

# **A plan for macromolecular crystallography at NSLS-II**

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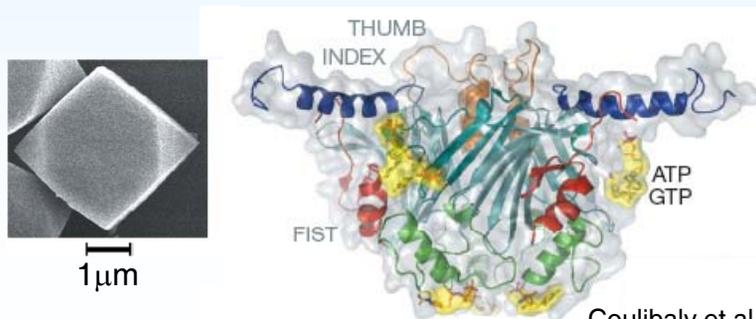
# The scientific case:

Macromolecular Complexes/Machines  
protein-protein, protein-DNA, ribosome, viruses

Protein ligand interactions  
rational drug design

## Microcrystals

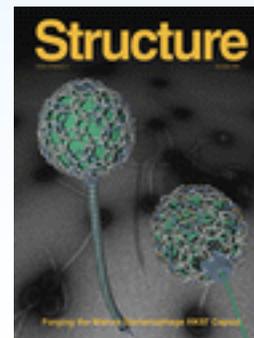
*The molecular organization of cypovirus polyhedra*



Coulibaly et al  
Nature (2007) 446, 97-101

## Large Unit Cells

*Forging the mature bacteriophage HK97 Capsid*



The HK97 virus capsid structure.

Unit cell dimensions 1010x 1010x 732 Å

## **MX at the NSLS:**

Provided venue for a Nobel prize for MX.

Strong production of premier pub's.

New developments – Mail-in, Automated Sample Centering, microcrystals, vis-light spectroscopy concurrent with MX

Strong automation for HTP.

A resource for Pharmas.

# Current NSLS programs:

## MX beam lines at the NSLS

X3A	Case Center for Proteomics
X4A/C	New York Structural Biology Center
X6A	NSLS/NIGMS
X8C	PXRR
X12B/C	PXRR
<b>X25*</b>	<b>NSLS/PXRR</b>
X26C	PXRR
<b>X29*</b>	<b>PXRR/Case</b>

\* Insertion Device Beam Lines

# User demand/productivity:

A good measure is PDB depositions

Year	ALS	APS	CHESS	NSLS	SSRL
2005	379	820	99	420	184
2006	468	1061	84	505	216
2007	290	899	58	398	261

**NSLS is very productive, and is competitive with the others.**

## **Goals:**

- Provide state of the art stations when NSLS-II comes on line.
- Continuity of service!

# **New NSLS-II Beam lines:**

Two sectors with one ID in each:

One, MX1, will serve the most challenging problems and be versatile (variable focusing, ancillary tools).

The other, MX2, will emphasize high throughput (automation).

# Moving NSLS Programs:

Three beam lines on three-pole-wigglers (3PW) to be built from appropriate optical elements and experimental stations now at the NSLS.

