Structural Bioinformatics Training Workshop & Hackathon 2017

Basic Spark

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Draft version under development

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mmtf-spark

- **Framework for parallel distributed analysis and mining of the PDB in MMTF file format with Apache Spark**
- **MMTF data sources**
  - Single <pdbId>.mmtf.gz files downloaded using RESTful web services
    - analyze a few PDB entries
  - Locally downloaded Hadoop Sequence file with MMTF records
    - analyze many or all PDB entries
  - See: http://mmtf.rcsb.org/download.html

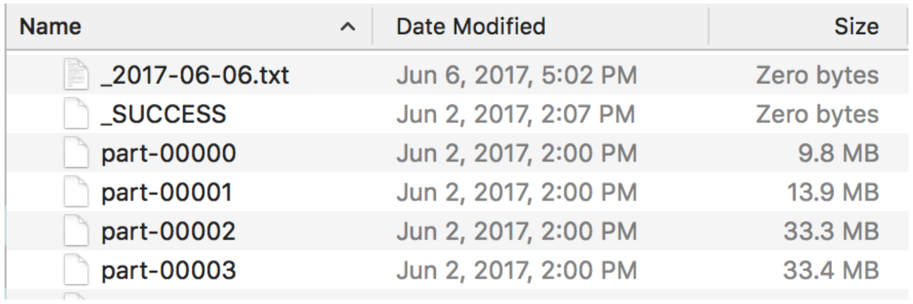
Hadoop "Sequence" Files

- **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

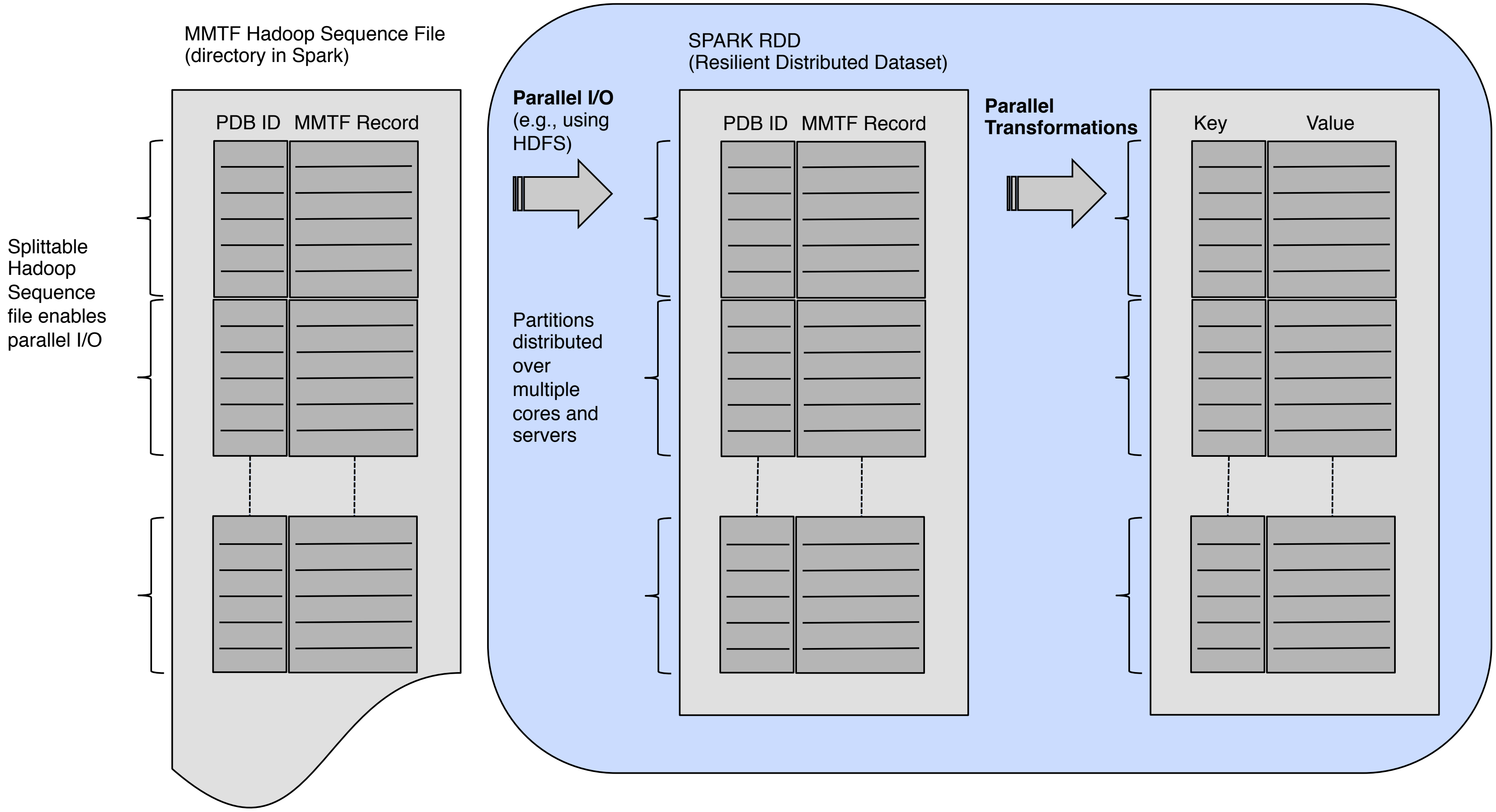
- **Example: full directory structure**



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**
- **> 300 sequence files**
  - part-00000 …
- **Download**
  - http://mmtf.rcsb.org/download.html

