Some Economic Considerations for Managing a Centralized Archive of Raw Diffraction Data

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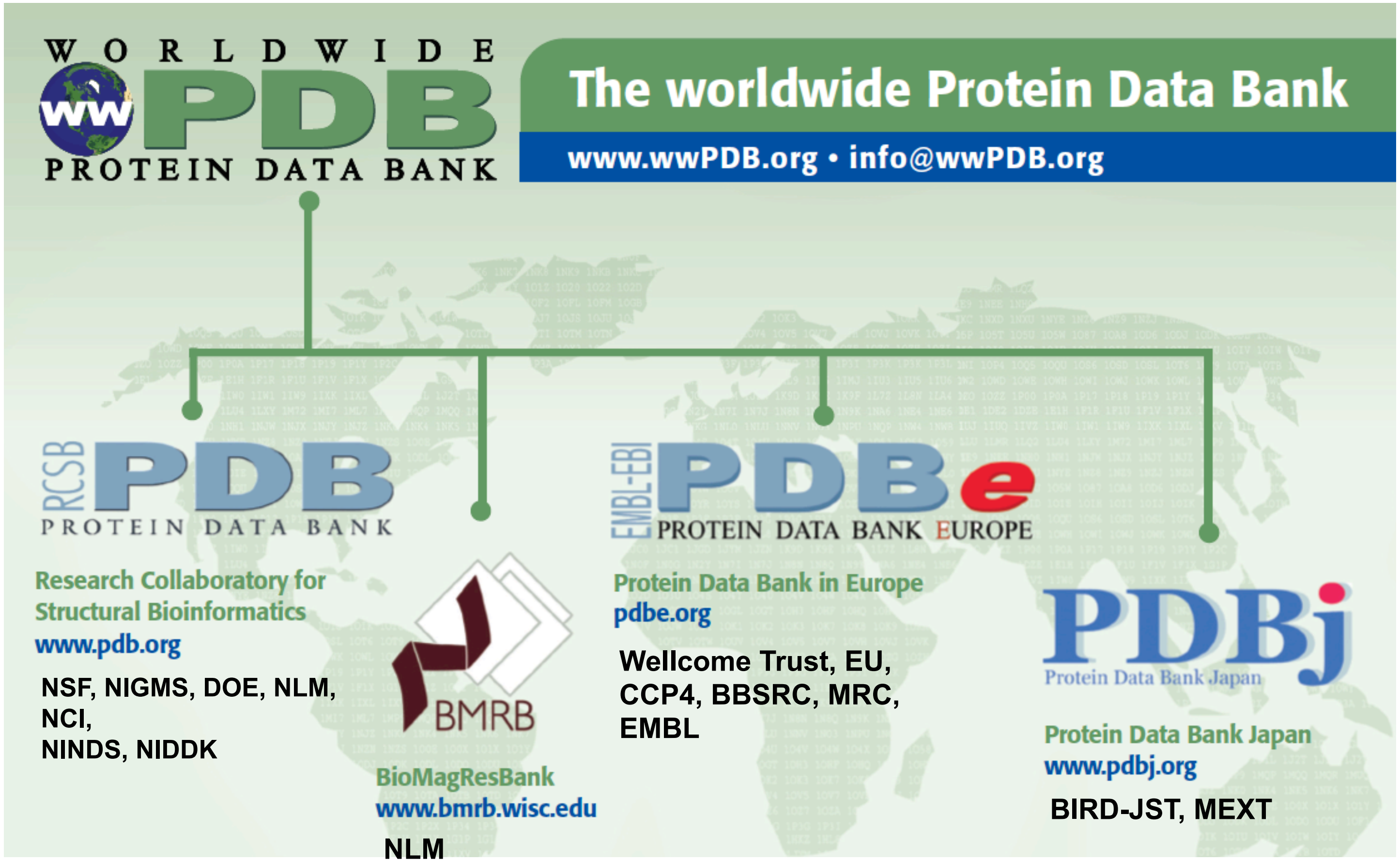
www.wwpdb.org

Overview

- PDB as a community partner
- Challenges and scope of archiving primary data
- Some technical and cost alternatives
- Possible incremental strategy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RCSB PDB PROTEIN DATA BANK
Research Collaboratory for Structural Bioinformatics
www.pdb.org
BMRB
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EMBL-EBI PDBe PROTEIN DATA BANK EUROPE
Protein Data Bank in Europe
pdbe.org
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NSF, NIGMS, DOE, NLM, NCI,
NINDS, NIDDK

NLM

Wellcome Trust, EU, CCP4, BBSRC, MRC, EMBL

BIRD-JST, MEXT

A unique scientific collaboration providing the authoritative global resource for experimentally determined 3D structures of important macromolecules.

