Design of the LCLS-2 Data Systems

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U.S. DEPARTMENT OF ENERGY
Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Outline

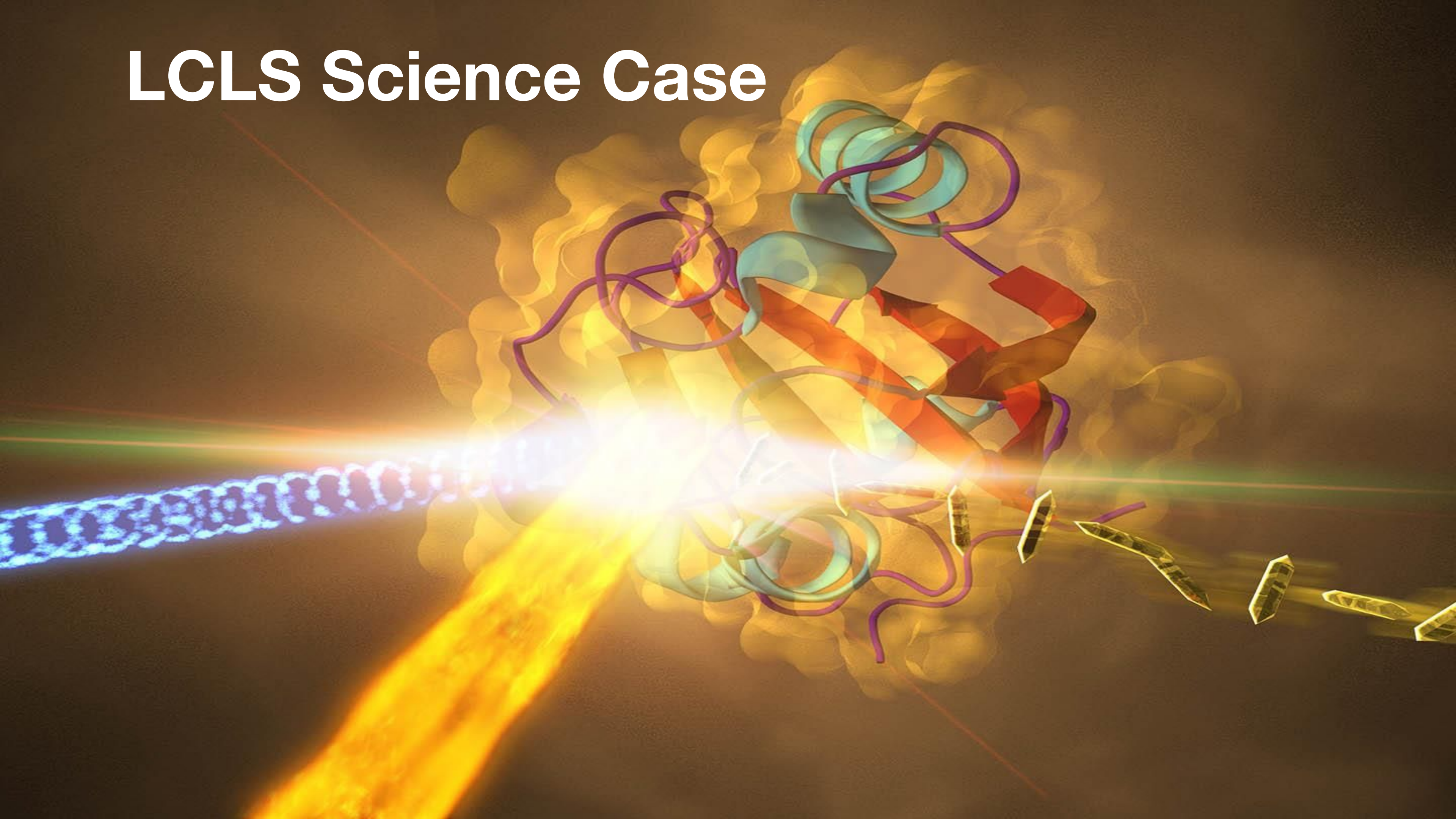
LCLS instruments and science case

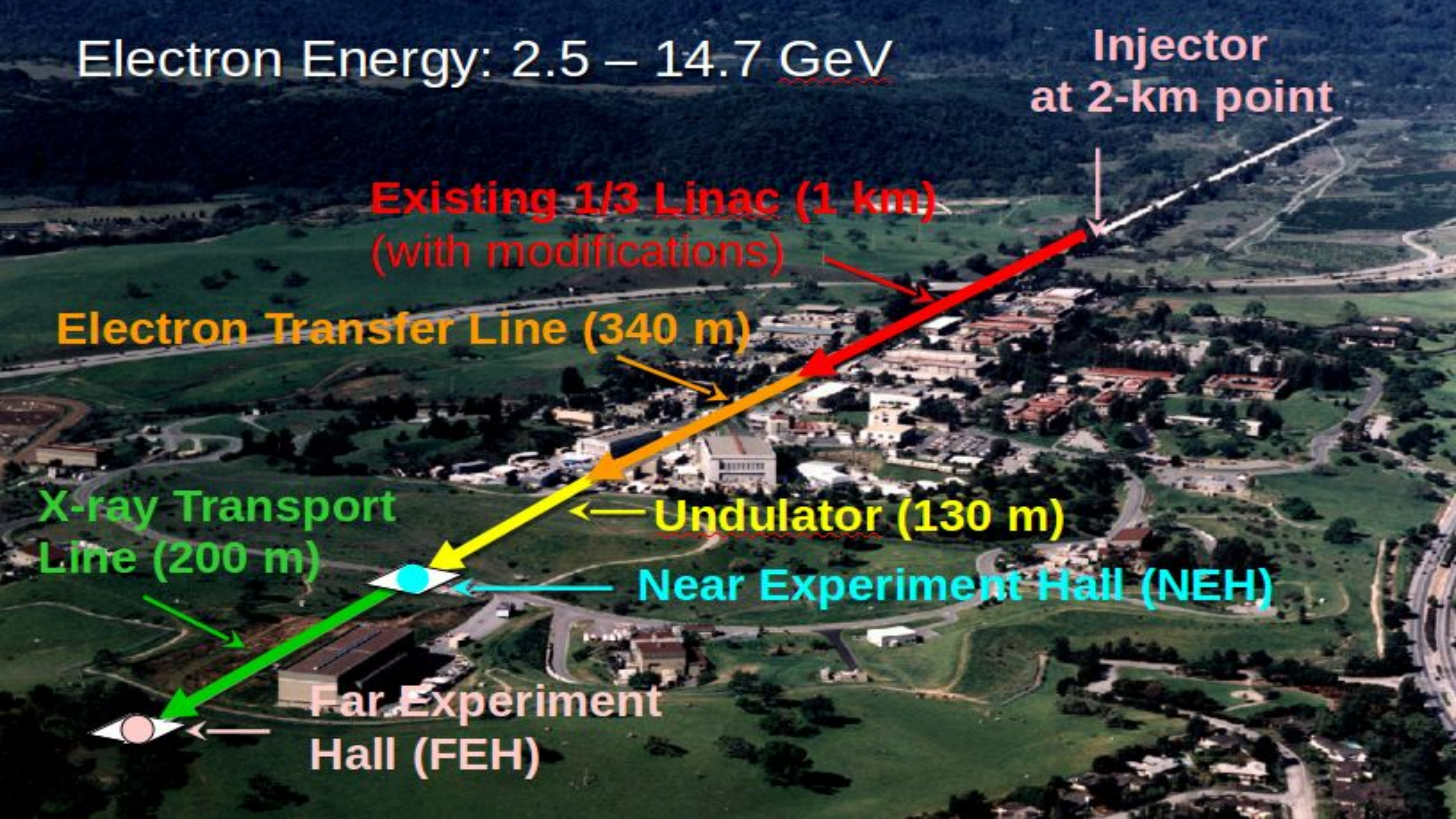
Guiding principles for the buildout of the LCLS-II data system

Projections

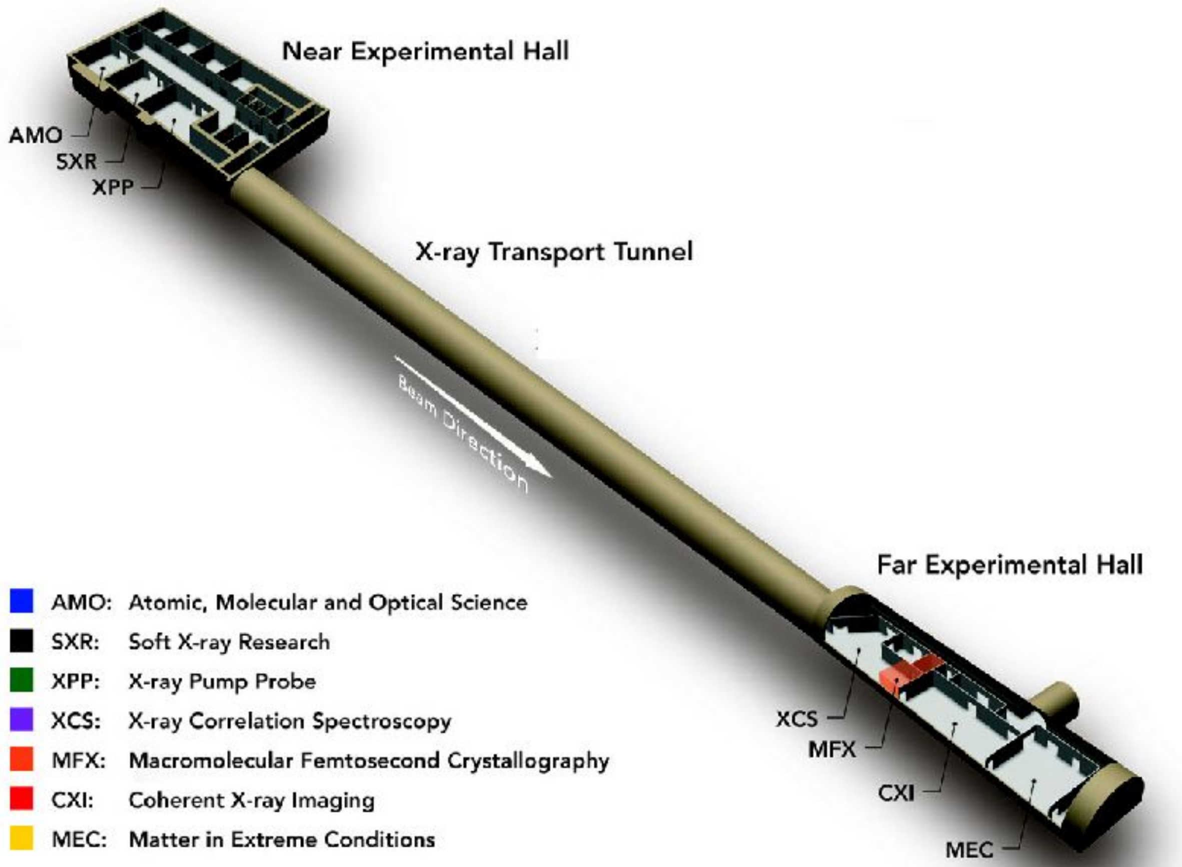
Design

LCLS Science Case




Electron Energy: 2.5 – 14.7 GeV
Injector
at 2-km point
Existing 1/3 Linac (1 km)
(with modifications)
Electron Transfer Line (340 m)
X-ray Transport
Line (200 m)
Undulator (130 m)
Near Experiment Hall (NEH)
Far Experiment
Hall (FEH)

LCLS Instruments



LCLS has already had a significant impact on many areas of science, including:

- ➔ Resolving the structures of macromolecular protein complexes that were previously inaccessible
- ➔ Capturing bond formation in the elusive transition-state of a chemical reaction
- ➔ Revealing the behavior of atoms and molecules in the presence of strong fields
- ➔ Probing extreme states of matter

