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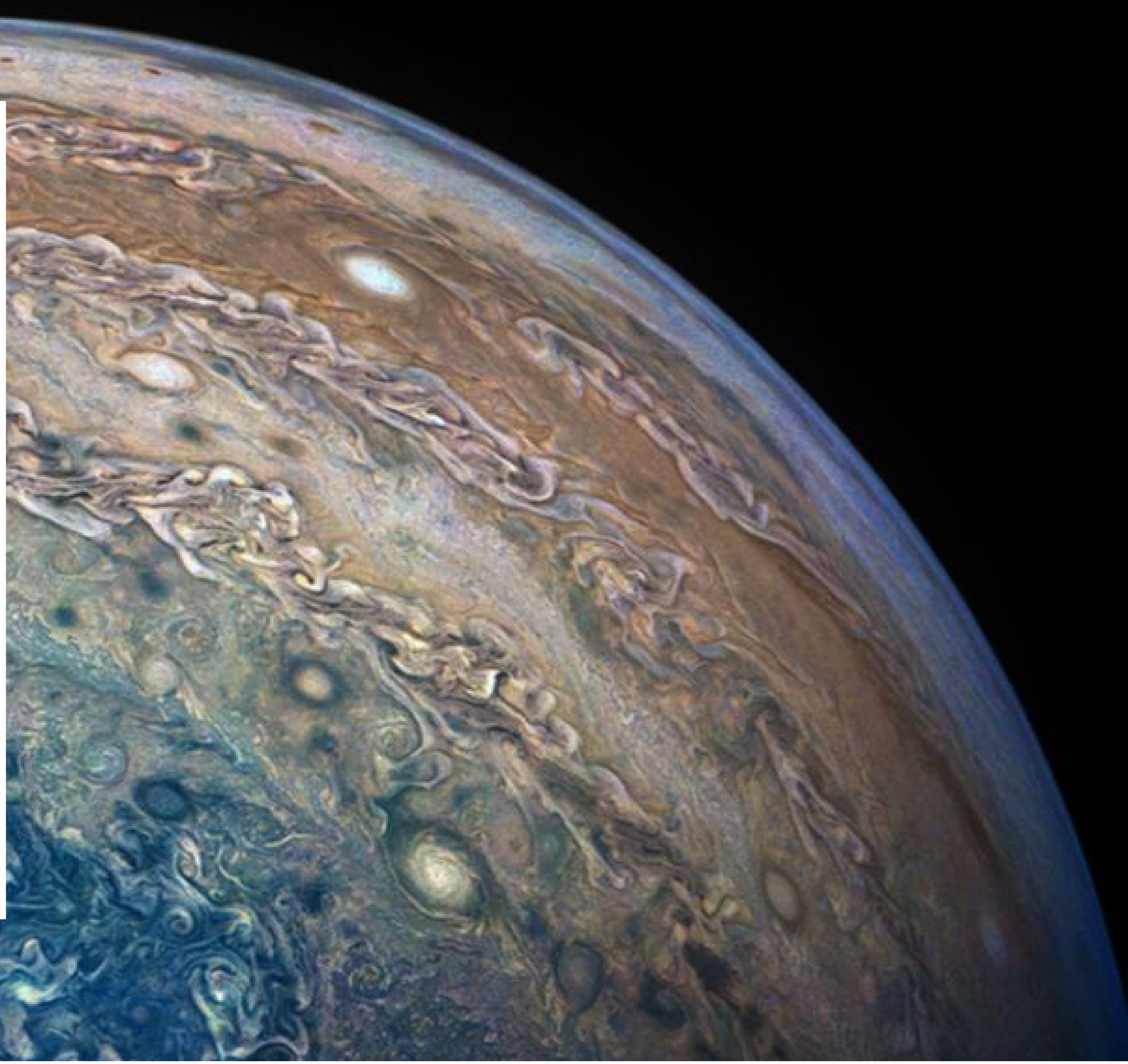

Understanding Matter under Extreme Conditions at the Nanoscale

Michael Bussmann @ NanoNet+ Annual Workshop

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CBG Max Planck Institute of Molecular Cell Biology and Genetics
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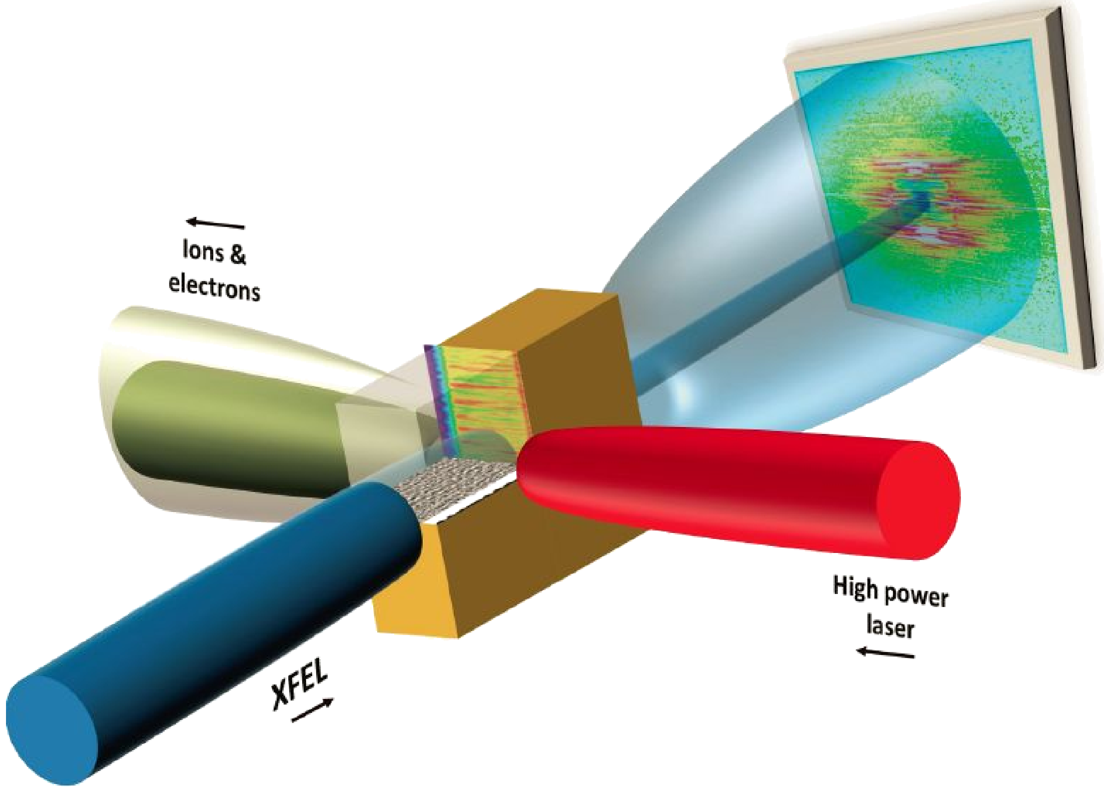
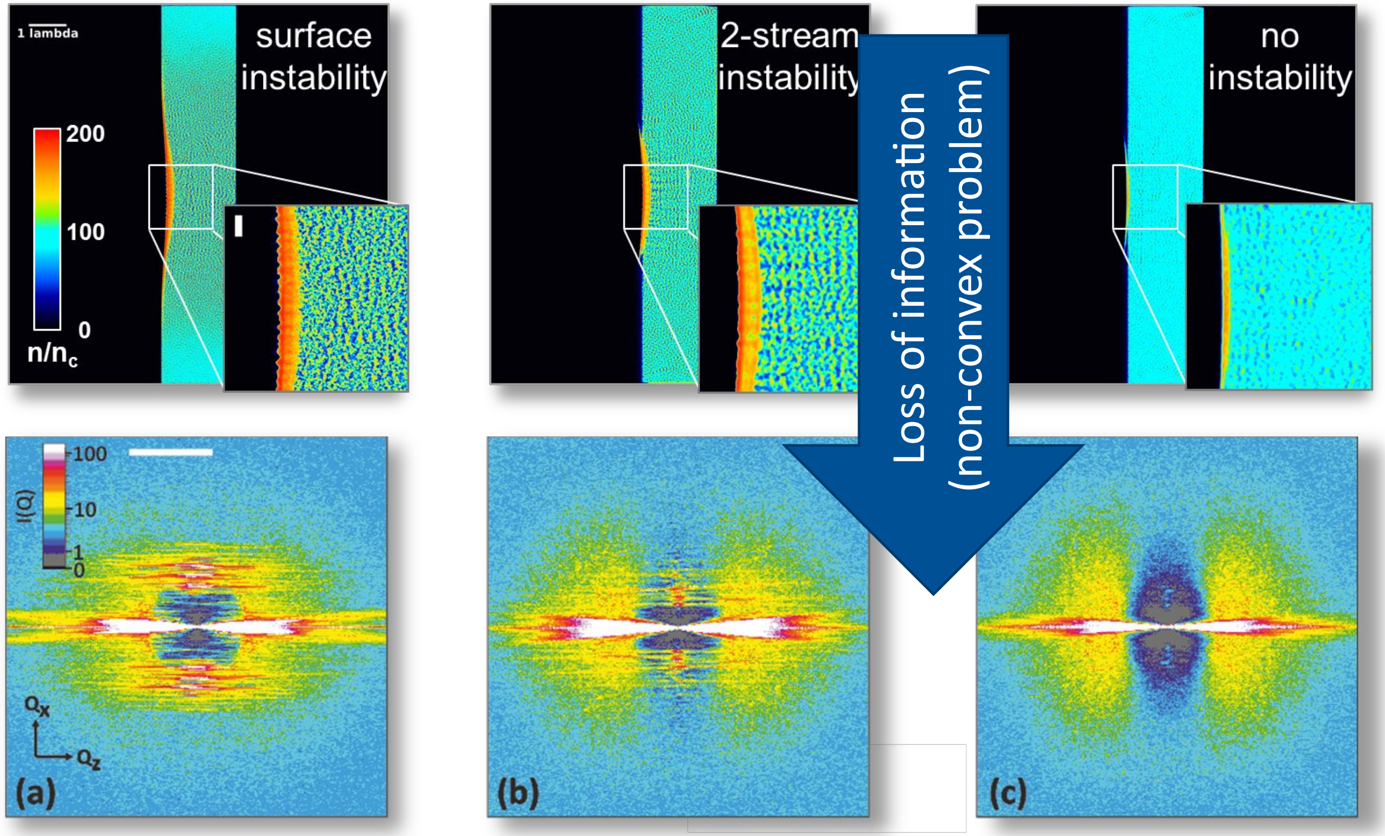
HiBEF