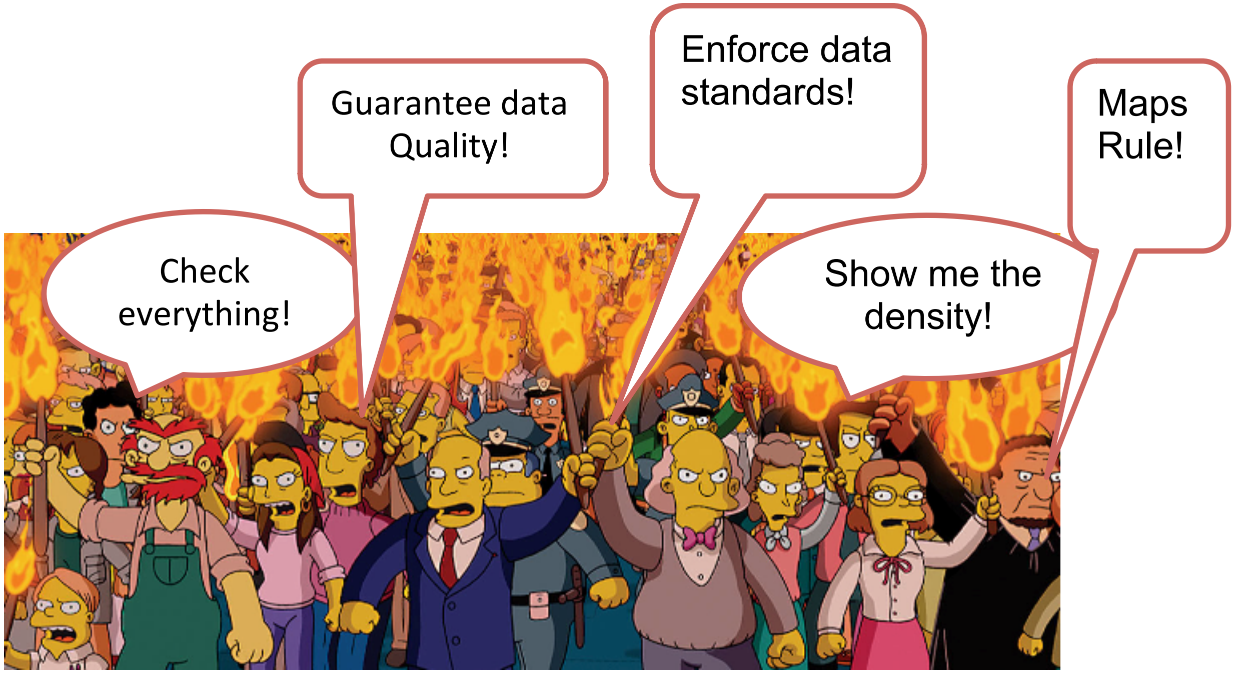
- Formalization of current working practice
- MOU signed July 1, 2003
- Announced in *Nature Structural Biology* November 21, 2003
- **Each partner funded locally**

Changing View of PDB

A Generally Hands-Off Role

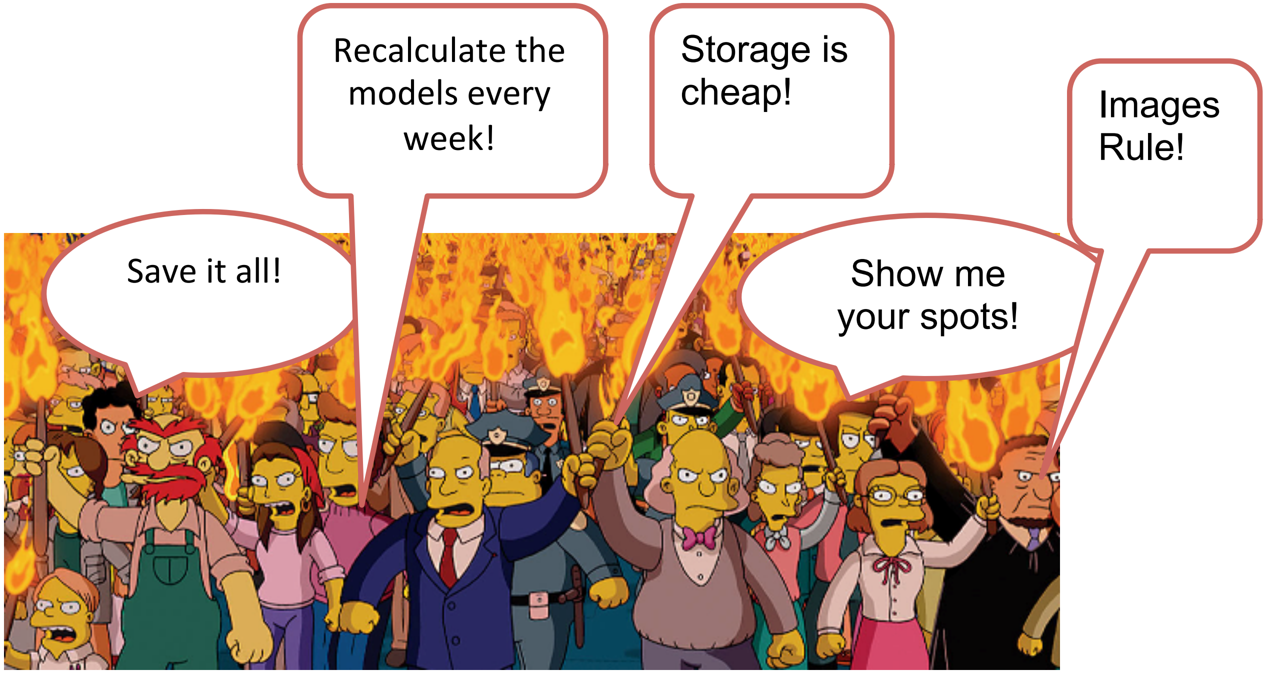
Changing View of PDB

Increasing Emphasis on Data Quality



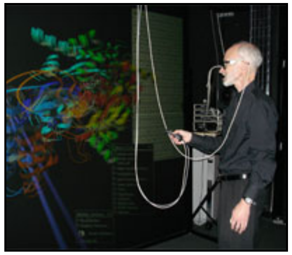
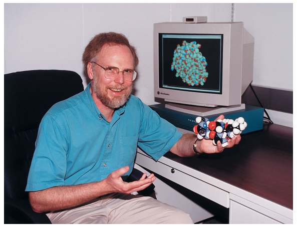
Changing View of PDB