MMTF-Spark Data Pipeline


MMTF Hadoop Sequence File
(directory in Spark)
PDB ID
MMTF Record
Splittable Hadoop Sequence file enables parallel I/O
SPARK RDD
(Resilient Distributed Dataset)
Parallel I/O (e.g., using HDFS)
Partitions distributed over multiple cores and servers
PDB ID
MMTF Record
Parallel Transformations
Key
Value

Basic MMTF-Spark Operations

- **Reading MMTF Files & Hadoop Sequence Files**
  - Full vs. Reduced
- **Filtering PDB structures**
  - Metadata, Polymer Types
- **Lambda Expression for Filter/Map/Reduce**
- **FlatMapping of PDB structures**
- **Writing custom Hadoop Sequence Files**
- **Filtering using RCSB PDB web services**

Downloading mmtf.gz files

…/io/demos/DownloadMmtfFiles.java

```
 // spark setup
JavaSparkContext sc = …

// download a list of PDB entries using mmtf web services
List<String> pdbIds = Arrays.asList("1AQ1","1B38","1B39","1BUH");

JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                                .downloadMmtfFiles(pdbIds, sc);
```

JavaPairRDD is a resilient distributed data structure of key/value pairs

key : String – structureId, e.g., pdbId (4HHB)
value: StructureDataInterface - structure representation in uncompressed form

Reading from a Sequence File

```
 // get path to full Sequence file from environment variable
String path = System.getProperty("MMTF_FULL");

 // spark setup
JavaSparkContext sc = …

// download a list of PDB entries
List<String> pdbIds = Arrays.asList("1AQ1","1B38","1B39","1BUH");

JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                                 .readSequenceFile(path, pdbIds, sc);

// or download all PDB entries
JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                                 .readSequenceFile(path, sc);
```

Demo

Reading files

Filtering by Quality Metrics

```
// download all PDB entries
JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                                 .readSequenceFile(path, sc);

// keep PDB entries with a resolution in the inclusive range [0, 2]
pdb = pdb.filter(new Resolution(0.0, 2.0));


// or more concise with method chaining
JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                                 .readSequenceFile(path, sc)
                                 .filter(new Resolution(0.0, 2.0));
```

Related filters: Rfree and Rwork

Note, these filters will eliminate any entries that do not have these metrics, e.g., NMR structures.

See http://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/introduction

Filtering by Polymer Chain Types

```
// keep PDB entries that contain at least one L-protein chain
JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                             .readSequenceFile(path, sc)
                             .filter(new ContainsLProteinChain());
```

```
// keep PDB entries that contain exclusively L-protein chains
boolean exclusive = true;

JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
                             .readSequenceFile(path, sc)
                             .filter(new ContainsLProteinChain(exclusive));
```

Related filters:
ContainsDProteinChain
ContainsDnaChain
ContainsRnaChain
ContainsDSaccharide (should this be chain?)
ContainsPolymerChain

Filtering by Heterogeneous Polymer Chain Types

```
// keep PDB that contain DNA, RNA, or both (DNA/RNA hybrid)
JavaPairRDD<String, StructureDataInterface> pdb = MmtfReader
        .readSequenceFile(path, sc)
        .filter(new ContainsPolymerChainType("DNA LINKING","RNA LINKING"));
```

Monomer types (most frequent types in bold)
PEPTIDE_LINKING (achiral, e.g., GLY)

D_PEPTIDE_LINKING
D_PEPTIDE_COOH_CARBOXY_TERMINUS
D_PEPTIDE_NH3_AMINO_TERMINUS

L_PEPTIDE_LINKING
L_PEPTIDE_COOH_CARBOXY_TERMINUS
L_PEPTIDE_NH3_AMINO_TERMINUS

DNA_LINKING
DNA_OH_3_PRIME_TERMINUS
DNA_OH_5_PRIME_TERMINUS

NON_POLYMER
SACCHARIDE (achiral)

D_SACCHARIDE
D_SACCHARIDE_14_and_14_LINKING
D_SACCHARIDE_14_and_16_LINKING

L_SACCHARIDE
L_SACCHARIDE_14_AND_14_LINKING
L_SACCHARIDE_14_AND_16_LINKING

RNA_LINKING
RNA_OH_3_PRIME_TERMINUS
RNA_OH_5_PRIME_TERMINUS

See http://mmcif.wwpdb.org/dictionaries/mmcif_mdb.dic/Items/_chem_comp.type.html