HELMHOLTZ INTERNATIONAL BEAMLINE FOR EXTREME FIELDS

Using the European XFEL & HIBEF as a microscope

Studying plasma accelerators at the atomic level

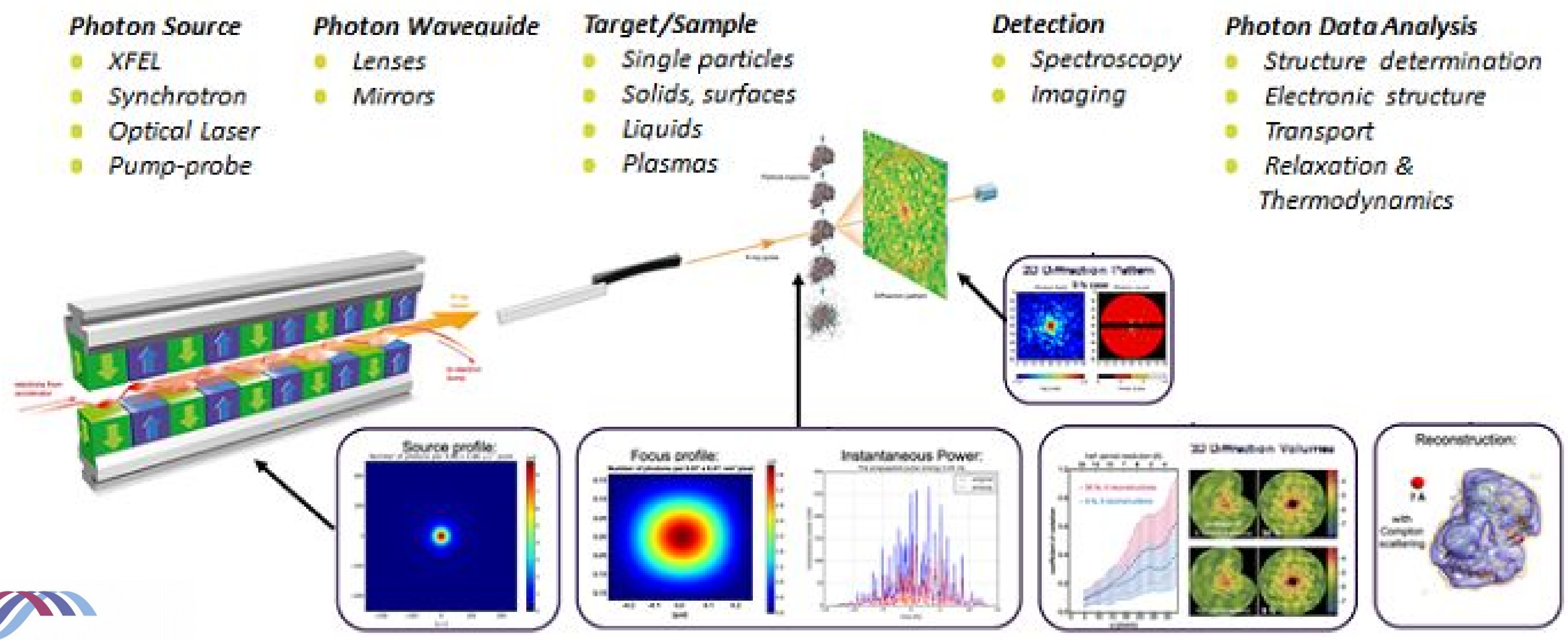




Thomas Kluge et al.

Recreating experiments virtually via digital twins

X-ray laser, complex system, scattering and detectors simulated

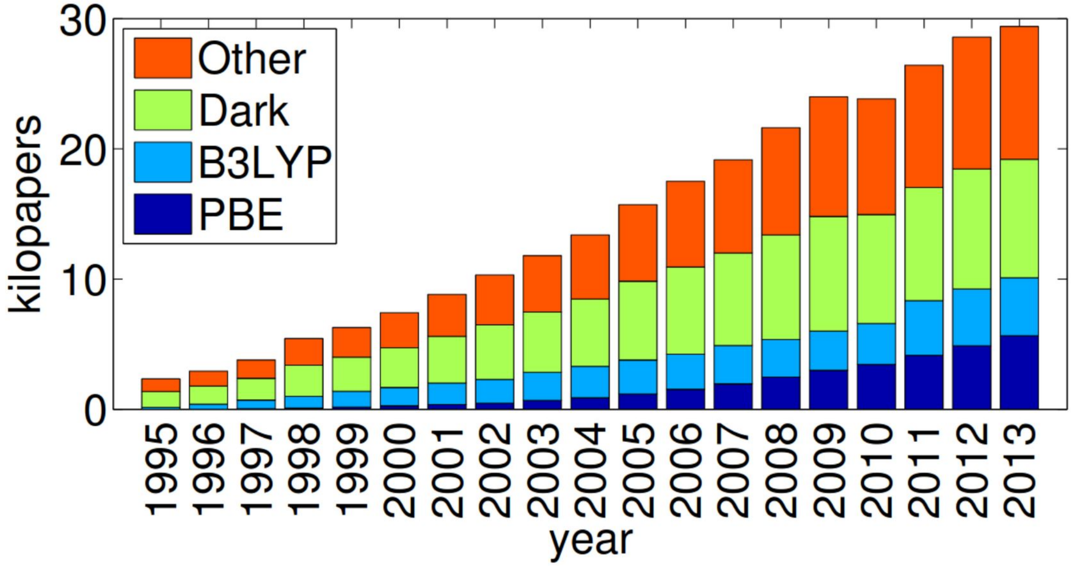


SIMEX Platform (see PANOSC VINYL)

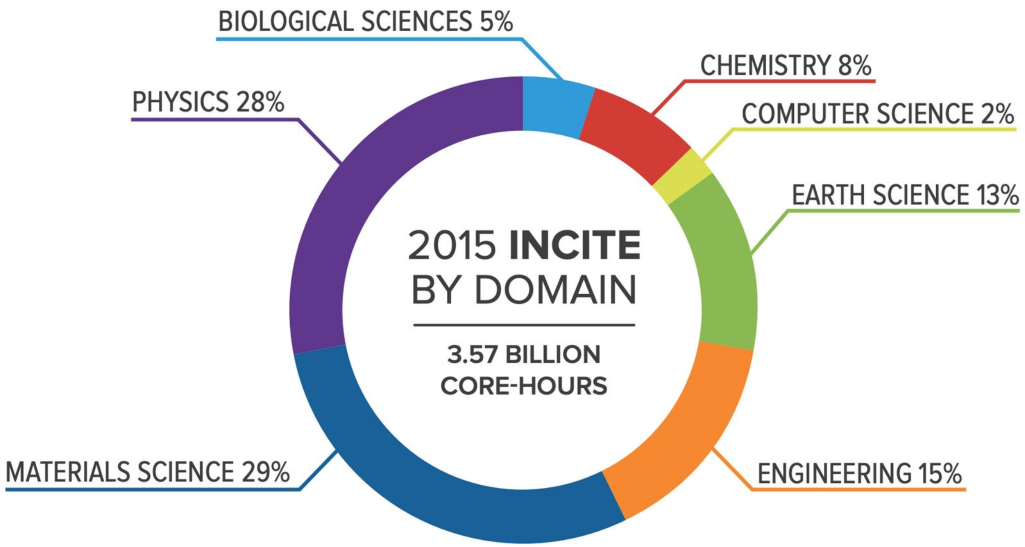
Carsten Fortmann-Grote et al.