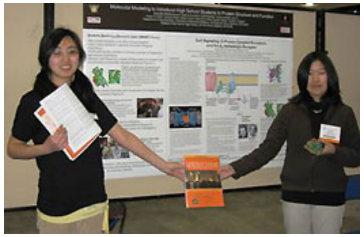
Increased Emphasis on Data Archiving

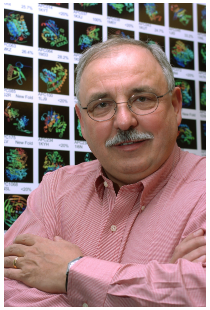


Who Downloads PDB data?

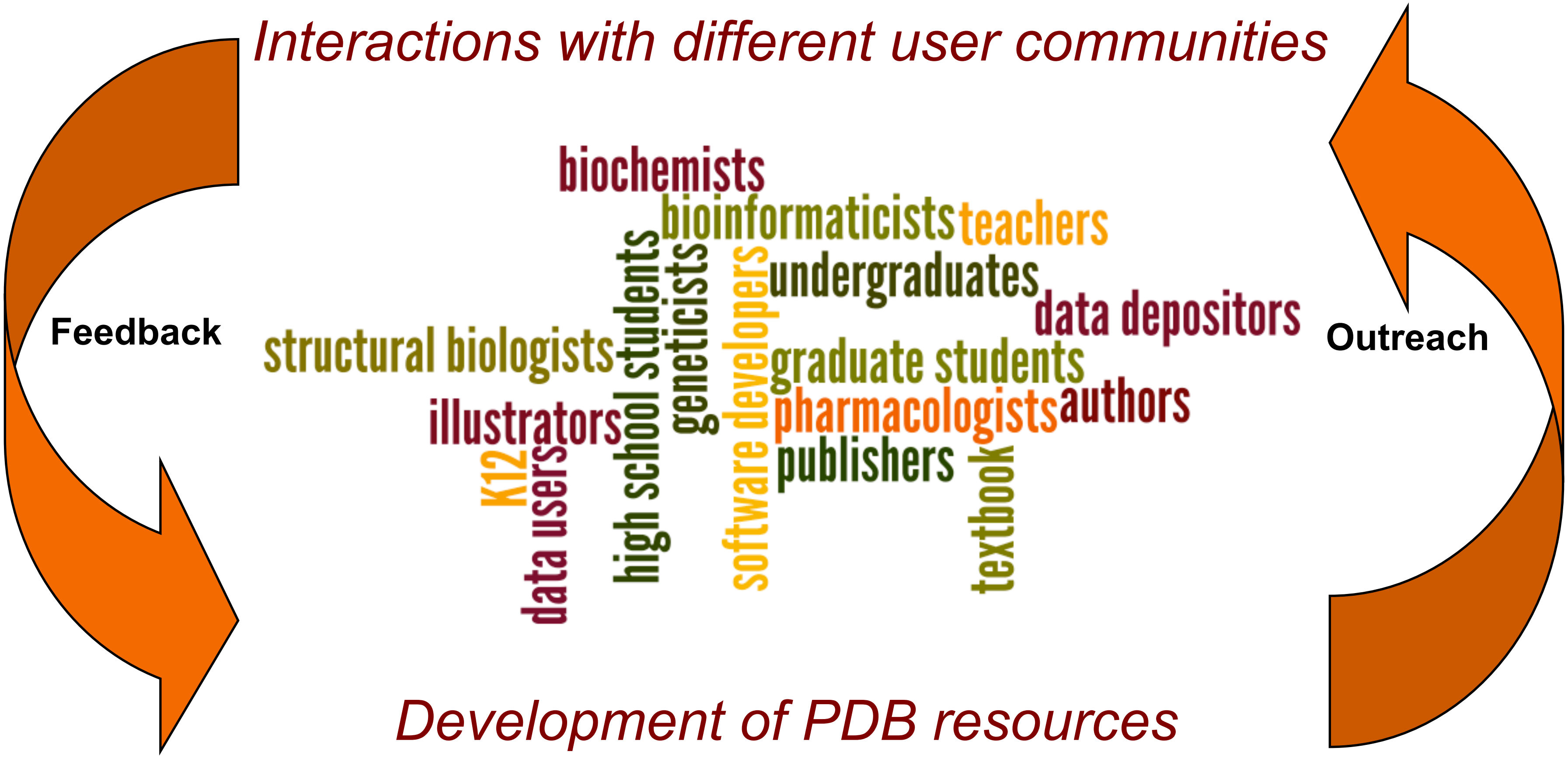
- Structural biologists
- Experimental biologists
- Computational biologists
- Biochemists
- Molecular biologists
- Educators
- Students





