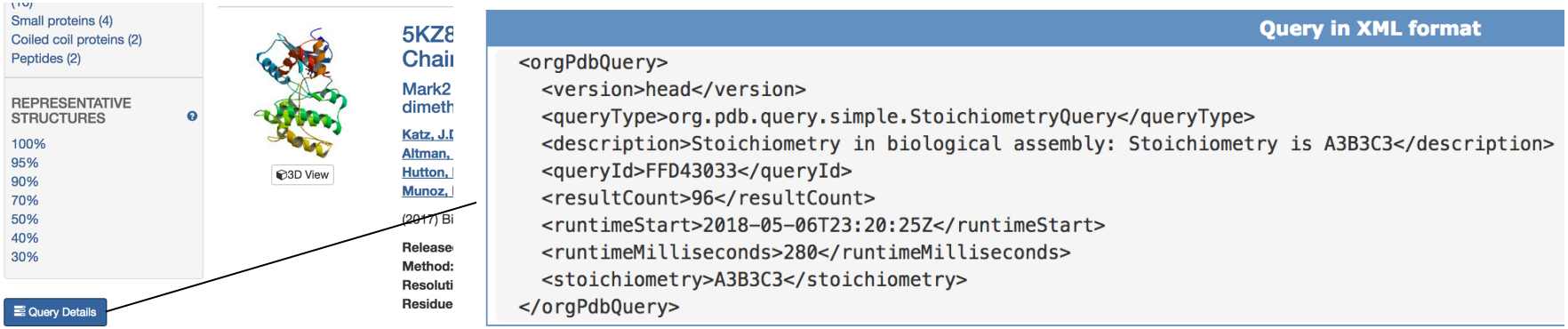
Jupyter Notebook Tutorials

https://github.com/sbl-sdsc/mmtf-workshop-2018/tree/master/3-mmtf-pyspark

- 1-Input
- 2-Filtering
- Problem-1 (Solution-1)
- 3-Webfiltering
- 4-Flatmapping
- 5-MapReduce
- Problem-1 (Solution-2)
- 6-Output
- 7-OutputTo3DViewer

Filtering Using AdvancedQuery

- Run any advanced query at http://www.rcsb.org
- Go to results page and click Query Details



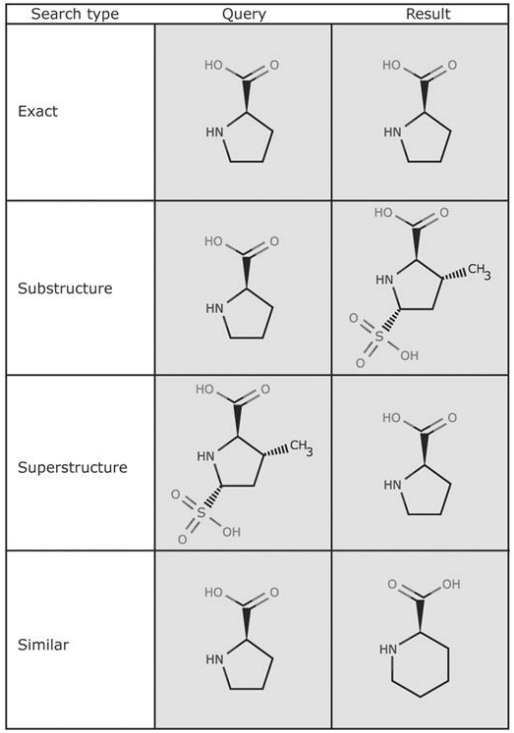

```
query = (
    "<orgPdbQuery>"
        "<queryType>org.pdb.query.simple.StoichiometryQuery</queryType>"
        "<stoichiometry>A3B3C3</stoichiometry>"
    "</orgPdbQuery>"
)
trimer_of_trimers = pdb.filter(AdvancedQuery(query))
```

Filtering by SMILES

```
// keep structures that contain a chemical component
// with this substructure
pdb = pdb.filter(
    ChemicalStructureQuery("OC(=O)CCCC[C@@H]1SC[C@@H]2N
    C(=O)N[C@H]12”,
    ChemicalStructureQuery.SUBSTRUCTURE, 0))
```

```
// keep structures that contain a chemical component
// that is >= 70% similar to the query structure
similarity = 70
pdb = pdb.filter(
    ChemicalStructureQuery("OC(=O)CCCC[C@@H]1SC[C@@H]2N
    C(=O)N[C@H]12”,
    ChemicalStructureQuery.SIMILAR, similarity))
```

Query Types:
EXACT
SUBSTRUCTURE
SUPERSTRUCTURE
SIMILAR



Summary

- **mmtfPyspark: Framework for parallel distributed mining of the PDB with Apache Spark**
- **MMTF Hadoop Sequence file is an efficient container format to process large number of structures**
- **PDB structures represented as key/value pairs**
- **Spark transformations**
  - filter, keys, map, flatMap
- **Spark actions**
  - count, reduce, collect

Resources

- **MMTF Website**
  - https://mmtf.rcsb.org
- **Git Repositories**
  - https://github.com/sbl-sdsc/mmtf-pyspark
  - https://github.com/sbl-sdsc/mmtf-spark
  - https://github.com/sbl-sdsc/mmtf-workshop-2017
- **MMTF File Format**
  - Bradley AR, et al. (2017) MMTF—An efficient file format for the transmission, visualization, and analysis of macromolecular structures. PLOS Computational Biology 13(6): e1005575. https://doi.org/10.1371/journal.pcbi.1005575
  - Valasatava Y, et al. (2017) Towards an efficient compression of 3D coordinates of macromolecular structures. PLOS ONE 12(3): e0174846. https://doi.org/10.1371/journal.pone.0174846

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