Recreating experiments virtually via digital twins

Simulations become extremely costly



Pribram-Jones et al., https://doi.org/10.1146/annurev-physchem-040214-121420



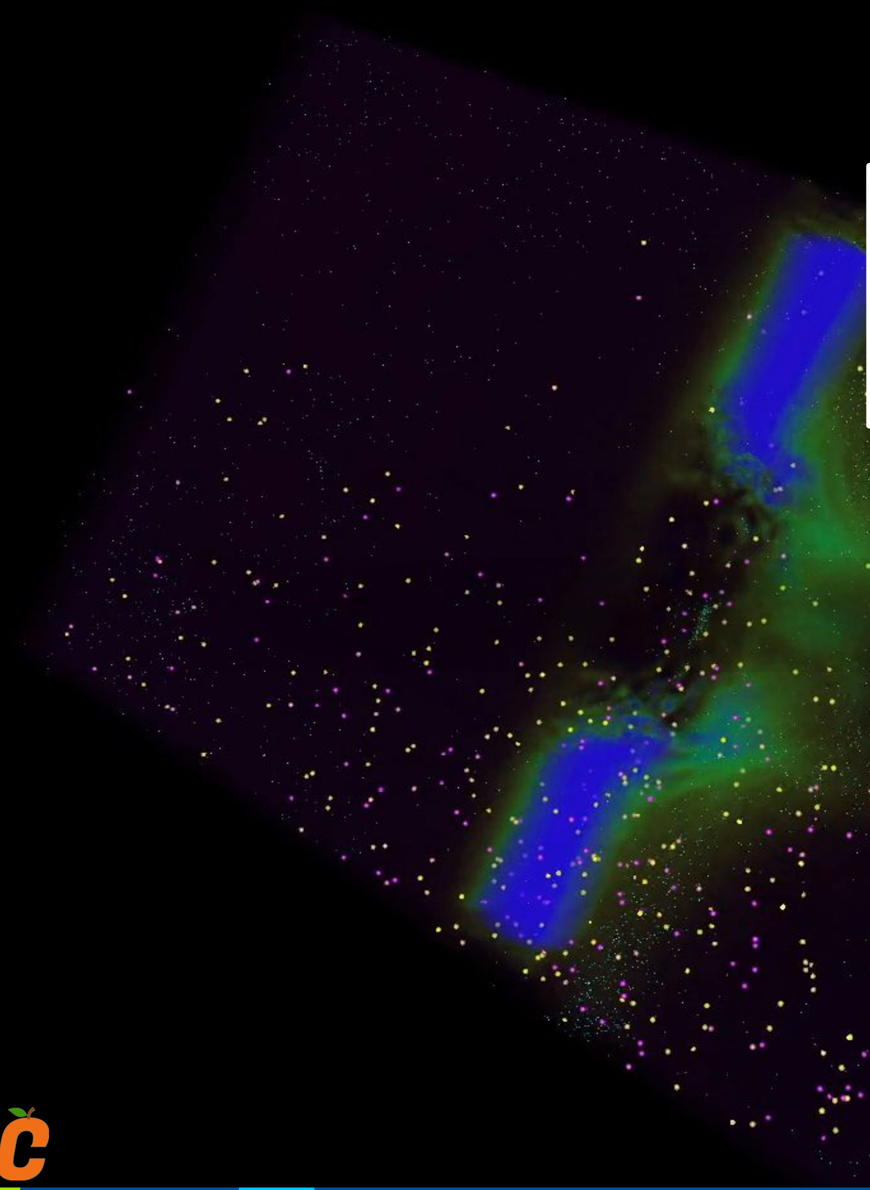
Argonne Leadership Facility Science Highlights 2015, https://alcf.anl.gov/files/alcfscibro2015.pdf

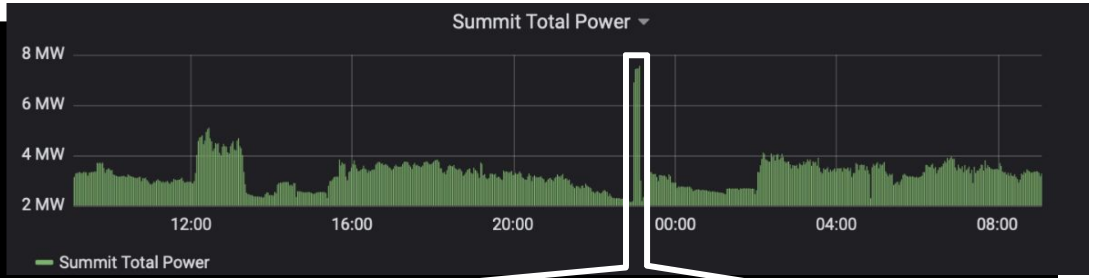
Simulations on Summit

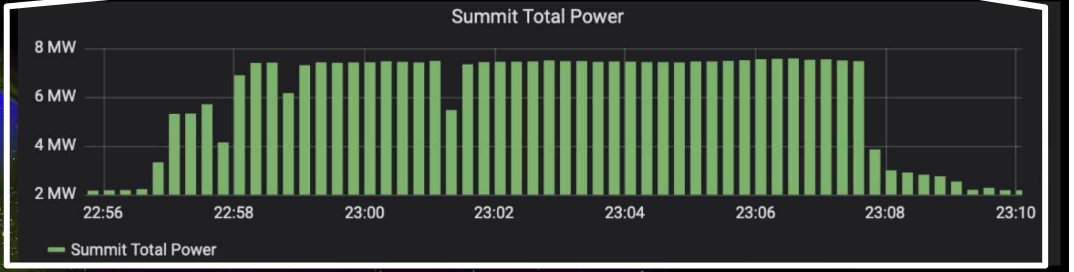
10 Trillion Particles

400 Billion Cells

27600 GPUs







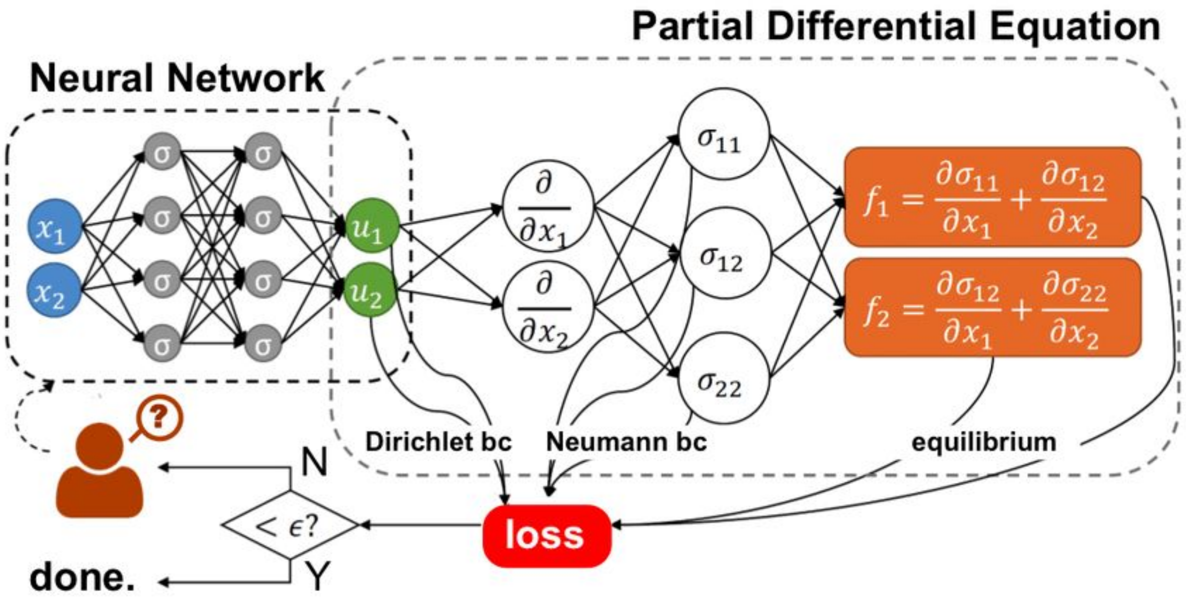
This is the way

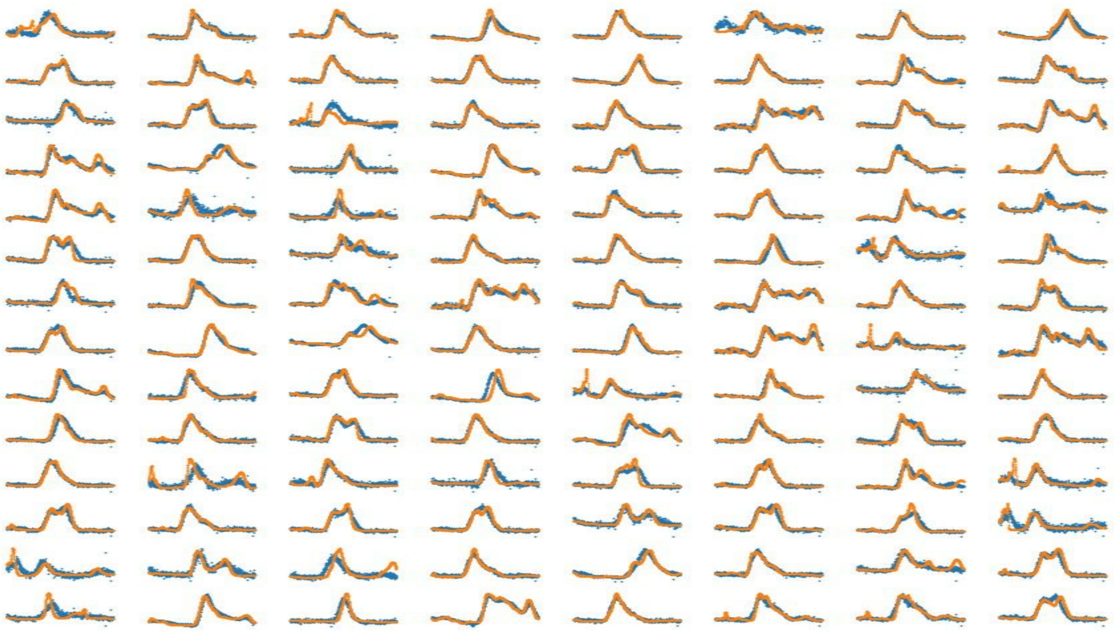
But how do we get there?