Data Analytics for high repetition rate Free Electron Lasers

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FEL data challenge:

- **Ultrafast X-ray pulses** from LCLS are used like flashes from a high-speed strobe light, producing stop-action movies of atoms and molecules
- Both **data processing** and **scientific interpretation** demand intensive computational analysis

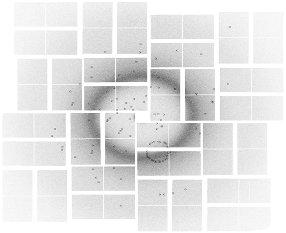
LCLS-II will increase **data throughput by three orders of magnitude** by 2025, creating an exceptional scientific computing challenge

LCLS-II represents SLAC’s largest data challenge by far

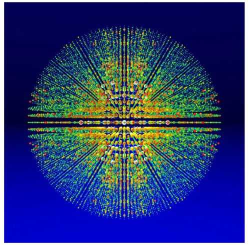
Example of LCLS Data Analytics: The Nanocrystallography Pipeline

Serial Femtosecond Crystallography (SFX, or nanocrystallography): huge benefits to the study of **biological macromolecules**, including the availability of femtosecond time resolution and the avoidance of radiation damage under physiological conditions (**"diffraction-before-destruction"**)

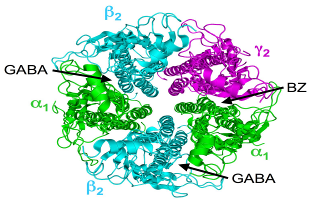
Megapixel detector



X-Ray Diffraction Image



Intensity map from multiple pulses



Electron density (3D) of the macromolecule

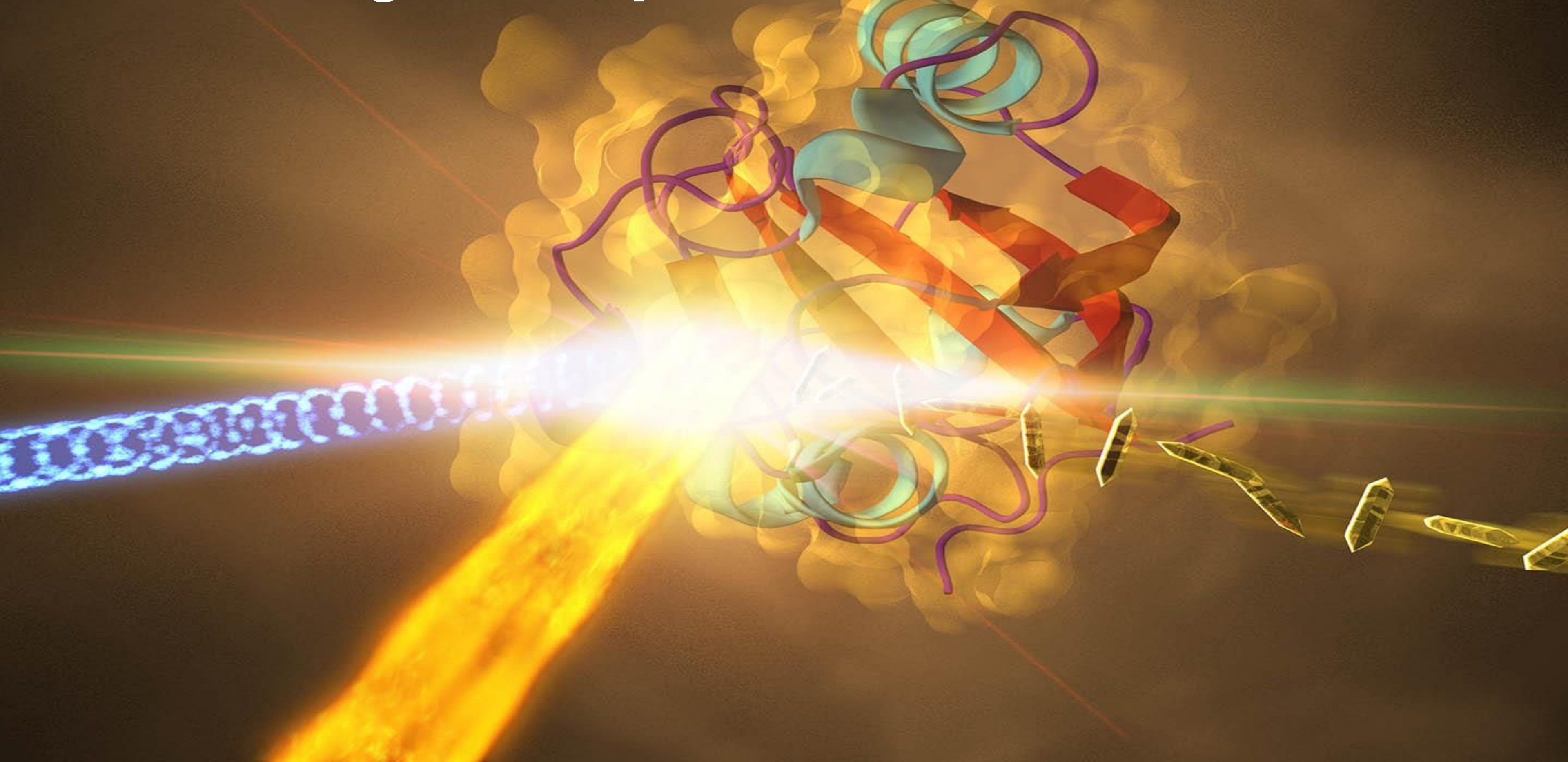
Well understood computing requirements

Significant fraction of LCLS experiments (~90%) use large area imaging detectors

Easy to scale: processing needs are linear with the number of frames

Must extrapolate from 120Hz (today) to 5-10 kHz (2022) to >50 kHz (2026)

Guiding Principles



Guiding Principles and Priorities

Key aspects LCLS-II data system:

1. **Fast feedback**
2. **24/7 availability**
3. **Short burst**
4. **Storage**
5. **Throughput**
6. Speed and flexibility of **development cycle** is critical

Hardware design guiding principles

Performance

Reliability

Ease of use

Software design guiding principles

Flexibility

User friendliness

Performance

When conflicts arise go back to the top guiding principle

Make full use of national capabilities

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LCLS-II will require access to **High End Computing Facilities (NERSC and LCF)** for highest demand experiments (exascale)

ESnet
Energy Sciences Network

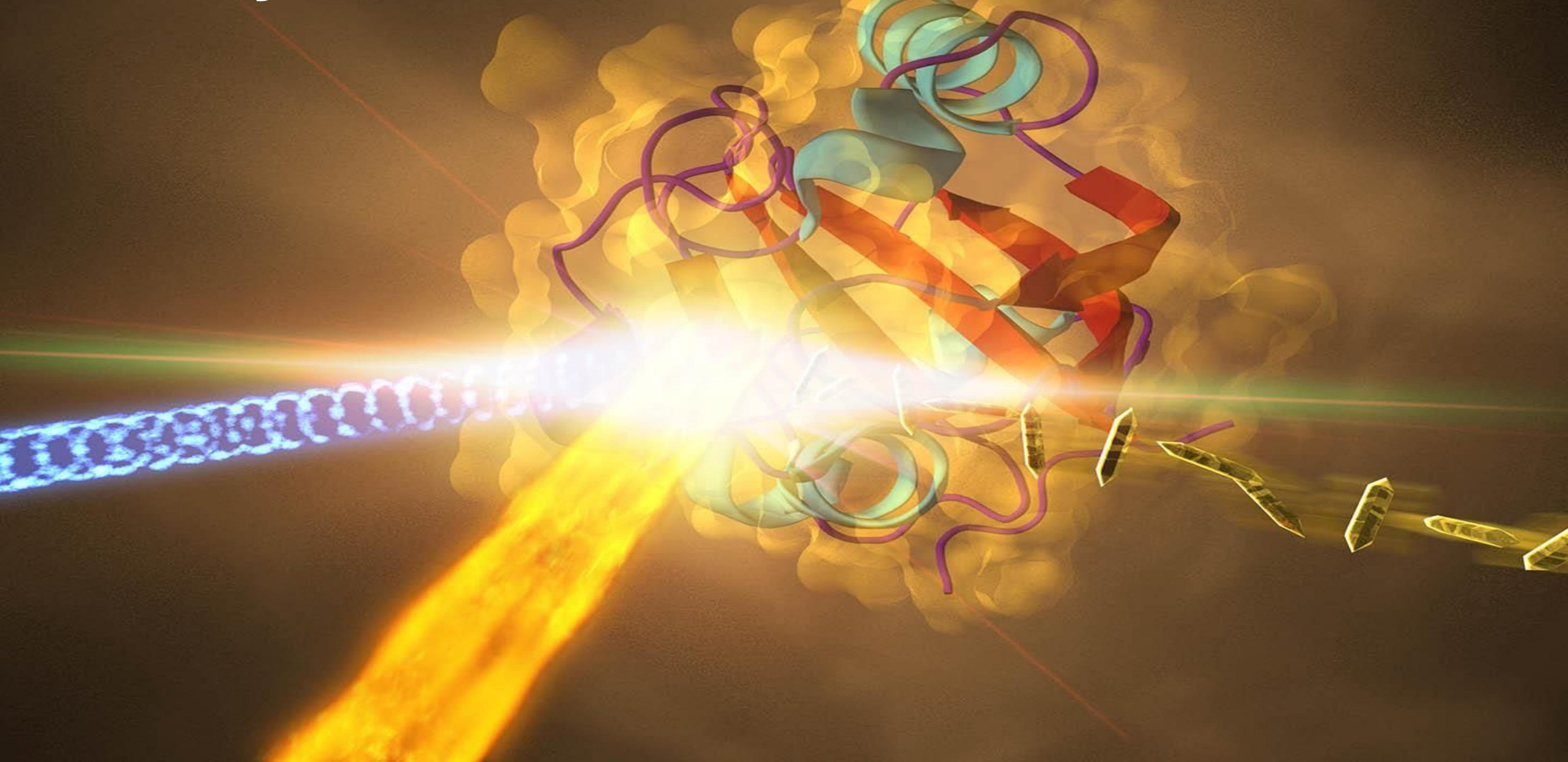
NERSC

Photon Science Speedway

Stream science data files on-the-fly from the LCLS beamlines to the NERSC supercomputers via ESnet

Very positive partnership to date, informing our future strategy

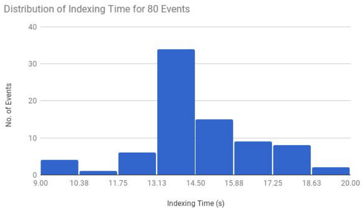
Projections



Process for determining future projections

Includes:

1. **Detector rates** for each instrument
2. **Distribution of experiments** across instruments (as function of time, ie as more instruments are commissioned)
3. Typical **uptimes** (by instruments)
4. **Data reduction** capabilities based on the experimental techniques
5. Algorithm **processing times** for each experimental technique



Time per event
x
Data rates

↓

Number of cores required

↓

FLOPS (~invariant)