How Do We Interact With These Communities



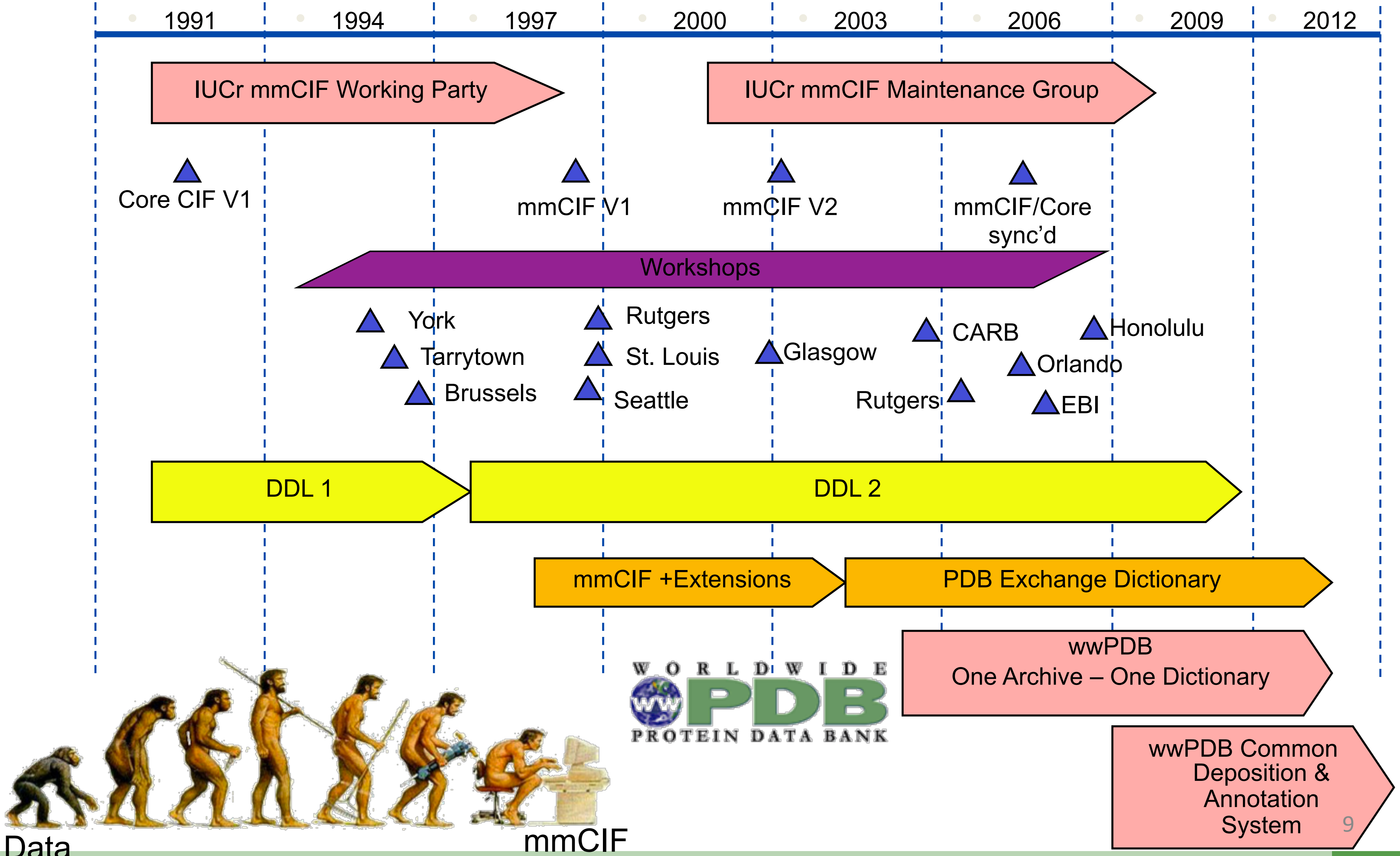
Interactions with different user communities

Feedback

Outreach

Development of PDB resources

Community Driven Data Standards PDBx/mmCIF



1991 1994 1997 2000 2003 2006 2009 2012

IUCr mmCIF Working Party

IUCr mmCIF Maintenance Group

Core CIF V1

mmCIF V1

mmCIF V2

mmCIF/Core sync'd

Workshops

York

Tarrytown

Brussels

Rutgers

St. Louis

Seattle

Glasgow

Rutgers

CARB

Orlando

EBI

Honolulu

DDL 1

DDL 2

mmCIF +Extensions

PDB Exchange Dictionary

wwPDB
One Archive – One Dictionary

wwPDB Common Deposition & Annotation System

WORLDWIDE PDB PROTEIN DATA BANK

Data

mmCIF

wwPDB Task Forces

To collect recommendations and develop consensus on method-specific issues, including validation checks that should be performed and identification of validation software applications.