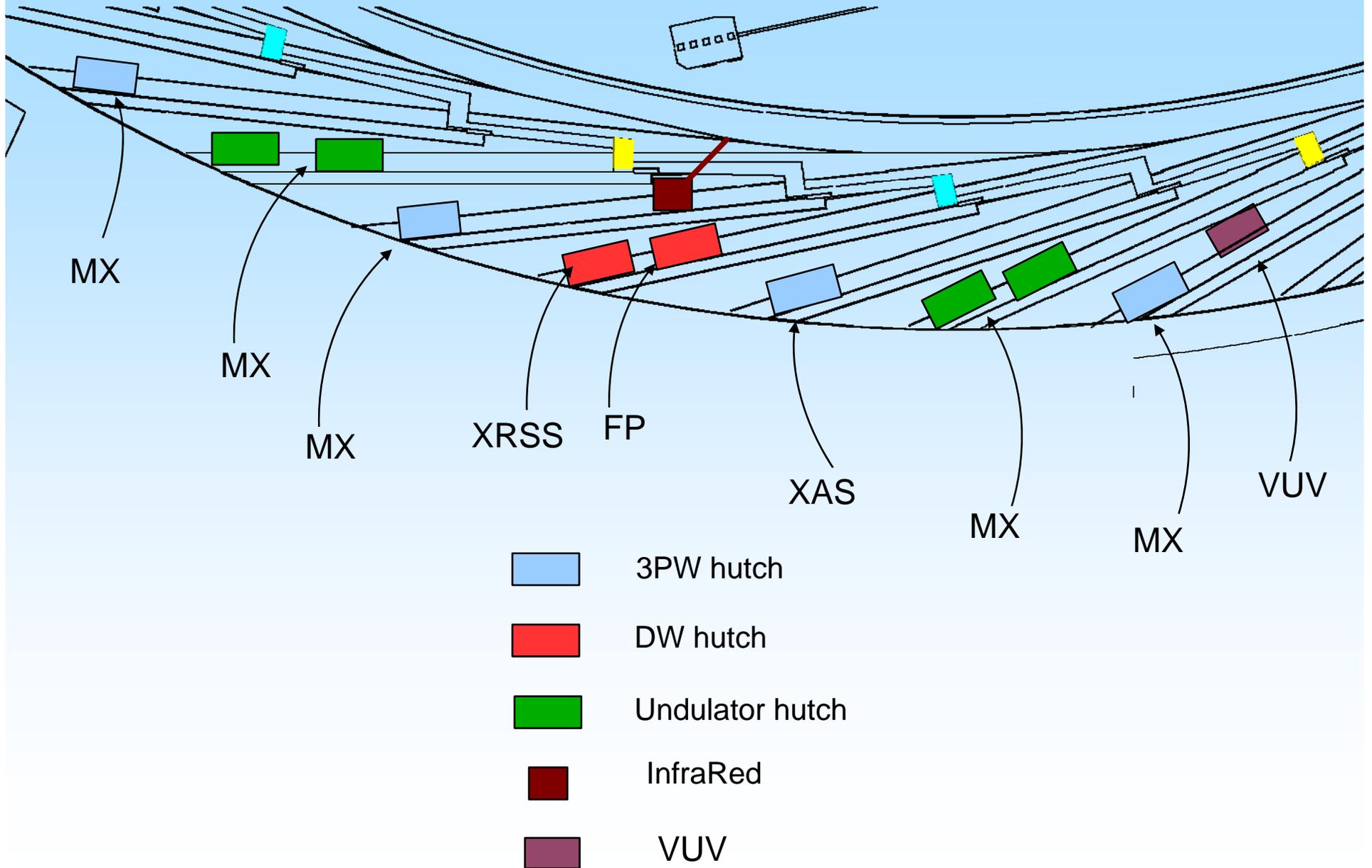
Would give **five** MX beam lines at NSLS-II.

## A coherent suite of beamlines

Already the Case community under Mark Chance, and we, have agreed to pursue a coherent design for three sectors:

- Low/high/low-beta sectors for two pairs of canted undulators for MX and a pair of canted DWs.
- Front of DW would be developed for footprinting.
- Back would be phase-II dev. for XAS, XRSS (x-ray solution scattering, both low and high angle), or MX.
- 3PW for XAS.

# A Suite of Structural Biology Beamlines



# Strategy I:

- Find agreement within the community on a basic start point.
- Create a Letter of Intent (LOI) for Phase I.
- Get EFAC approval.
- Take the plan to appropriate funding agencies.
- Write a grant proposal.
- Build beam lines in coordination with other life science beam lines



# Strategy II:

*What needs to be done over the next couple of months*

1. Transform the white paper to a LOI, while recruiting a beam line development team
2. Create advisory committees
3. Seek continuing funding from DOE/NIH for R&D projects and beam-line upgrades.

# Transition Timeline

	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017
White paper, LOI, EFAC										
Submission of Grant Proposal										
Funding for construction of two ID BL										
Design ID BL										
Order components for ID BL										
Construction ID BL										
Commissioning ID BL										
NSLS-NSLSII										
Select NSLS BL's for decommission										
NSLS BL decommission										
Rebuild NSLS BLs at NSLS II										
Commissioning										
Proposal for more MX beam lines, LOI, EFAC, grant proposal, funding, etc.										

# **Current funding:**

NSLS programs are currently funded by:

NIH – NCRR, NIGMS, NIBIB

DOE – BES

New York Structural Biology Center

## **Future funding:**

These agencies have been already approached but a strategy needs to be developed. We hope this effort will seed other BDTs and other funding sources.

## **The bottom line:**

We believe that structural biology in the US will be well served by there being state-of-the-art macromolecular crystallography stations at the NSLS-II from the beginning of its operation. This plan should achieve that.

## **Development research –**

The life-science community should be able to create long-term funding for personnel in J-→ building.

Could improve x-ray detectors, x-ray optical systems, and automated systems for specimen manipulation.

# Structural biology research –

Something like the Partnership for  
Structural Biology – <http://psb.esrf.fr/>



## **Multi-disciplinary research –**

Include all the SR-based disciplines.

Vertically integrated research laboratory with facilities for cell growth, macromolecule purification, crystal growth, and characterization by other methods than light-based ones – NMR, mass spectrometry, and electron microscopy.