Undulator	Instrument	Endstation	Technique	Detector	Detector Size	Detector Rate (Hz)	Data Rate (aggregate) (GB/s)	Ultilization Factor (0-1)	Data Reduction Type (1st Cut)	DR Factor (1st cut)	Data Reduction Type (Optimistic))	DR Factor (Optimistic)	FY20 Q1	FY20 Q2	FY20 Q3	FY20 Q4	FY21 Q1	FY21 Q2	FY21 Q3	F
SXU	NEH 1.1	DREAM	COLTRIMS	Digitizer	800000	100000	160.0	0.75	Zero suppression	0.020	Peak Finding	0.0020		1.00	1.00	0.50	0.25	0.25	0.25	0
SXU	NEH 1.1	DREAM	Time of Flight	Digitizer	1000000	100000	200.0	0.75	Zero suppression	0.020	Peak Finding	0.0020				0.13	0.13	0.13	0.06	0
SXU	NEH 1.1	LAMP	Time of Flight	Digitizer	1000000	100000	200.0	0.75	Zero suppression	0.020	Peak Finding	0.0020				0.13	0.13	0.13	0.06	0
SXU	NEH 1.1	LAMP	Imaging	SXR Imag. + Digi.	4000000	10000	82.0	0.45	Veto	0.100	N.A.	0.1000							0.13	0
SXU	NEH 2.2	LJE	XAS / XES	TES	1000	100000	20.0	0.60	Zero suppression	0.100	Binning	0.0000								0
SXU	NEH 2.2	LJE	XAS / XES	TES	10000	100000	200.0	0.60	Zero suppression	0.100	Binning	0.0000								
SXU	NEH 2.2	LJE	XAS / XES	RIXS-ccd	4096	1000	0.0	0.60	N.A.	1.000	Accumulating	0.0010				0.25	0.50	0.25	0.25	0
SXU	NEH 2.2	RIXS	IXS / RIXS	RIXS-ccd	4096	1000	0.0	0.60	N.A.	1.000	Accumulating	0.0010						0.13	0.13	0
SXU	NEH 2.2	RIXS	XRD / RXRD	SXR Imaging	1000000	10000	20.0	0.60	ROI	0.100	Accumulating	0.0001						0.06	0.06	0
SXU	NEH 2.2	RIXS	XPCS	SXR Imaging	1000000	10000	20.0	0.60	Compression	0.500		0.1000						0.06	0.06	0
SXU	NEH 1.2	---	X-ray/X-ray	SXR Imaging	1000000	10000	20.0	0.30	ROI	0.100	Binning	0.0001								
SXU	NEH 1.2	---	Imaging	epix100-HR + Digi.	4000000	5000	42.0	0.45	Veto	0.100	N.A.	0.1000								
SXU	NEH 1.2	---	XAS / XES	RIXS-ccd	4096	1000	0.0	0.60	N.A.	1.000	Accumulating	0.0010								

Scale of the LCLS-II Data Challenge: Throughput and Processing Projections

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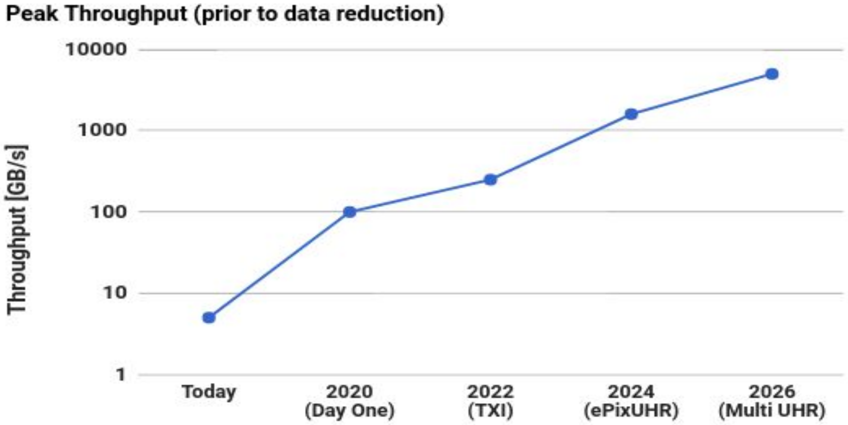
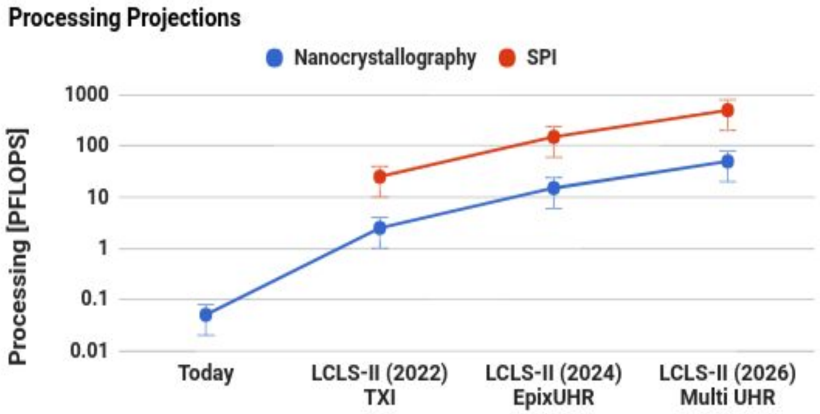




Example data rate for LCLS-II (early science)

- 1 x 4 Mpixel detector @ 5 kHz = **40 GB/s**
- 100K points fast digitizers @ 100kHz = **20 GB/s**
- Distributed diagnostics 1-10 GB/s range