X-ray Validation

- 2008 Workshop
- 2011 *Structure* publication
- Chair: Randy J. Read (University of Cambridge)

3DEM Validation

- 2010 Meeting
- Chairs: Richard Henderson (Maps, MRC-LMB), Andrej Sali (Models, UCSF)
- White paper in progress

NMR Validation

- Meetings held 2009, 2011
- Chairs: Gaetano Montelione (Rutgers), Michael Nilges (Institut Pasteur)
- Report in progress

Small-Angle Scattering

- 2012 Meeting
- Members: Jill Trewhella (Univ Sydney), Dmitri Svergun (EMBL Hamburg), Andrej Sali (UCSF), Mamoru Sato (Yokohama City Univ), John Tainer (Scripps)

NMR

X-ray

EM

Workshops and Working Groups

3DEM Data Exchange

I2PC Workshop 2012 - Madrid

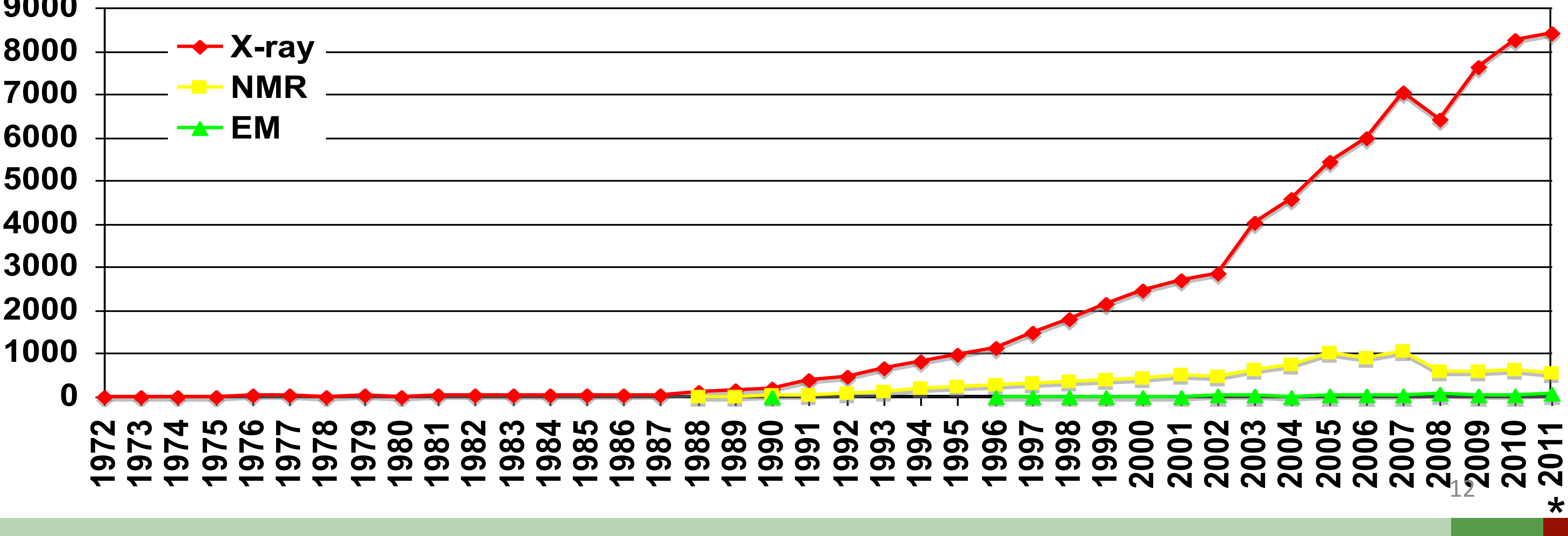
PDBx Deposition Working Group

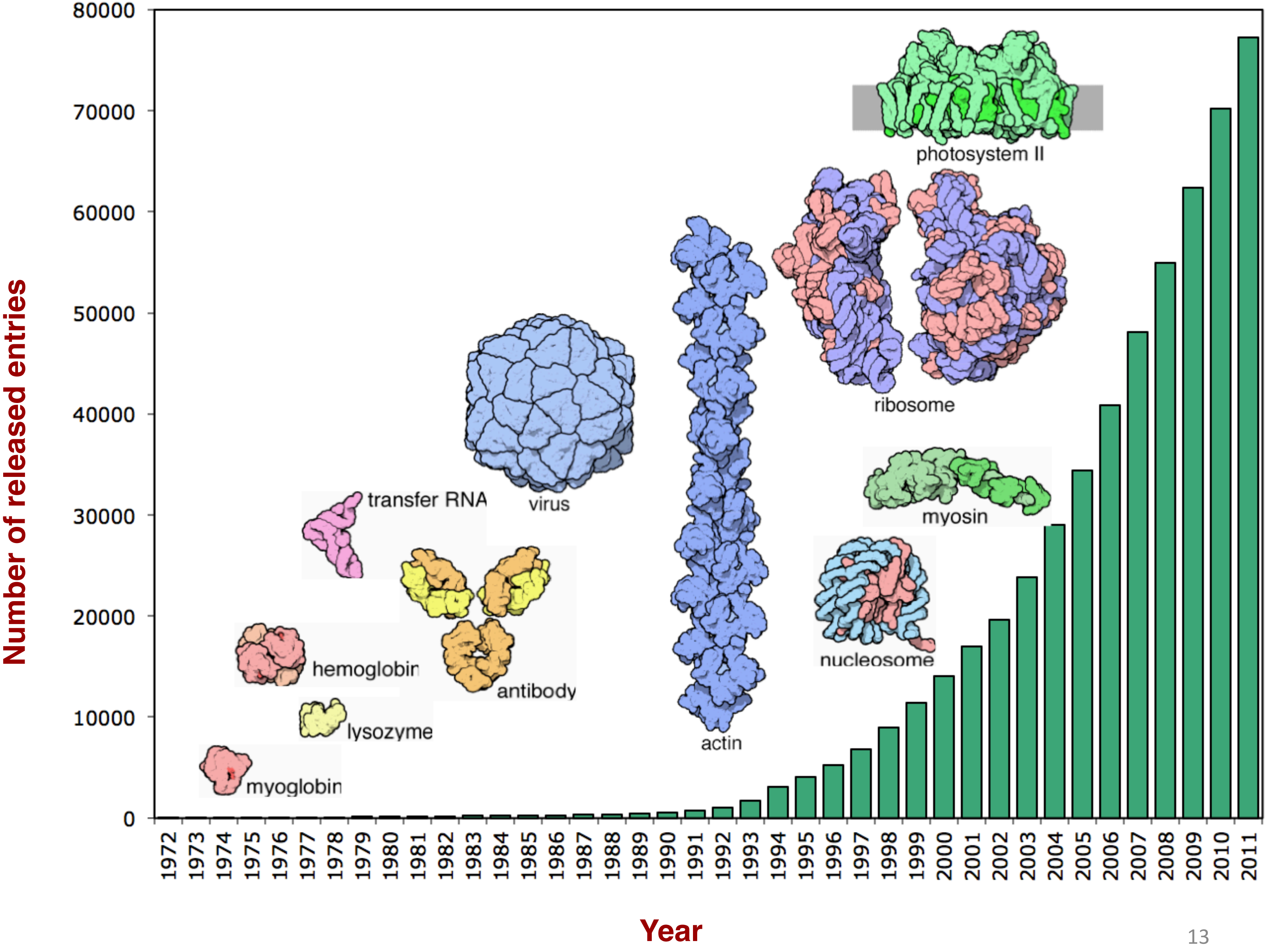
Refinement Developers Workshop 2011 - EBI

10,000-Fold Growth in Four Decades

- 83,400 entries
- 2012 will see ~10,000 depositions
- Over 85% entries include structure factor data used in the final refinement

Depositions in a calendar year by experimental method





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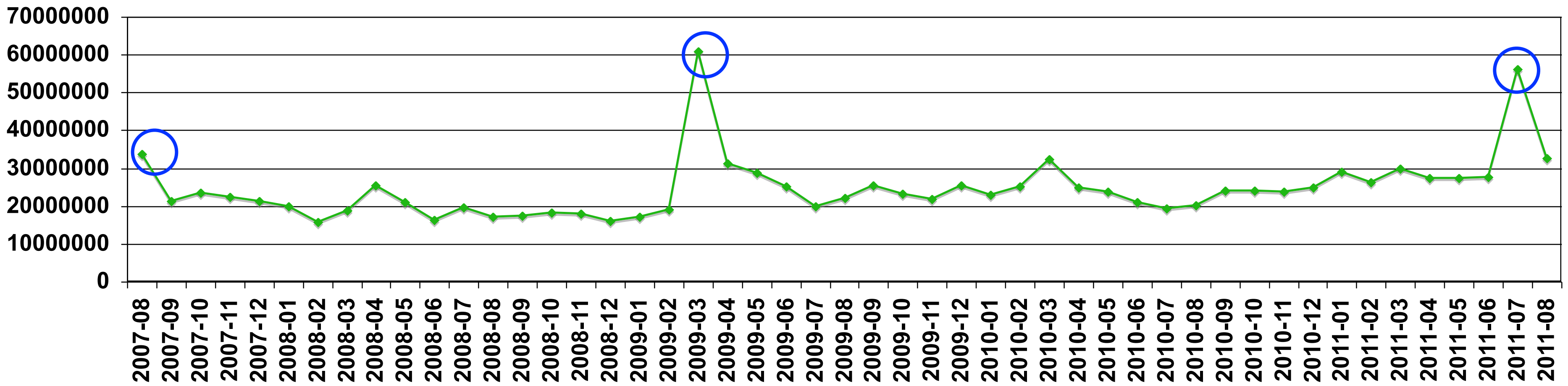
PDB FTP Downloads