1. Run full digital twin of planned experiment on Top 10 HPC
2. Create AI surrogate model from HPC simulations
3. Use for real time interpolation of data during experiment
4. Use inversion to reduce data on-the-fly by orders of magnitude

Digital Twins and AI on Top 10 HPC Systems

Physics-informed Neural Networks FTW!





blue: ground truth **orange: PINN prediction**

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Creating Surrogate Models of Plasma Targets

NEURAL SOLVERS

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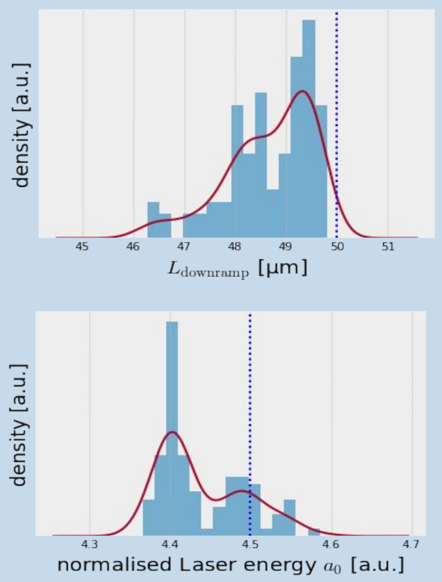
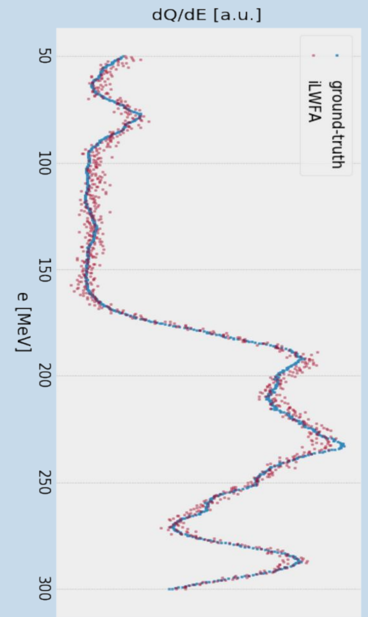


Invertible Neural Network



Benefits

- Recover ambiguous mapping
- Uncertainty quantification

Inputs:
Laser Energy
& Plasma Density Profile

Output:
Particle Energy Spectrum

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A single, scalable invertible PINN for multiple Modalities

NEURAL SOLVERS

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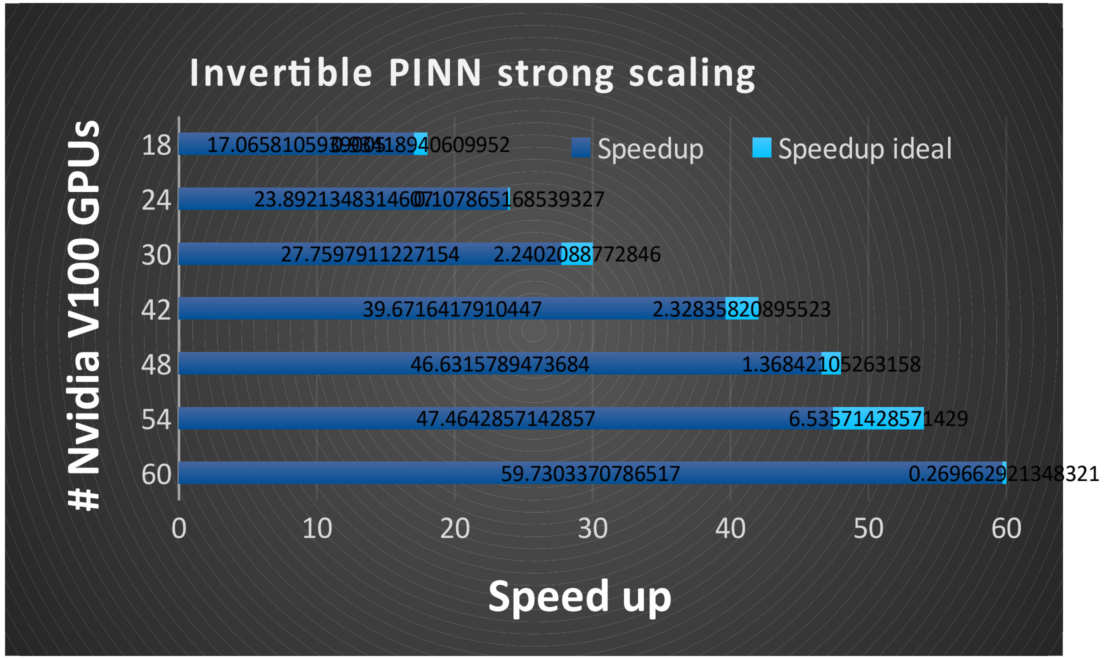

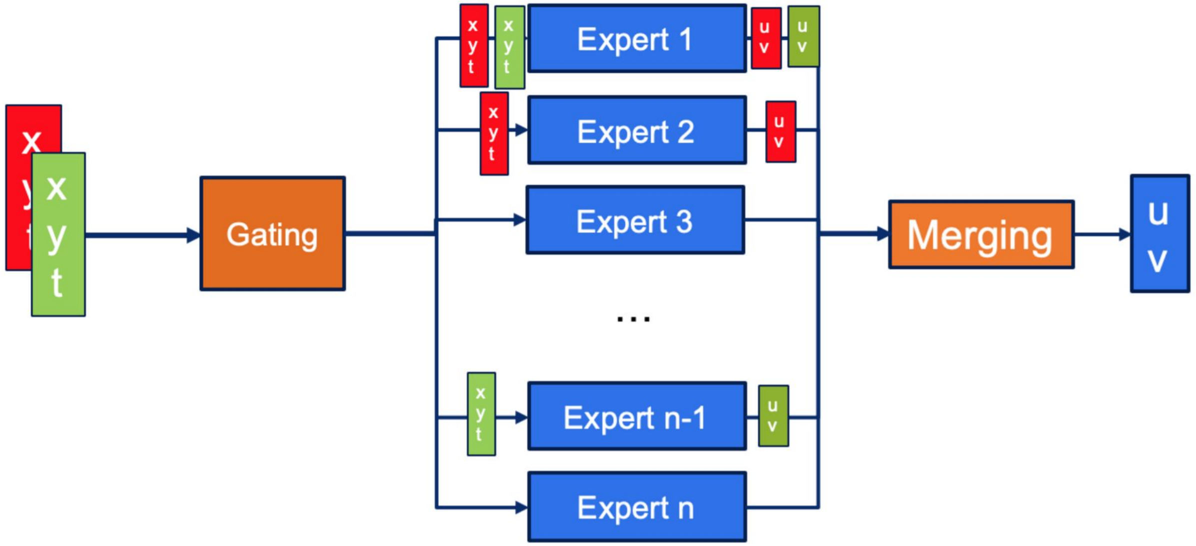

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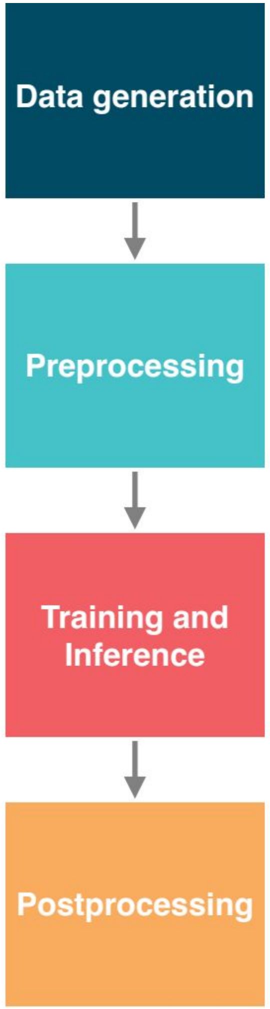
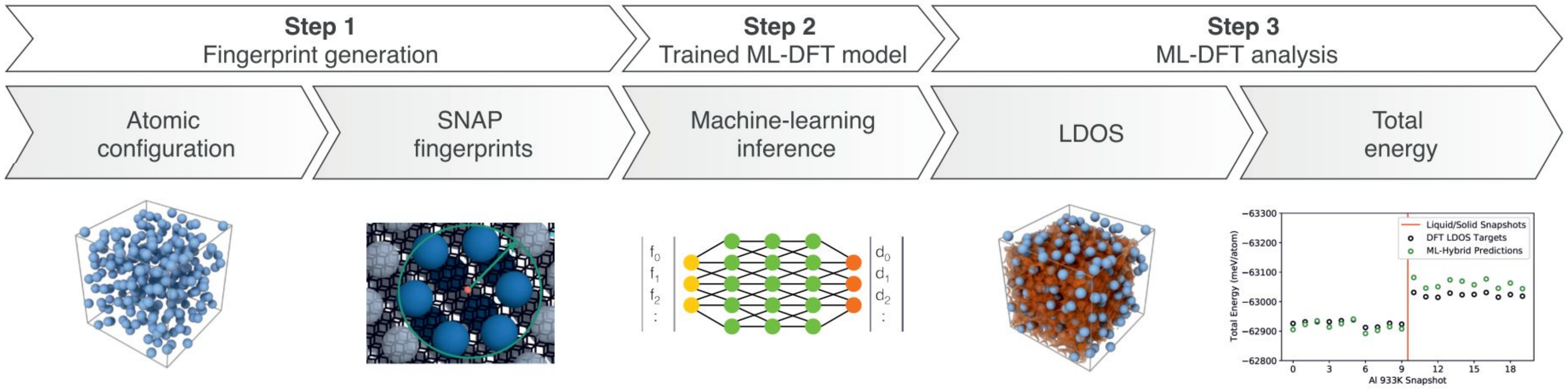
Surrogate Modeling for various physical Systems (PIC, DFT, …)





(a) Snapshot of an atomic configuration.

