



# Structural Molecular Biology at SSRL: Computer Hardware

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Hardware Session

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# Macromolecular Crystallography Group



- Operates 6 beamlines at SPEAR3
- Typical crystallography experiment
  - 16 – 48 hours of beamtime
  - Multiple samples
  - 100GB – 1TB data
  - Processing of data as it becomes available



# Our Users

- User Program
  - 130+ Active user groups
  - More than 90% remote
  - Data collection and processing
  - Large proportion of interactive usage.
- JCSG Structure Determination Core
  - Large number of data sets collected
  - Structure determination by evaluating multiple solutions in parallel
  - Mostly batch processing
  - Spare cycles used by Kornberg group at Stanford for EM image processing
- Staff research and development



# Hardware

- User program
  - 32, 8 Core, Nehalem based blades
  - 360TB effective storage, HA NAS
  - Moderate addition of processing power expected due to increase in automation of data analysis.
- JCSG
  - 40, 8 Core, mostly Nehalem based, rack servers
  - 80TB mirrored storage, NAS
  - Expecting to stay at the present amount of hardware, gradually updating to “current” technology



# Publications

Some publications related to scientific computing originating in our group.

Xsolve: parallel processing of JCSG diffraction datasets

H. van den Bedem, G. Wolf, Q. Xu and A. M. Deacon "**Distributed structure determination at the JCSG**" *Acta Cryst.* (2011). D**67**, 368-375

Xpleo: publicly available web application for modeling missing loops into electron density

H. van den Bedem, I. Lotan, J.-C. Latombe and A. M. Deacon "**Real-space protein-model completion: an inverse-kinematics approach**" *Acta Cryst.* (2005). D**61**, 2-13

Qfit: publicly available web application for modeling multiple sidechain conformations

H. van den Bedem, A. Dhanik, J.-C. Latombe and A. M. Deacon "**Modeling discrete heterogeneity in X-ray diffraction data by fitting multi-conformers**" *Acta Cryst.* (2009). D**65**, 1107-1117

Web-Ice: Data collection via web interface.

A. González, P. Moorhead, S. E. McPhillips, J. Song, K. Sharp, J. R. Taylor, P. D. Adams, N. K. Sauter and S. M. Soltis "**Web-Ice: integrated data collection and analysis for macromolecular crystallography.**" *J. Appl. Cryst.* 41, 176-184 (2008)