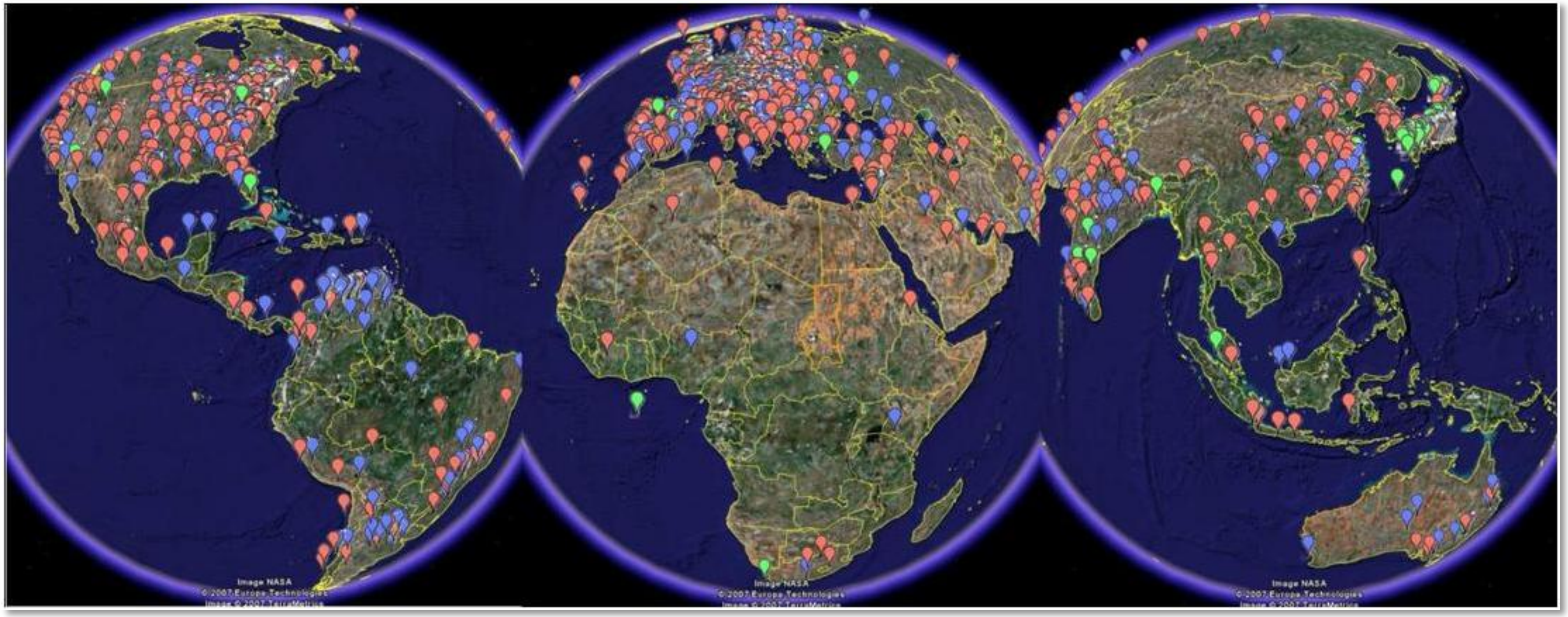
*
Version 3.0/3.1 files released

*
Version 3.15 files released

*
Version 4.0 files released

~2 M downloads/year of structure factor data files 2009-present

2010 FTP Traffic



🟥 **RCSB PDB**
159 million
entry downloads

🟦 **PDBe**
34 million
entry downloads

🟩 **PDBj**
16 million
entry downloads

Challenges and Scope

- Target content
- Longevity
- Example applications
- Audience
- Representation

What are the Content Targets?

- Laboratory data files
- Laboratory data files with supporting metadata
- Archival storage of standardized data and metadata

Expected Duration of Storage?

- Through publication review
- A few years not to exceed the availability of supporting hardware & software
- Longer …