(b) Bispectrum components at each point on a Cartesian grid

(c) Feed-forward neural network.

(d) ML-DFT prediction of the local density of states (LDOS) on Cartesian grid.

(e) ML-DFT prediction of the total energy for both solid and liquid phases.

Materials Learning Algorithms

Attila Cangi et al.

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Assuming locality enables domain decomposition of learning

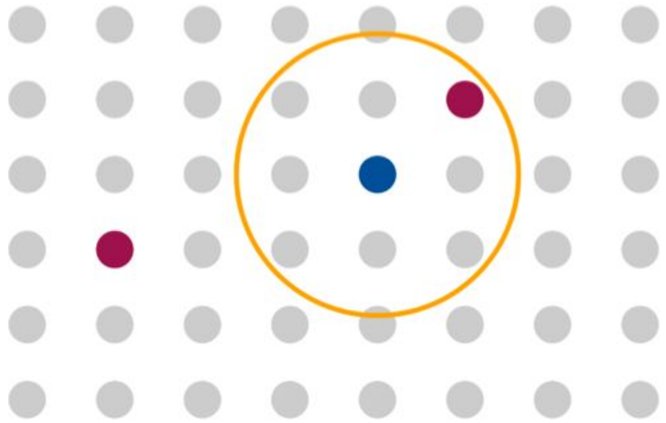
SNAP descriptors

- ***Assumption***: LDOS at any point in space can be approximated by a function that depends only on the positions and chemical identities of atoms within some finite neighborhood of the point.

- We construct a fingerprint that maps the neighborhood of any point to a set of scalar values called descriptors.

- A good descriptor must satisfy certain minimum requirements:
  - invariance under permutation, translation, and rotation of the atoms in the neighborhood
  - continuous differentiable mapping from atomic positions to descriptors, especially at the boundary of the neighborhood.

- At each grid point on the Cartesian mesh we use SNAP descriptors
  - expand in the basis of 4D hyperspherical harmonic functions
  - Vector with 91 scalar entries



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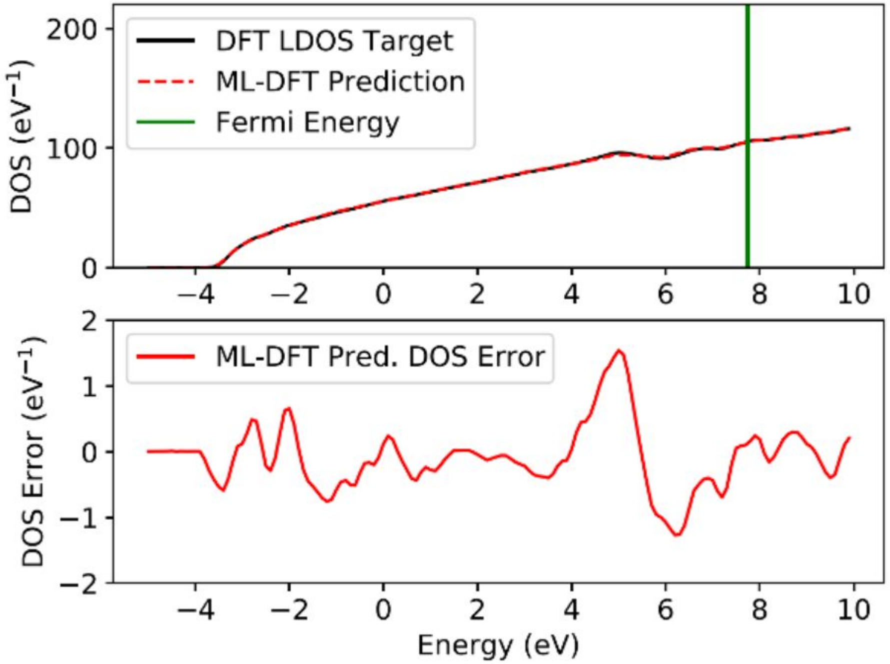
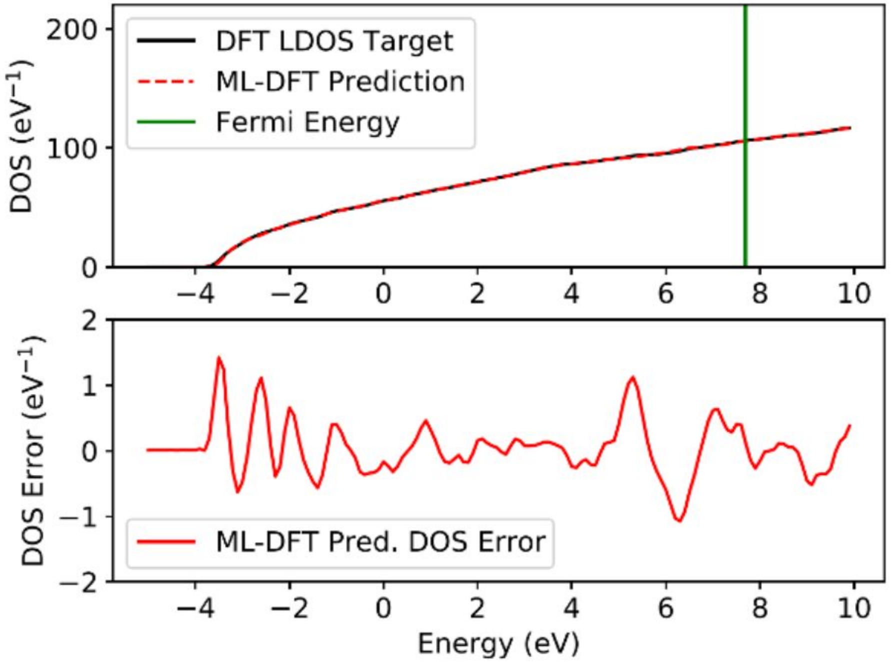
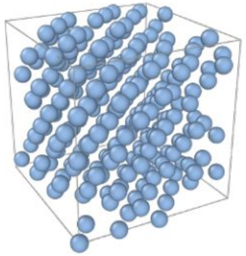
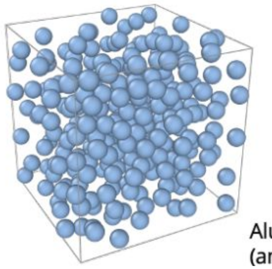
Surrogate Modeling for Aluminum at the Melting Point







Aluminum in solid phase
(ambient density, melting point)



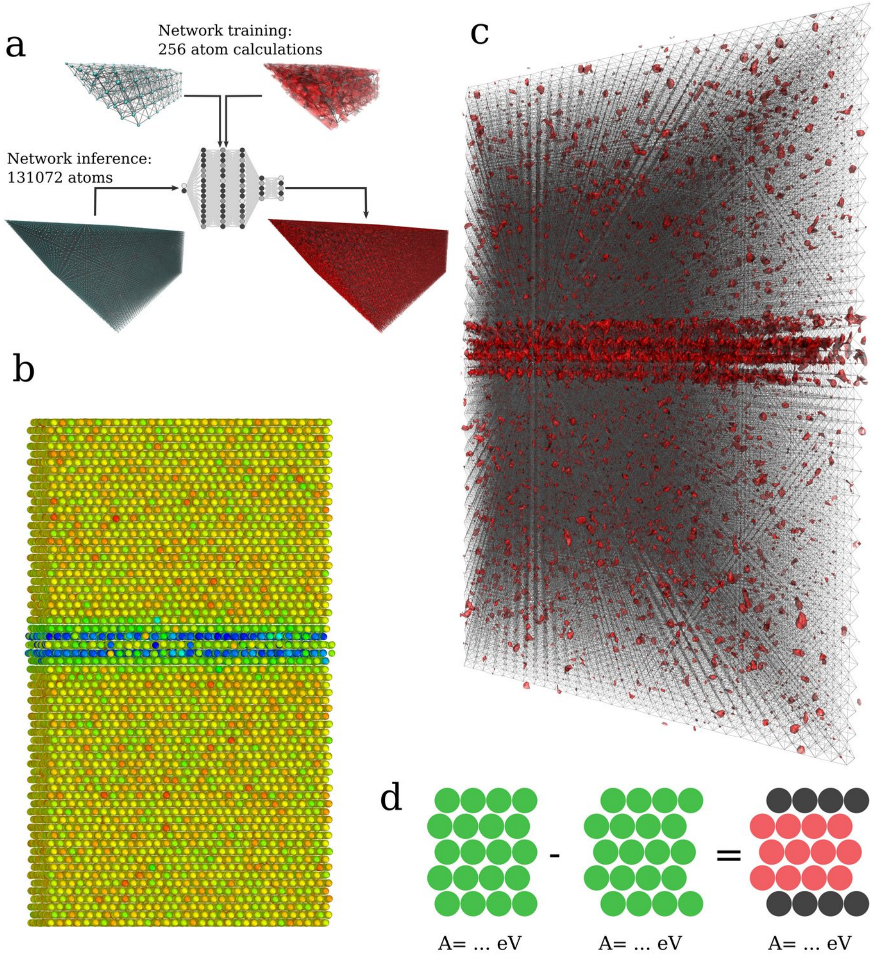
Aluminum in liquid phase
(ambient density, melting point)

