# Serial Femtosecond Crystallography at the Linac Coherent Light Source

Chunhong Yoon

Research Software Developer

BASCD2016, 3/Dec/16









Eadweard Muybridge, 1878 Horse in motion

# **Femtosecond Photography of Small Particles**









Office of Science



The Linac Coherent Light Source (LCLS) is world's first hard X-ray free-electron laser which can be used for determining the molecular structure of proteins.

SFX at the LCLS

# Why femtoseconds?

### SLAC

#### Diffraction before destruction



Ultrabright, ultrashort X-ray pulses outrun radiation damage producing sharp images of atoms and molecules.

# **Selenium-SAD at LCLS**

--SLA

Sample: Selenobiotinyl-streptavidin crystal

Photon energy: 12.8 keV (Se K-edge: 12.6 keV)

Anomalous difference  $\Delta F/F$ : 1%



Hunter, M. S., Yoon, C. H., ..., Boutet, S. et. al. (2016). Selenium single-wavelength anomalous diffraction de novo phasing using an X-ray Free Electron Laser. *Nature Communications*.

# Serial Femtosecond Crystallography (SFX) Setup

Detector Liquid Jet KB Mirrors Primary Interaction Point Undulator (420 m upstream)

Diffraction before destruction Number of pulses/sec: 120 Millions of diffraction patterns from crystals Classification Problem: Hit or Miss?



## **Selenium-SAD: Setup**















# Selenium-SAD: 3D Merge

- Num. of images: 7,601,841 (35TB)
- Num. of hits: 1,567,793 (20%)
- Indexed patterns: 481,079 (31%)







# **Selenium-SAD: Phase Retrieval**

- Selenium anomalous signal is used to pinpoint the selenium sites.
- This is enough information to solve the entire structure of streptavidin.
- First ever demonstration of Se-SAD with a free-electron laser.

Figure of Merit:  $R_{split}$ : 0.048  $CC_{1/2}$ : 0.998  $CC_{ano}$ : 0.177 Resolution: 32.51-1.90 A  $R_{work}$  /  $R_{free}$ : 0.166 / 0.199

Selenobiotin is shown in balls and sticks model and its electron-density colored in blue.



SLAC

LCLS-II: Two RA positions available for exascale computing.

Email: yoon82@stanford.edu