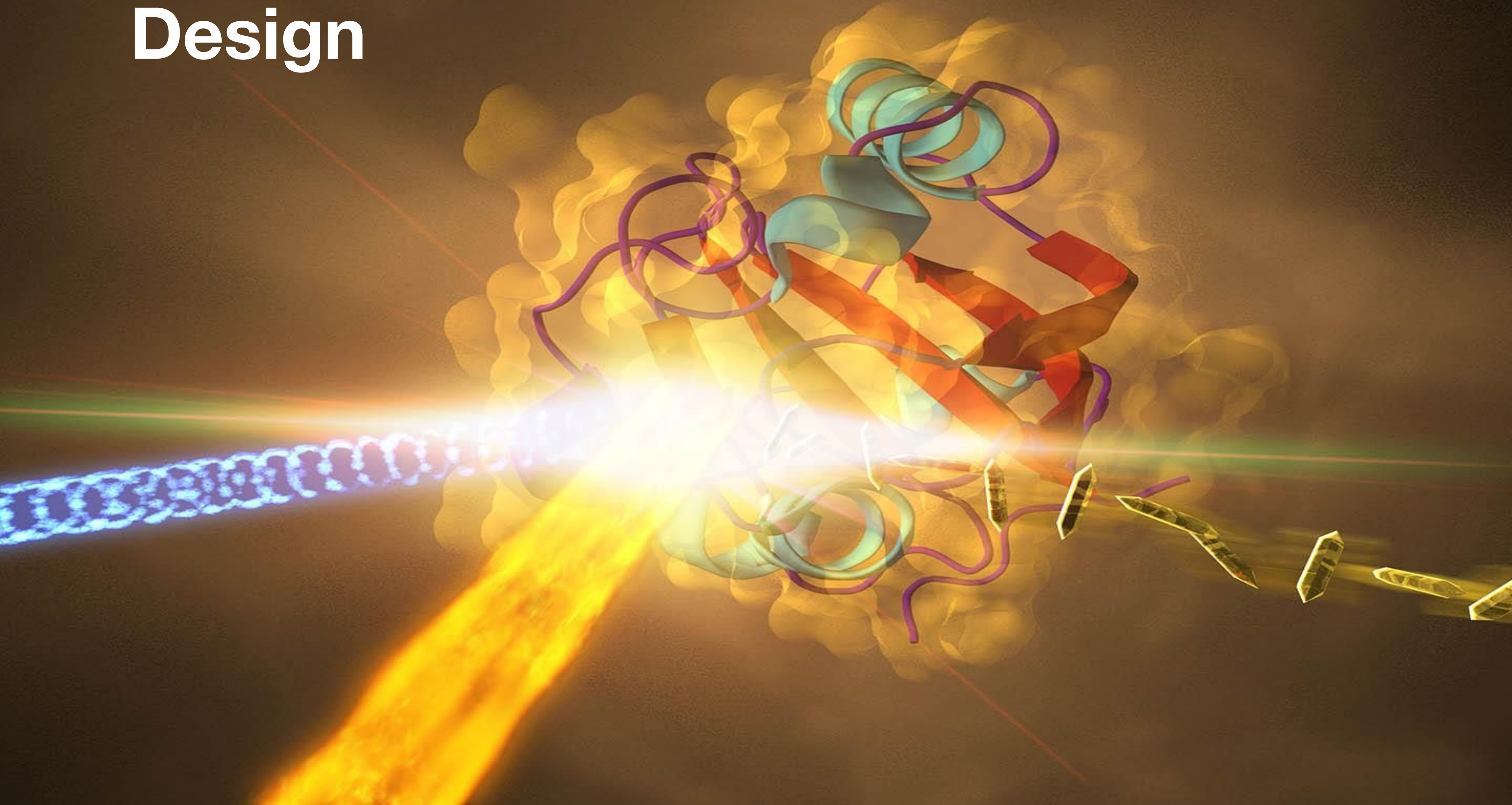
Example LCLS-II and LCLS-II-HE (mature facility)

- 2 planes x 4 Mpixel ePixUHR @ 100 kHz = **1.6 TB/s**

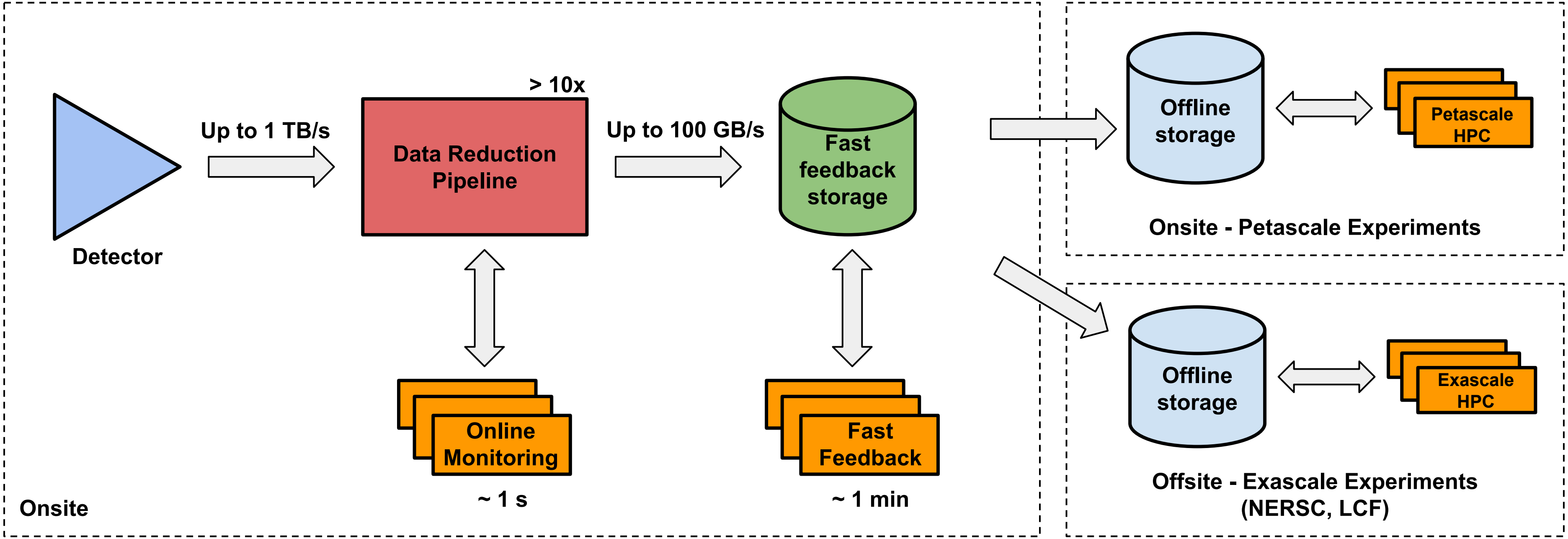
More sophisticated algorithms currently under development (e.g., for single particle imaging) will require exascale machines