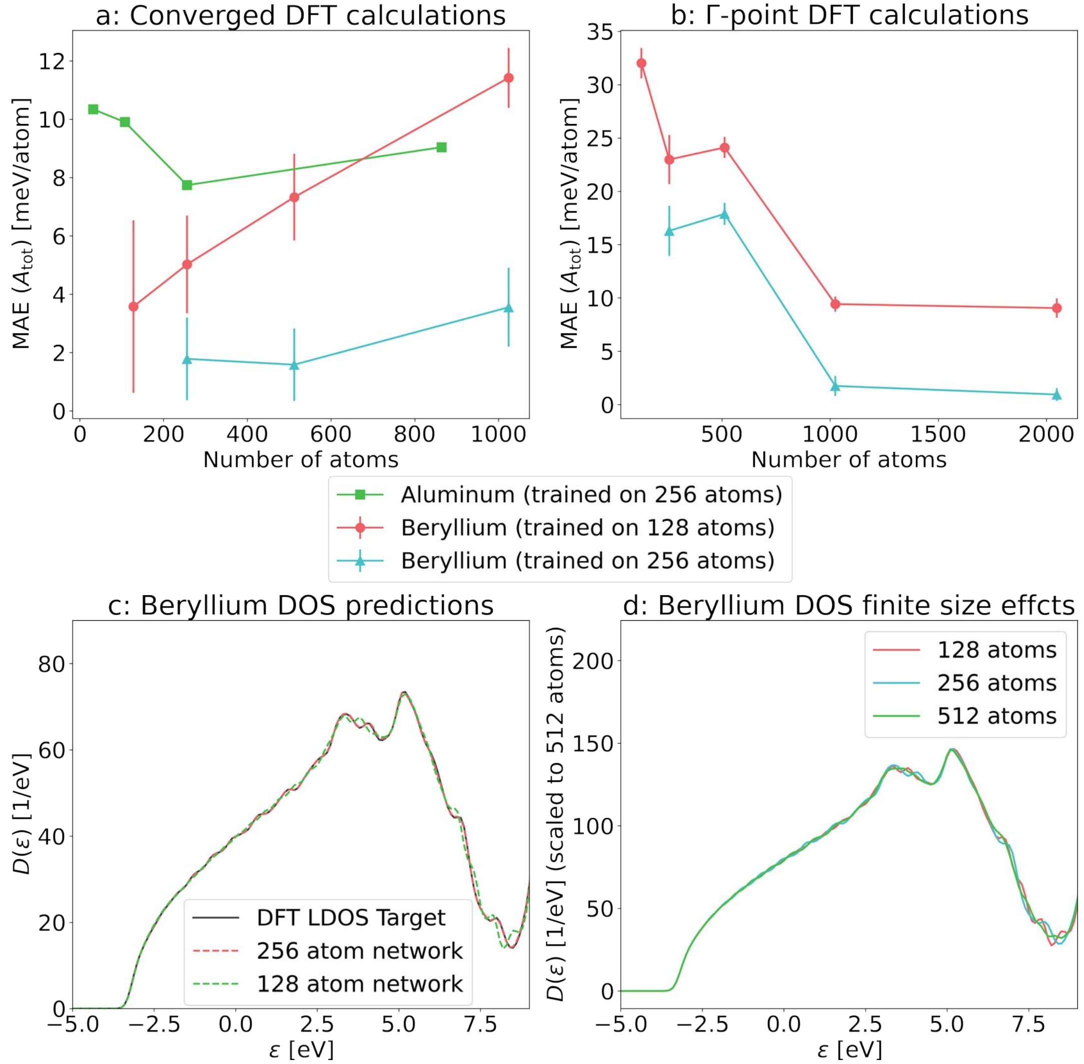
Attila Cangi et al.

Digital Twins and AI on Top 10 HPC Systems

Surrogate Modeling of Beryllium

DFT from 256 atoms to 131072 atoms





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Surrogate Modeling of Beryllium

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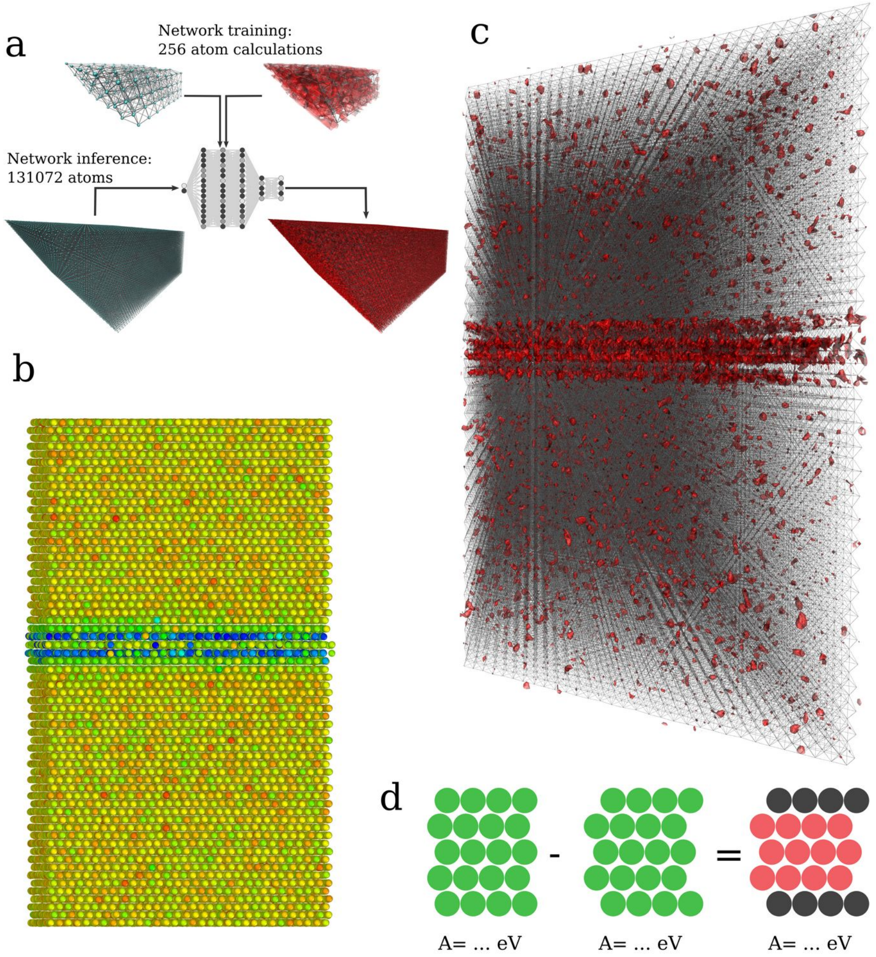