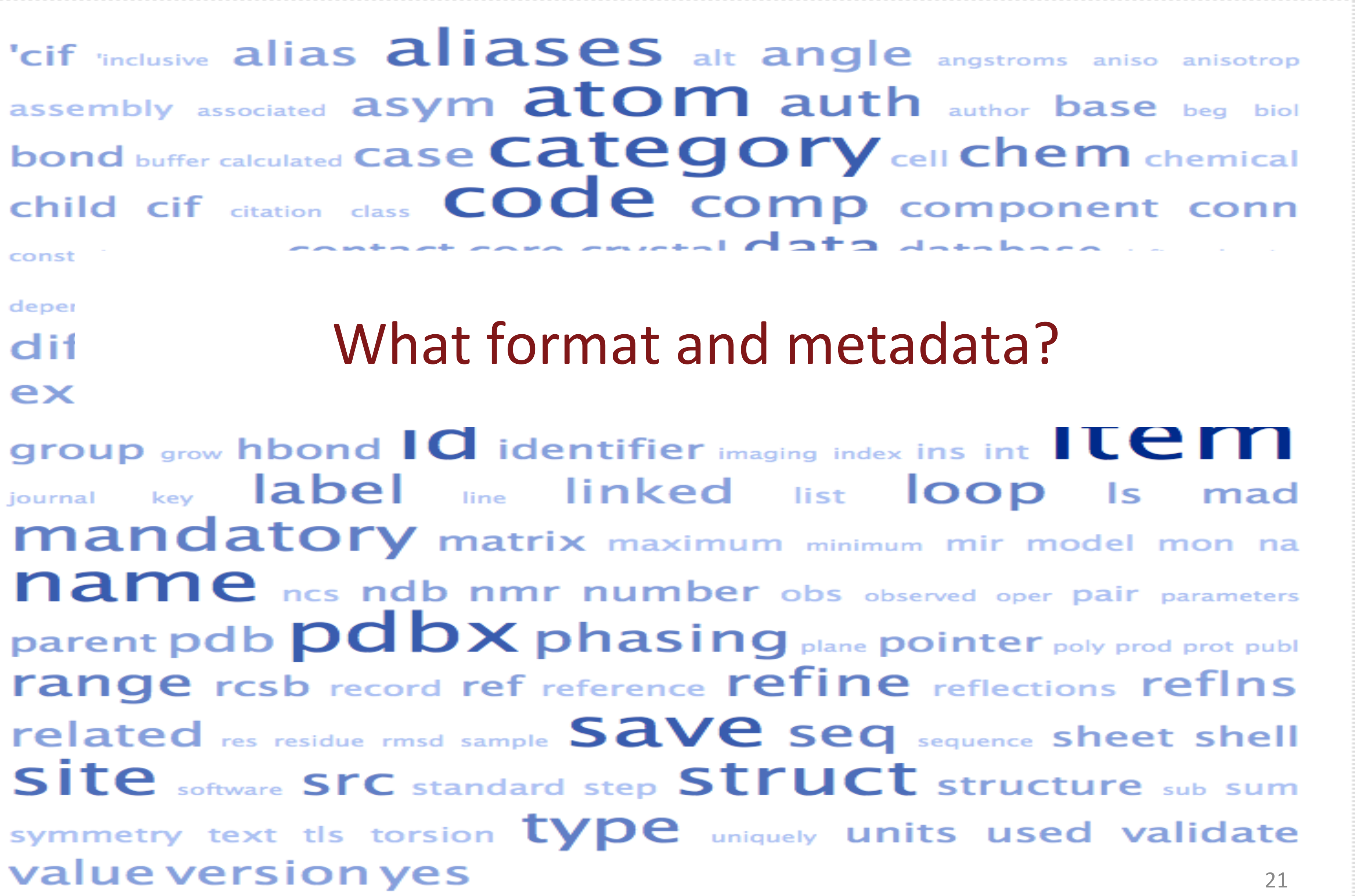
Use Cases

- Recover laboratory data files
- Satisfy philosophical/ethical/funding requirements
- Support peer review, reproduction, and validation of published results
- Extend on published results
- Provide test cases/benchmarks for methods development
- Preserve data from difficult cases

Audiences Impacted

- Direct Impact
  - Methods developers
  - Expert users
- Indirect Impact
  - Novice or non-specialist users

What format and metadata?



Archival Format and Metadata

- Solid metadata foundation for archiving -
  - CBF/imgCIF
  - PDBx/mmCIF
- Not widely used at early stages of the structure determination pipeline.
- How will working formats and process details be standardized for archiving?
  - Tar ball containing 1000 files from multiple data collections, multiple crystals, with multiple wavelengths …

Format and Metadata Targets

- Existing efforts provide data in program formats and limited software accessible metadata (e.g. TARDIS & JCSG)
- To what extent does this limit the audience and the useful lifetime of this data?

Technical Options

- Self-publishing
- Institution/facility hosting and delivery
- Centralized cloud delivery
- Centralized delivery by the PDB

Self-Publishing

- Contributor posts contents to a file sharing resource
  - Institution or facility storage resources
  - Google Drive –
    - 25GB $2.50/month - 16TB $800/month
  - Egnyte Hybrid Cloud
    - 150GB $300/yr
  - FileSwap
    - Up to 50 GB for $9.95/month
- Contributor registers DOI and digital signatures with archive

Centralized Cloud Delivery

Target one year ~ 10,000 x 5GB data sets

- Leased storage from a major provider
  - Amazon –
    - Storage - $0.125/GB/month
    - Access - ~$0.12-0.05/GB + $0.01/request
  - Google
    - Storage - $0.095/GB/month
    - Access - ~$0.21-0.08/GB + $0.01/request
- Application developed to manage depositions
- DOIs and signatures registered with archive

$75K storage + $5100/download in yr 1
$450K storage + $15.3K/download after yr 3

Archive Centralized Storage Hardware Costs

Target one year ~ 10,000 x 5GB data sets

- Cheap RAID or JBOD
  - 50TB ~ $30K or ~ $600/TB w/ 3yr maintenance
- NAS Expansion (disks and shelves only)
  - NetApp –
    - 50 TB ~ $83K or $1675/TB w/ 3yr maintenance
  - DDN -
    - 50 TB ~ $51K or $1025/TB w/ 3yr maintenance

Archive Centralized Storage

Minimum System Requirements

- Deposition site primary and backup copy
- Distribution site primary and backup copy
- Assume data requirement of 50 TB per year for the first 3 years -
  - Cheap RAID - $360 K
  - NetApp expansion - $ 996K
  - DDN expansion - $612 K
- In year 4, replace existing disk hardware + new storage for year four data.

At each wwPDB site

Archive Curation Costs

wildly optimistic estimates

- Early Stages –
  - 1 crystallographic application programmer
  - 1-2 annotators with deep expertise and troubleshooting experience with a variety of data collection, integration and phasing applications.
  - 1 scientific programmer to implement deposition and data processing automation

Comparable staffing requirements at each wwPDB site

Some Possible Practical Steps

- Tackle unmerged intensities first
- Register DOIs and digital signatures for locally store/self-published image data sets.
- Develop metadata extensions for all processing steps.
- Implement standard formats and metadata with facility control systems and pipeline software
- Pilot an automated data capture system with standard data format and metadata.

Acknowledgements

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RUTGERS

UCSD

SDSC • SKAGGS SCHOOL of PHARMACY and PHARMACEUTICAL SCIENCES

The RCSB PDB is a member of the

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