Throughput requirements are extremely challenging: data reduction needed

Design

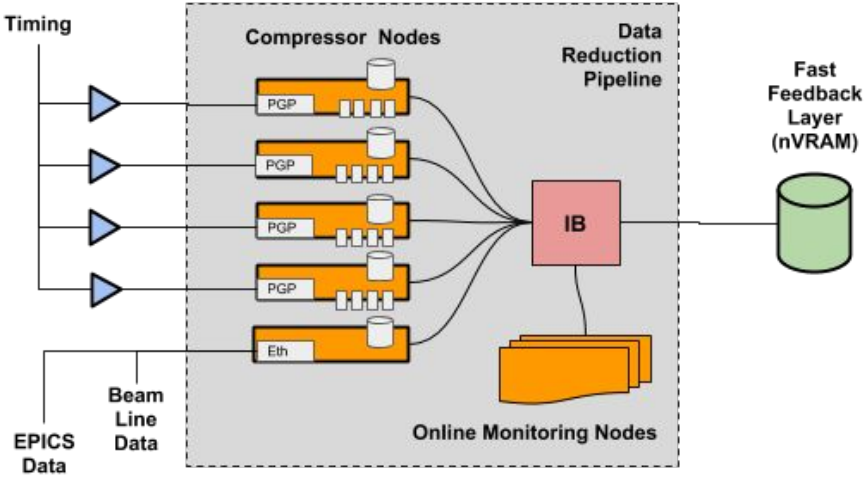


LCLS-II Data Flow



Data Reduction Pipeline

- Besides cost, there are **significant risks** by not adopting on-the-fly data reduction
  - Inability to move the data to HEC, system complexity (robustness, intermittent failures)
- Developing toolbox of techniques (**compression, feature extraction, vetoing**) to run on a **Data Reduction Pipeline**
- Significant **R&D effort**, both engineering (throughput, heterogeneous architectures) and scientific (real time analysis)

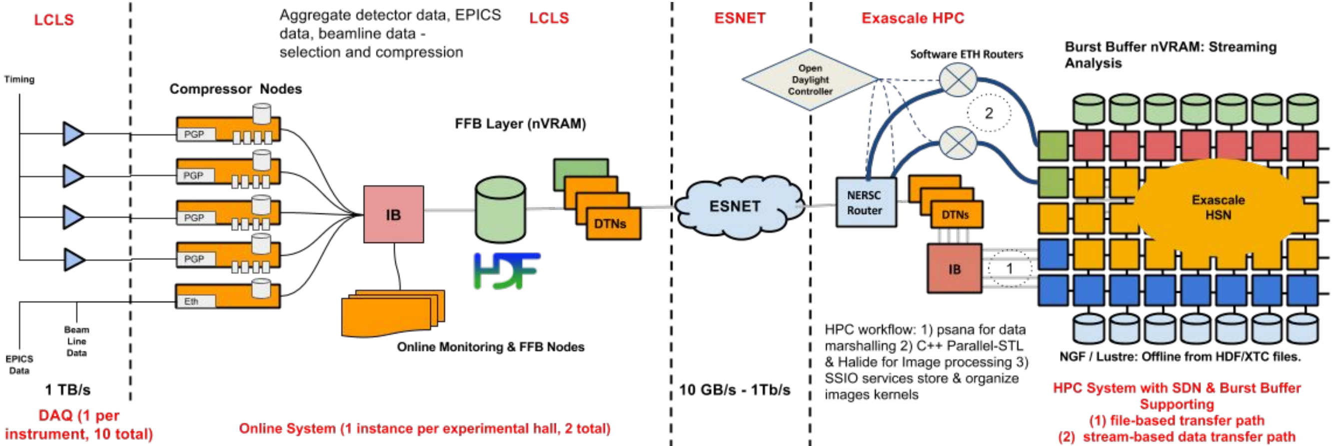


Without on-the-fly data reduction we would face unsustainable hardware costs by 2026

ExaFEL:
Data Analytics at the Exascale for Free Electron Lasers

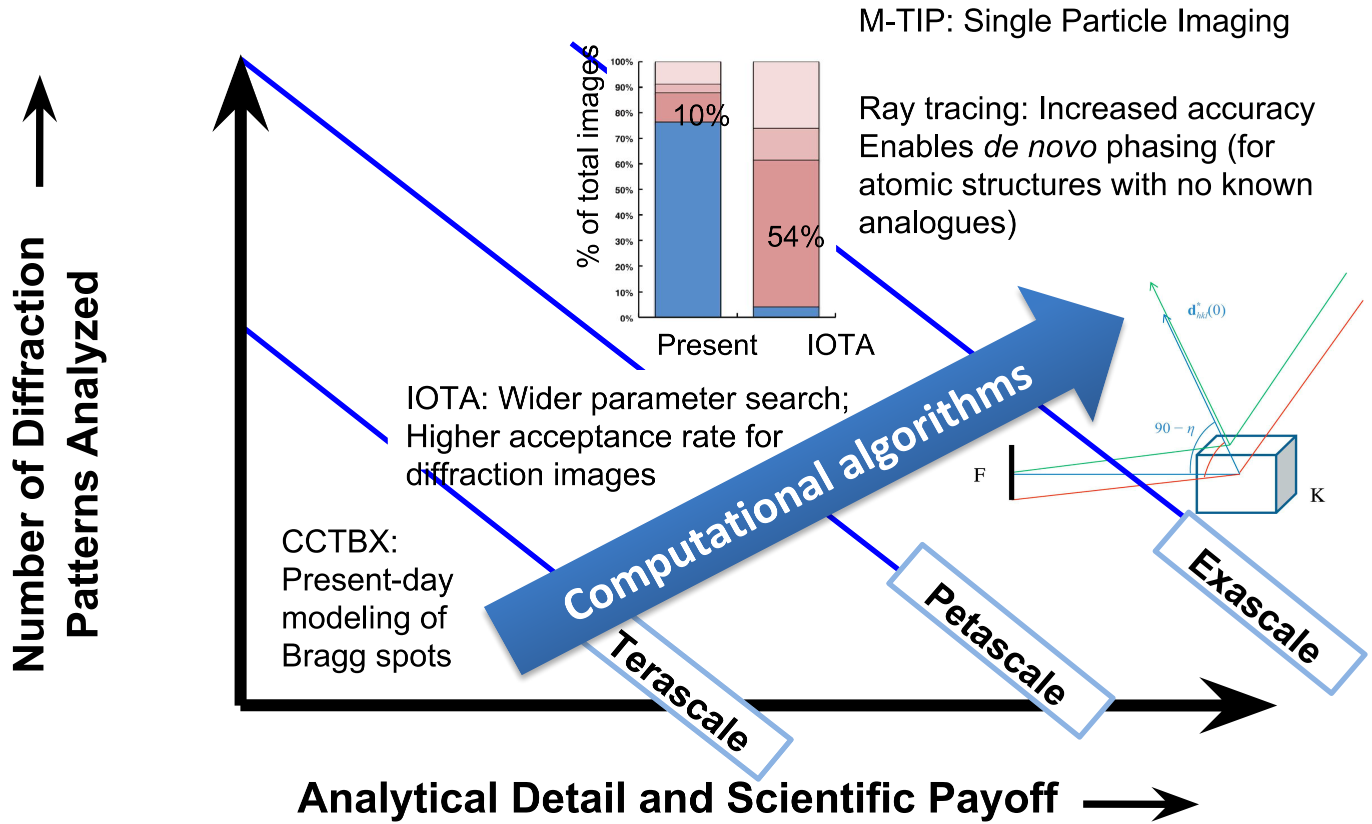
Application Project within Exascale Computing Project (ECP)