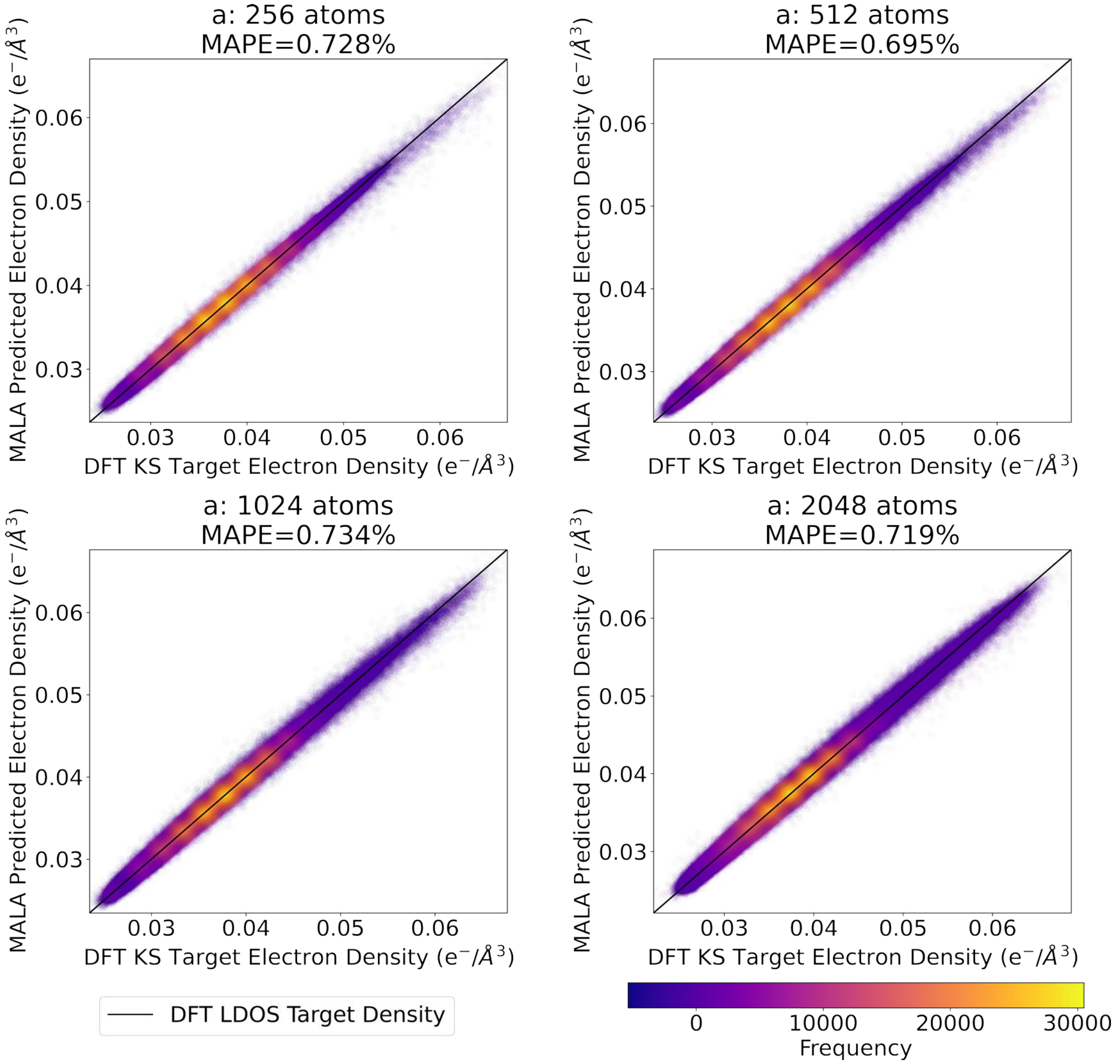

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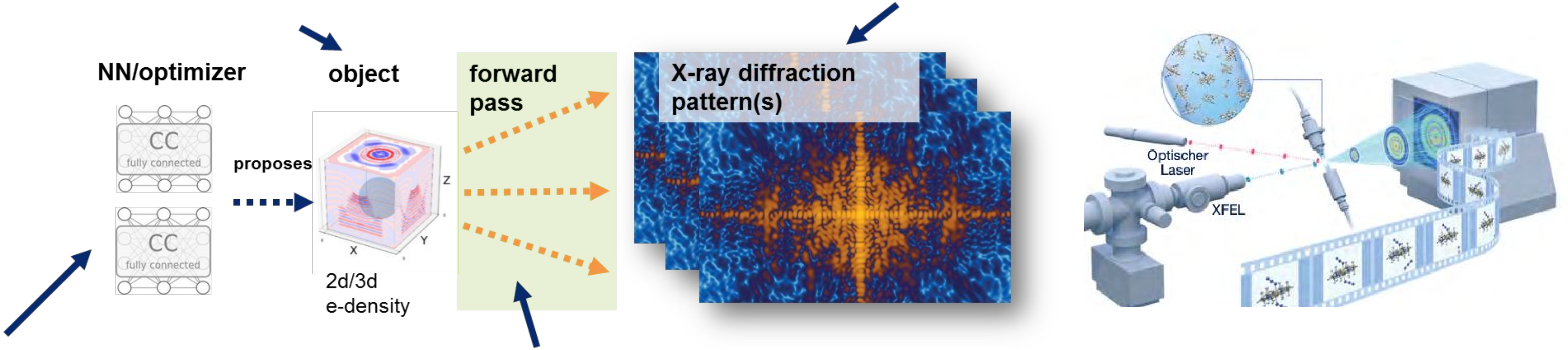
Surrogate Models of Experiments

Surrogate Models of Scattering Diagnostics



Solver of IIP
generative model of
solution space

(Deep) Physics Prior
analytical expression or surrogate model*

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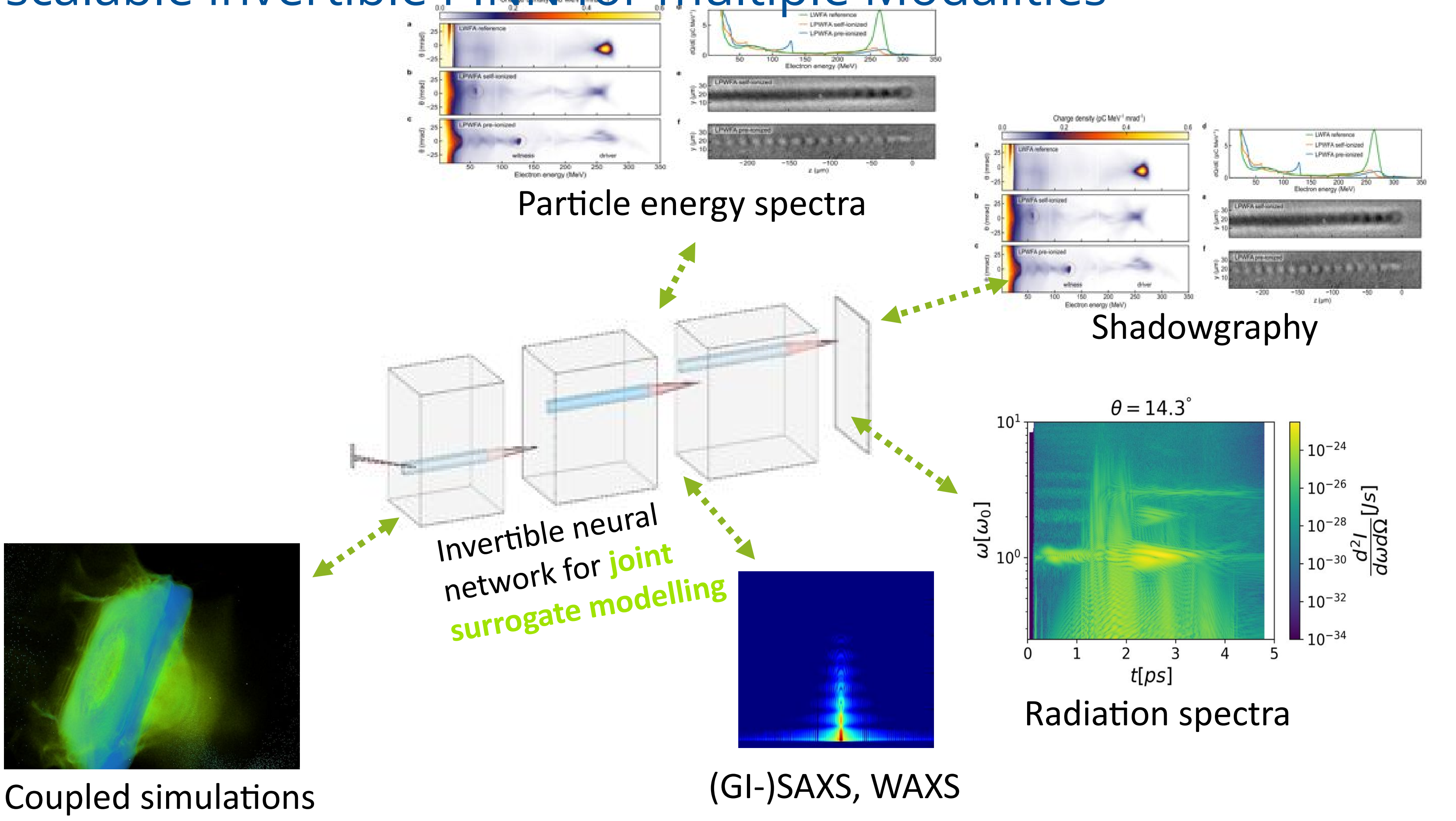
Surrogate Models of Experiments

