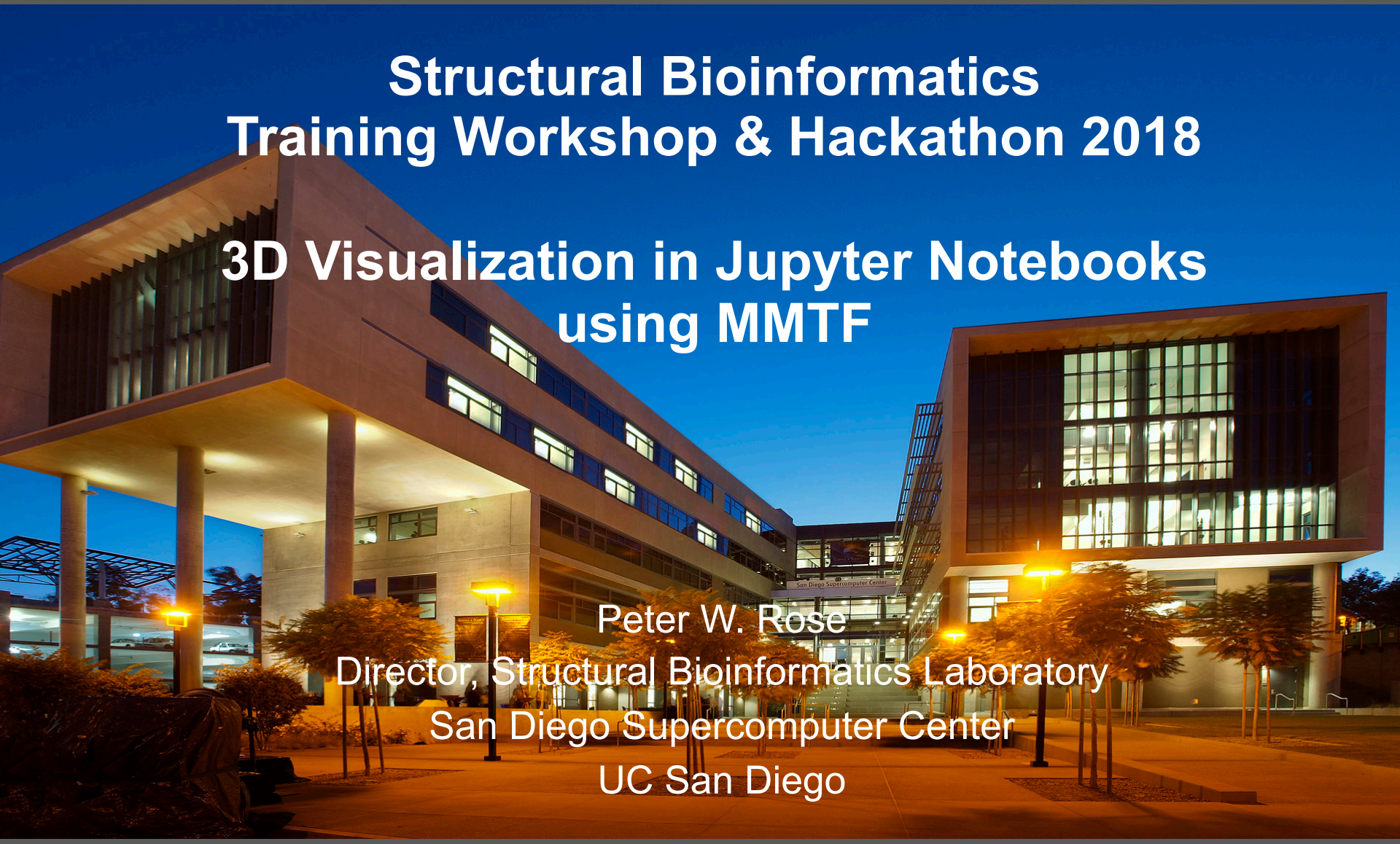
Structural Bioinformatics Training Workshop & Hackathon 2018

3D Visualization in Jupyter Notebooks using MMTF



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3D Visualization using MMTF

3D viewer fetches structures using MMTF web services
http://mmtf.rcsb.org/download.html

Data are decompressed on the client side using MMTF decoder libraries.

Jupyter Notebook Widgets for 3D Visualization

NGLview

- **Wrapper around NGL**
- WebGL-based JavaScript viewer
- MMTF-JavaScript API
- Subset of NGL features
- Supports visualization of trajectories

- Website: http://nglviewer.org
- https://github.com/arose/nglview

py3Dmol

- **Wrapper around 3Dmol.js**
- WebGL-based JavaScript viewer
- MMTF-JavaScript API

- Website: http://3dmol.csb.pitt.edu
- https://github.com/3dmol

Resources

- **NGL**
  - Rose AS, et al. (2016) Web-based molecular graphics for large complexes. In Proceedings of the 21st International Conference on Web3D Technology (Web3D '16). ACM, New York, NY, USA, 185-186. https://doi.org/10.1145/2945292.2945324
  - Nguyen, H, et al. (2018) NGLview–interactive molecular graphics for Jupyter notebooks, Bioinformatics 34, 1241–1242, https://doi.org/10.1093/bioinformatics/btx789

- **3Dmol.js**
  - Rego, N, Koes, D (2015) 3Dmol.js: molecular visualization with WebGL, Bioinformatics 31, 1322–1324, https://doi.org/10.1093/bioinformatics/btu829

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