High data throughput experiments	LCLS data analysis framework	Infrastructure
Algorithmic improvements and ray tracing - Example test-cases of Serial Femtosecond Crystallography, and Single Particle Imaging	Porting LCLS code to supercomputer architecture, allow scaling from hundreds of cores (now) to hundred of thousands of cores	Data flow from SLAC to NERSC over ESnet



We need to build from this very important early engagement with ASCR

From Terascale to Exascale



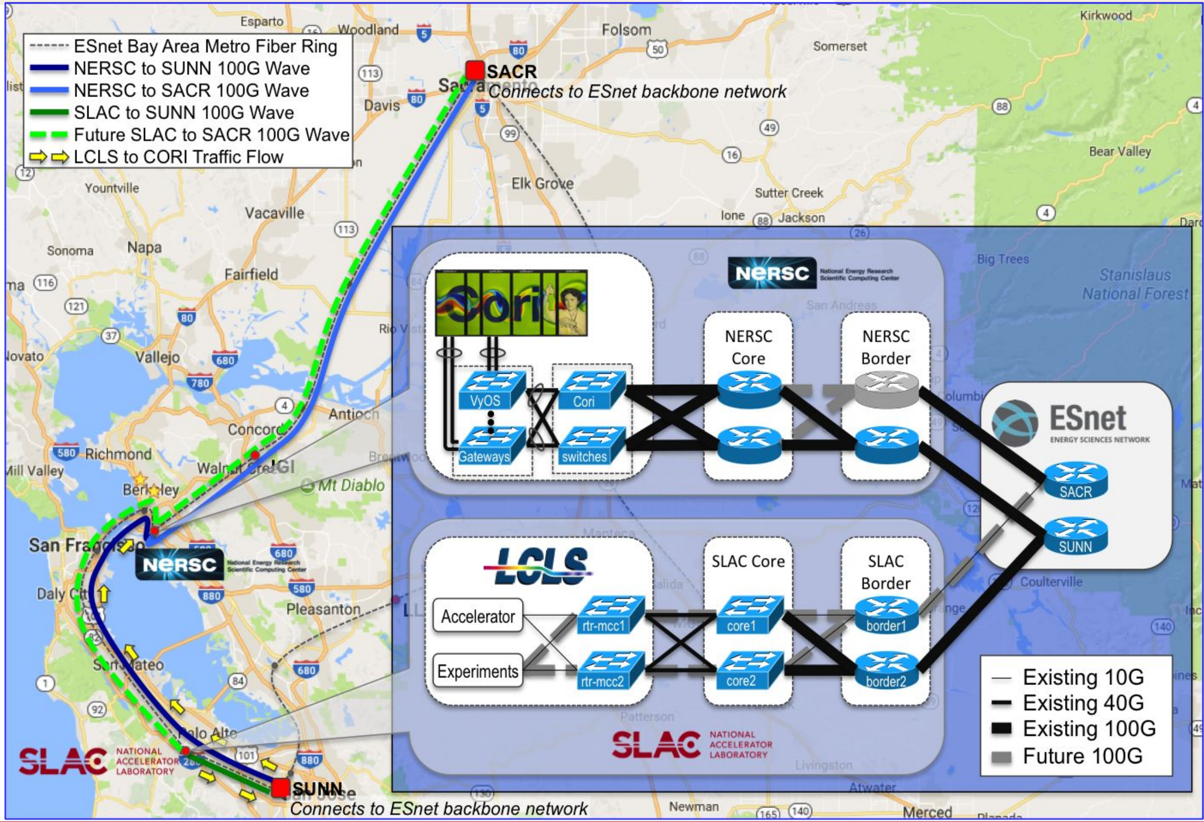
Exascale vastly expands the experimental repertoire and computational toolkit

Picture credit: Kroon-Batenburg et al (2015) Acta Cryst D71:1799

The Role of ESnet

By 2022 we'll need > **200-Gb/s** capabilities between the LCLS beamlines and ESnet

By 2026 we'll require **Tb/s** capabilities



ESnet will be instrumental in providing LCLS-II access to exascale

DOE High End Computing (HEC) Facilities will play a critical role, complemented by dedicated, local systems

LCLS-II will require:

- Access to **HEC Facilities**
  - For highest demand experiments (exascale)
- **Dedicated, local** capabilities
  - **Data Reduction Pipeline**: Data compression, feature extraction, vetoing (trigger)
  - **Fast feedback**: Real time analysis

A viable approach will have to combine local and complex-wide facilities