A single, scalable invertible PINN for multiple Modalities



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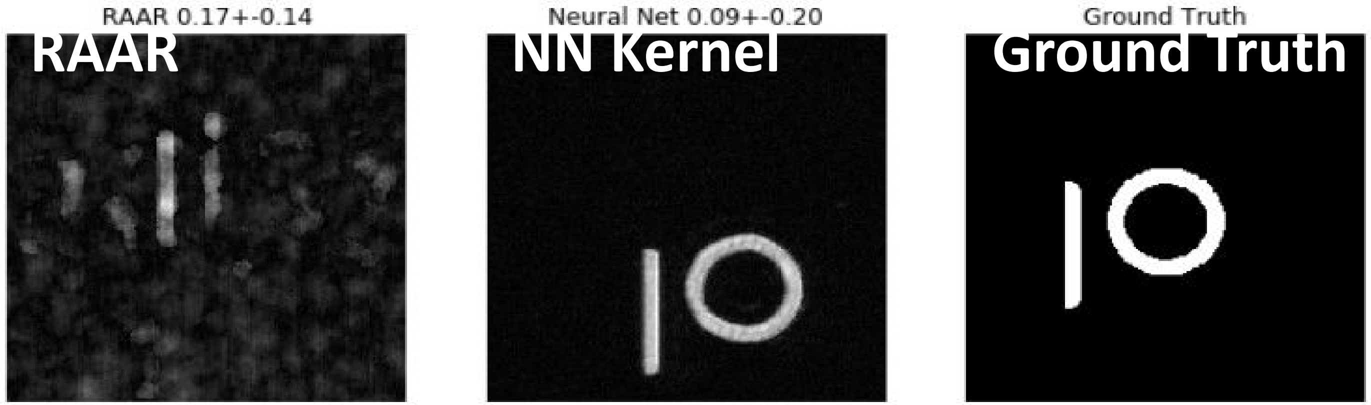
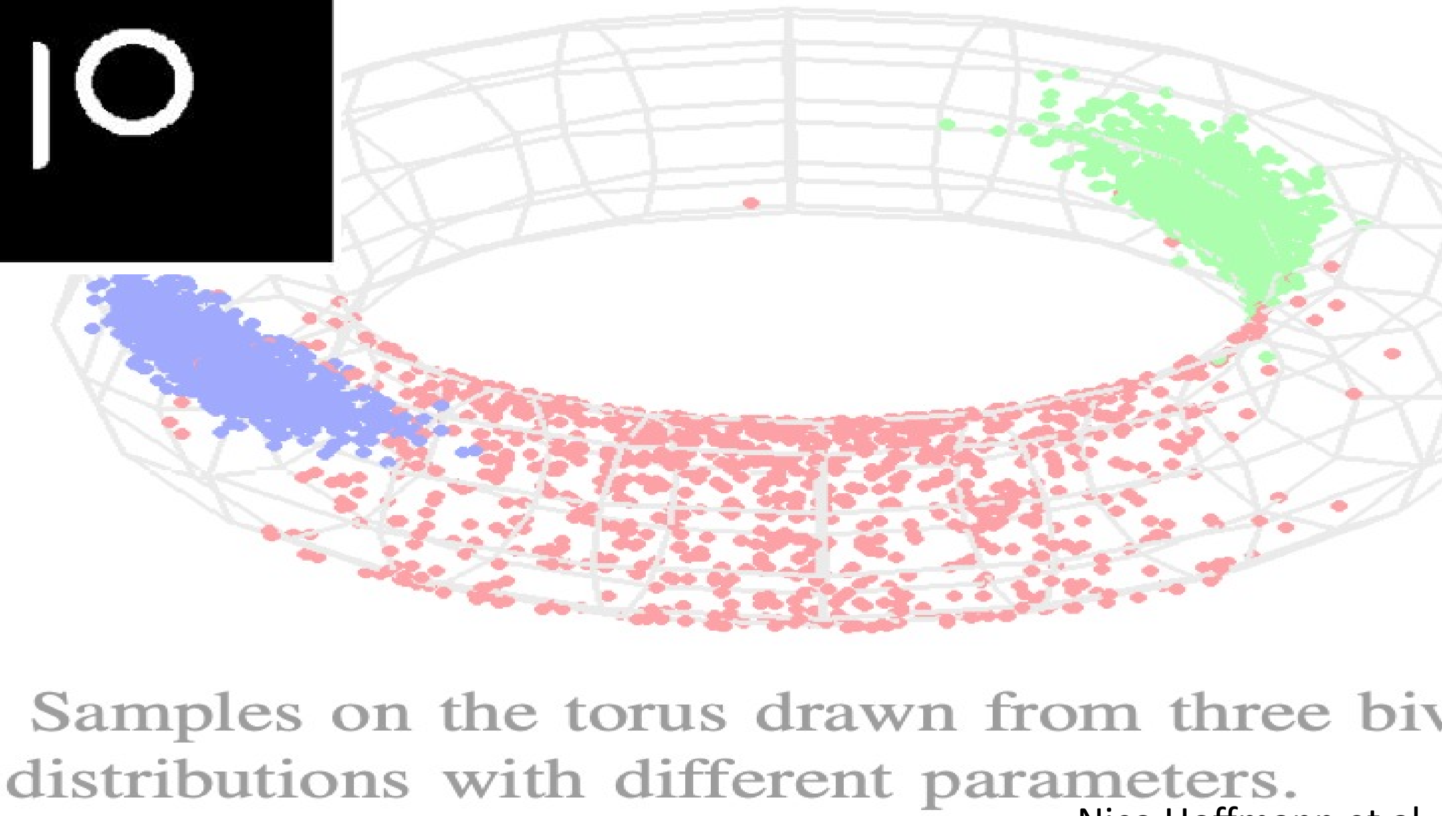
Retrieve System Parameters from Experiments in Real Time

Fast, robust Phase Retrieval from Small Angle X-Ray Scattering





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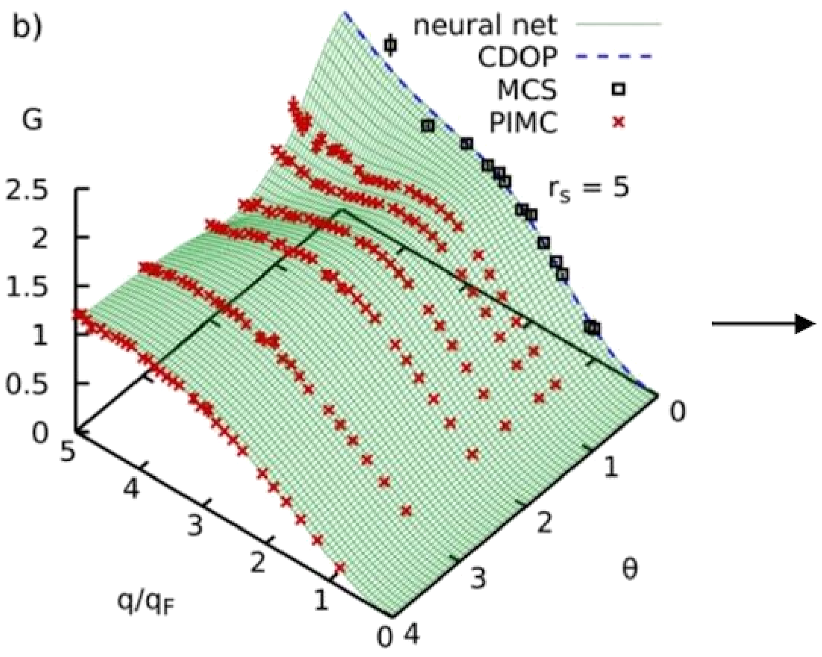
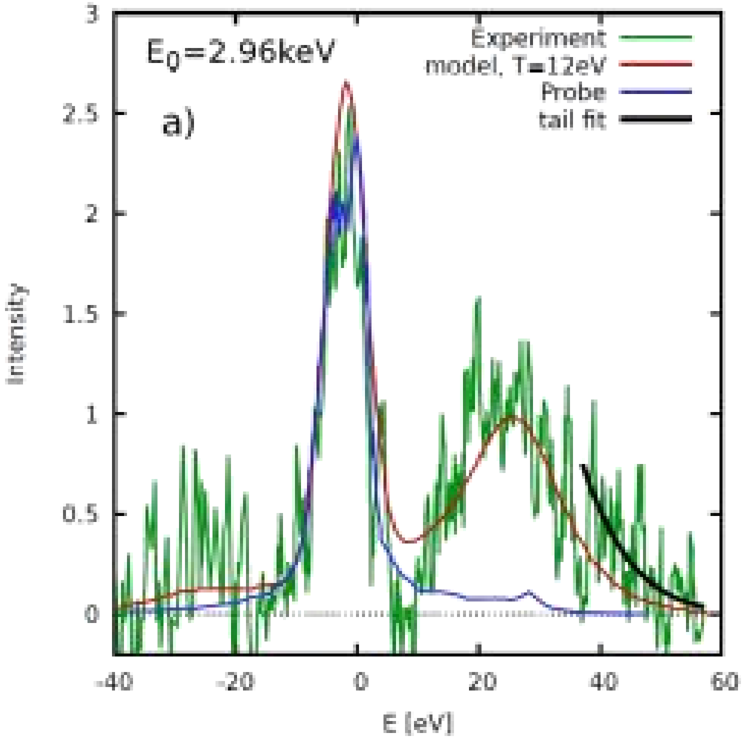
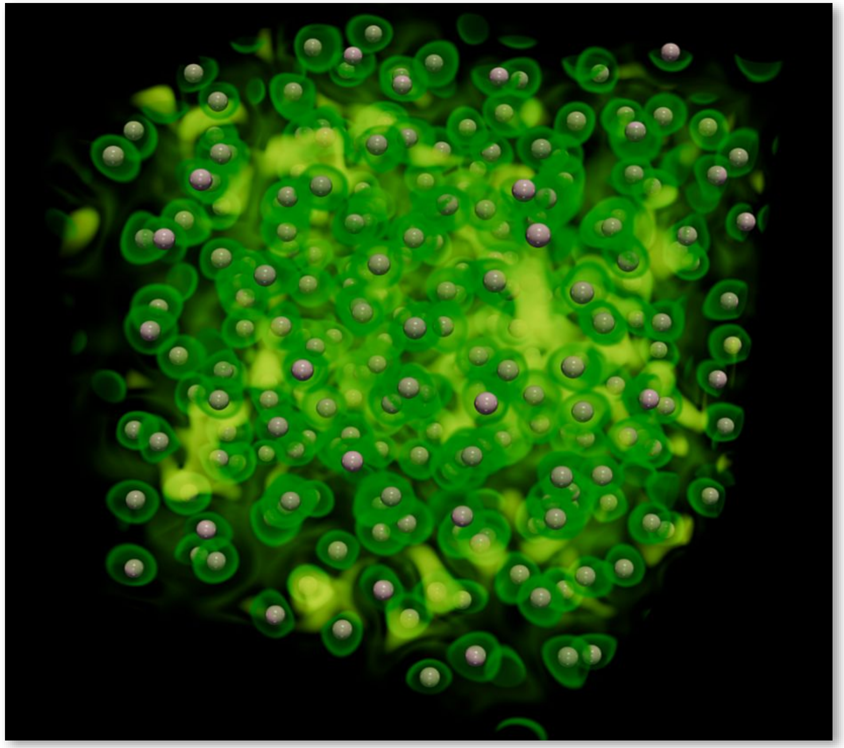
Retrieve System Parameters from Experiments in Real Time

From Ab-Inition PIMC to realistic XRTS temperature estimates







Tobias Dornheim et al.

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