

# 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

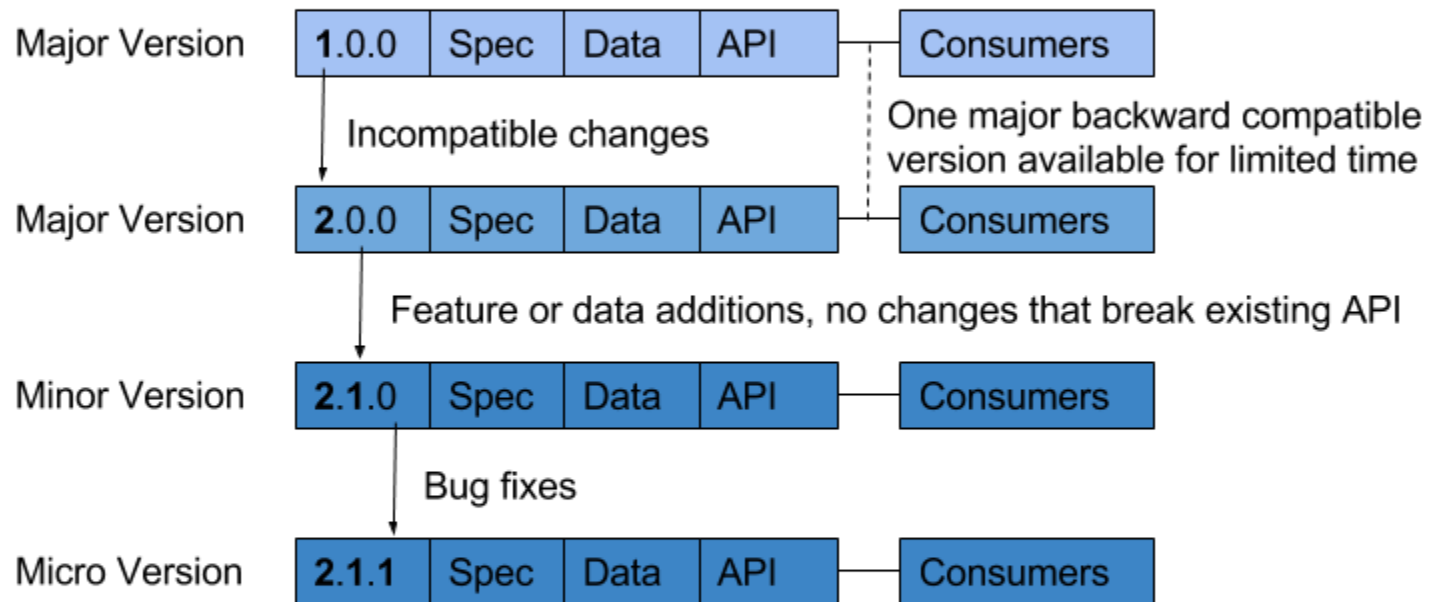
- **Cloud Providers**
  - Academic
    - NSF XSEDE Supercomputers
      - <https://www.xsede.org/>
      - Example: <https://www.xsede.org/rosie-blooms>
    - NIH Commons Cloud Credits
      - <https://www.common-credit-portal.org/>
  - Commercial
    - Azure, AWS, Google
- **Share instructions how to 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 - Semantic Versioning



# 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](mailto:mmtf@rcsb.org)
- Join Google Group: MMTF-Users



# Funding

This workshop was supported by the National Cancer Institute of the National Institutes of Health under Award Number U01CA198942. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health.

