Aurora ESP Projects







Anouar Benali (ANL)

Extending Moore's Law computing with Quantum Monte Carlo

Martin Berzins (U. Utah)

Design & evaluation of highefficiency boilers for energy production using a hierarchical V/UQ approach

CS Chang (PPPL)

High fidelity simulation of fusion reactor boundary plasmas

Theresa Windus (Ames)

NWChemEx: Tackling Chemical, Materials & Biochemical Challenges in the Exascale Era

Katrin Heitmann (ANL)

Extreme-Scale Cosmological Hydrodynamics

Ken Jansen (U. Colorado)

Extreme Scale Unstructured Adaptive CFD: From Multiphase Flow to Aerodynamic Flow Control

Norman Christ (Columbia)

Lattice Quantum
Chromodynamics Calculations
for Particle and Nuclear Physics

Aiichiro Nakano (USC)

Metascalable Layered Materials Genome

Benoit Roux (U. Chicago)

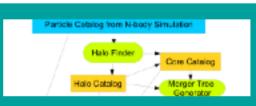
Free Energy Landscapes of Membrane Transport Proteins

David Bross (ANL)

KinBot initiates

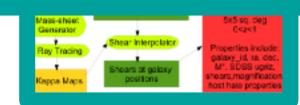
Exascale Computational Catalysis

in database the surface



Salman Habib (ANL)

Dark Sky Mining



Ken Jansen (U. Colorado)

Data Analytics and Machine Learning for Exascale CFD



Walter Hopkins(ANL)

Simulating and Learning in the ATLAS detector at the Exascale

Amanda Randles (Duke U.)

Extreme-scale In Situ Visualization and Analysis of Fluid-Structure-Interaction Simulations

Will Detmold (MIT)

Machine Learning for Lattice Quantum Chromodynamics

Nicola Ferrier (ANL)

Enabling Connectomics at Exascale to Facilitate Discoveries in Neuroscience

Noa Marom (CMU)

Many-Body Perturbation
Theory Meets Machine
Learning to Discover Singlet
Fission Materials

Rick Stevens (ANL)

Virtual Drug Response Prediction

Bill Tang (Princeton)

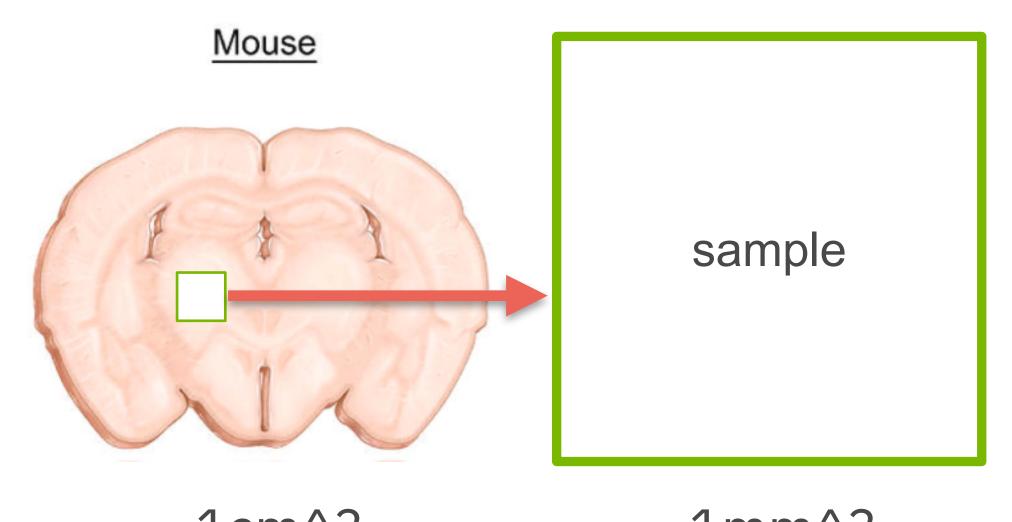
Accelerated Deep Learning Discovery in Fusion Energy Science





Connectomics Data-Driven Models



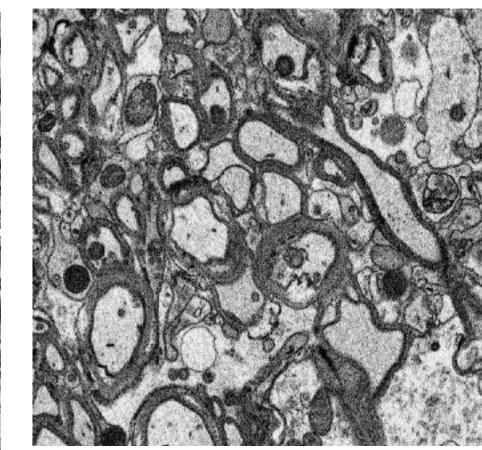


~1cm^3 ~1mm^3

25000 40nm sections 1mm x 1mm (6nm resolution)

section

Each section
imaged with EM as
N tiles (8 bit)
80K x 40K pixels



Sections stitched together

How much image data is 1mm³? 1×10¹⁵ voxels --> ~1 PB



Mouse brain: 70M neurons

