Structural Bioinformatics Training Workshop & Hackathon 2017

MMTF Plans

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Plans

- **MMTF-Spark**
  - Feedback from community (e.g., this workshop)
- **MMTF-PySpark**
  - Python version with Jupyter Notebook & 3D viewer
    Datasets -> Pandas -> machine learning methods
- **Parallelize algorithms**
  - Parallelize conventional algorithms using the latest advances in computer science
- **Webinars and online tutorials**

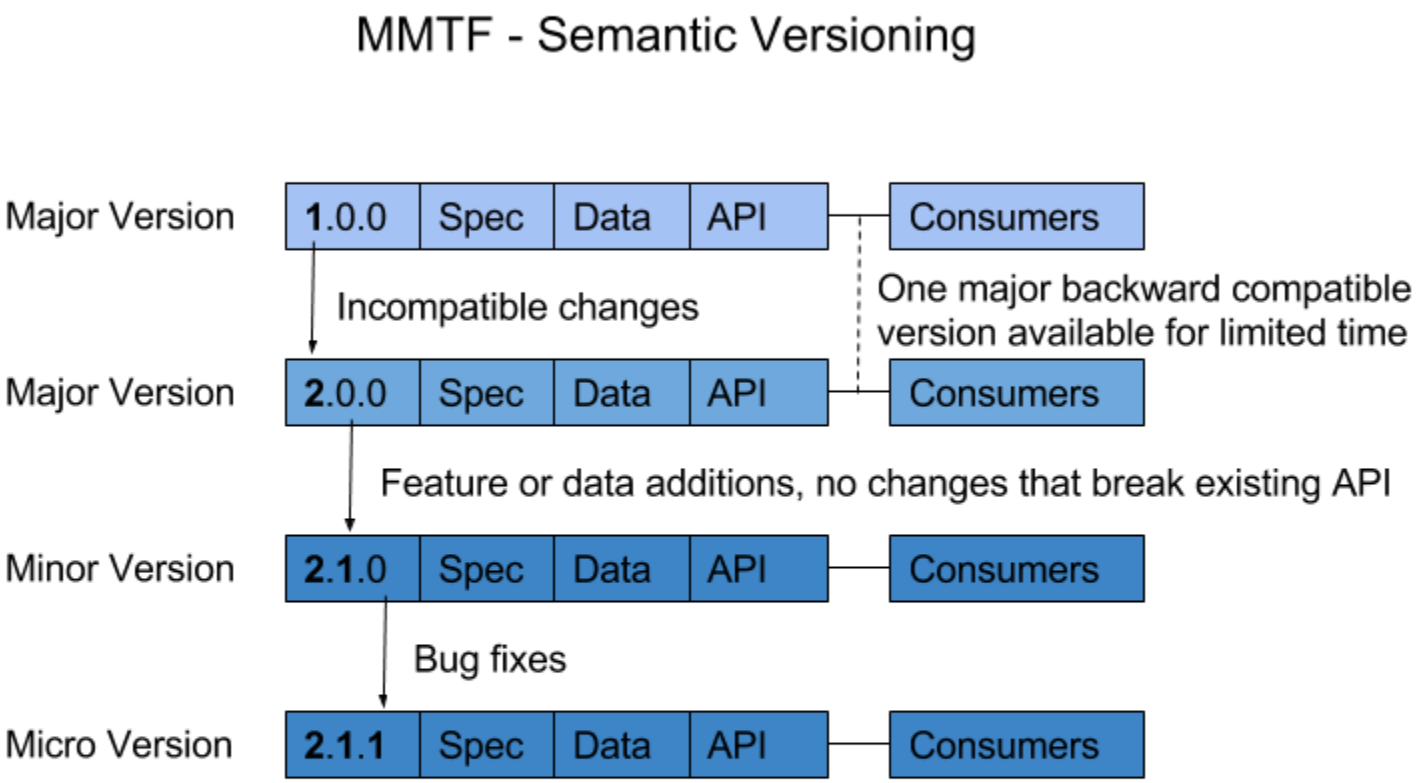
Support Large Scale Calculations

- **Cloud Providers**
  - Academic
    - NSF XSEDE Supercomputers
      - https://www.xsede.org/
      - Example: https://www.xsede.org/rosie-blooms
    - NIH Commons Cloud Credits
      - https://www.commons-credit-portal.org/
  - Commercial
    - Azure, AWS, Google
- **Share instructions how to setup and run calculations**
- **Scaling Benchmarks**

MMTF Format

- **Use provided API's**
  - Protects from future changes to underlying format
- **Medium term: Support annotations**
  - Structure, model, chain, group, atom, and bond level
- **Long term: Support Integrated Hybrid Models**
  - Multiscale
  - Multistate
  - Time series (reaction cycle/pathway)
  - https://github.com/ihmwg/IHM-dictionary

MMTF API Changes



MMTF Community

- **Crowdsource, share, and reuse code**
- **Collaborate on projects**
- **Provide a support network**
- **Incubator projects for mmtf-spark/pyspark**
  - mmtf-spark-incubator (Java)
  - mmtf-pyspark-incubator (Python)
  - Require
    - Full documentation (e.g., JavaDoc)
    - Unit tests for all classes/methods
    - Demos showcasing capabilities
  - Productionize methods -> mmtf-spark/mmtf-pyspark

How Can you Support MMTF/Spark

- Spread the word (tweet #mmtf_spec)
- Contribute code
- Work on joint projects/grants
- Collaborate
- Provide letters of support
- Cite papers (see: http://mmtf.rcsb.org)
- Star Git Repositories
- Email: mmtf@rcsb.org
- Join Google Group: MMTF-Users