



# PROGRESS IN HPC + AI CONVERGENCE

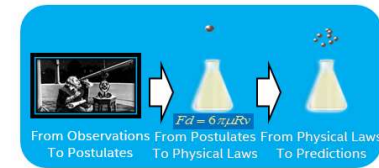
**Victor Lee**  
**Intel Corporation**



**THE NEW CENTER OF POSSIBILITY**

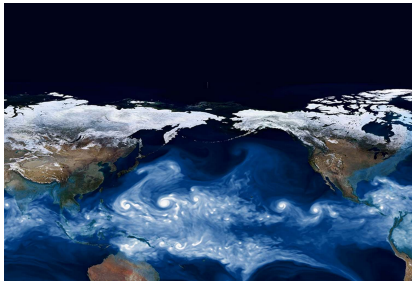
# HIGH PERFORMANCE COMPUTING (HPC)

Traditional HPC models and simulates theoretical science through first principle or experimentally. Human is involved in every step.



*Human Centric*

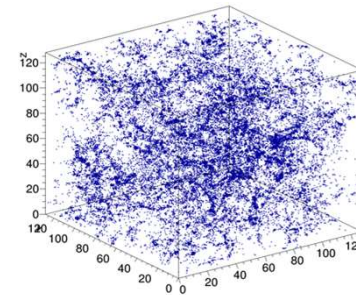
Climate Modeling



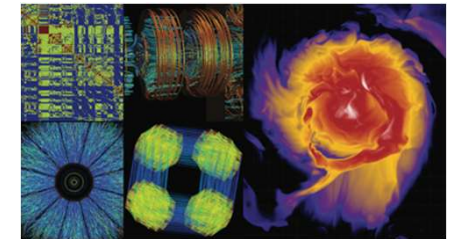
Weather



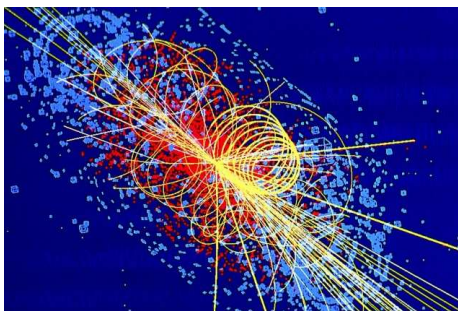
Cosmology



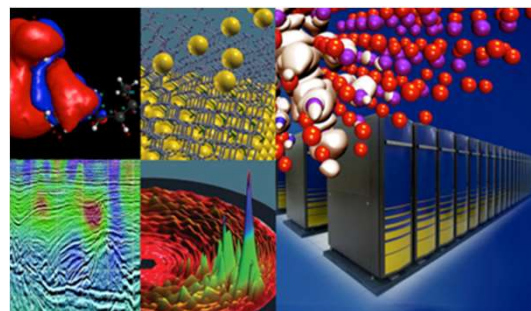
Nuclear Physics



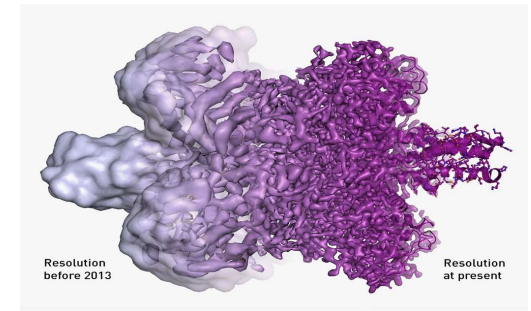
Fundamental Physics



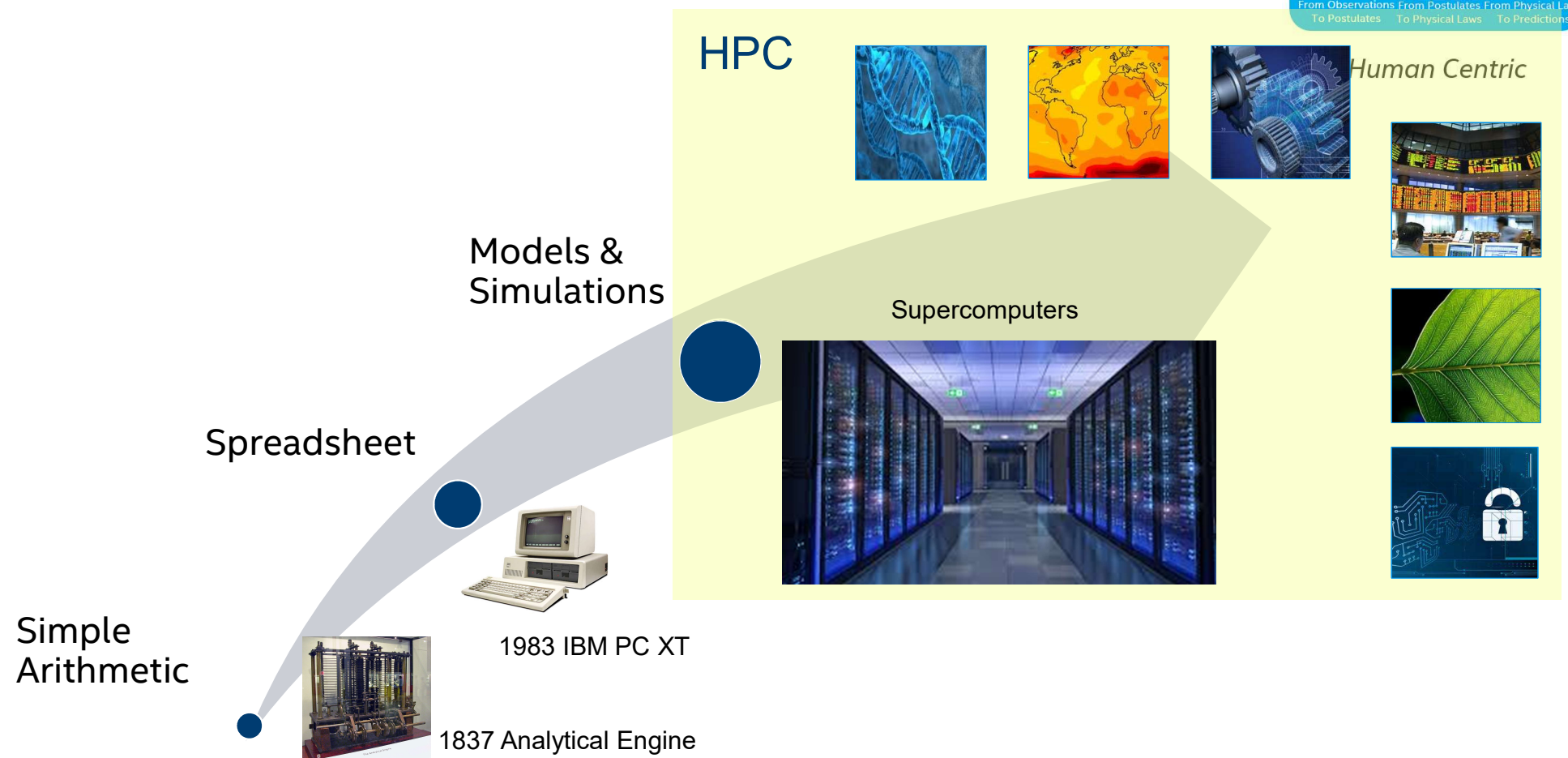
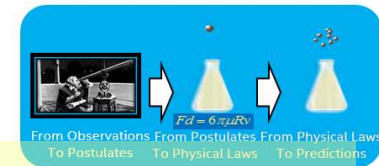
Material Simulations



Drug Discovery

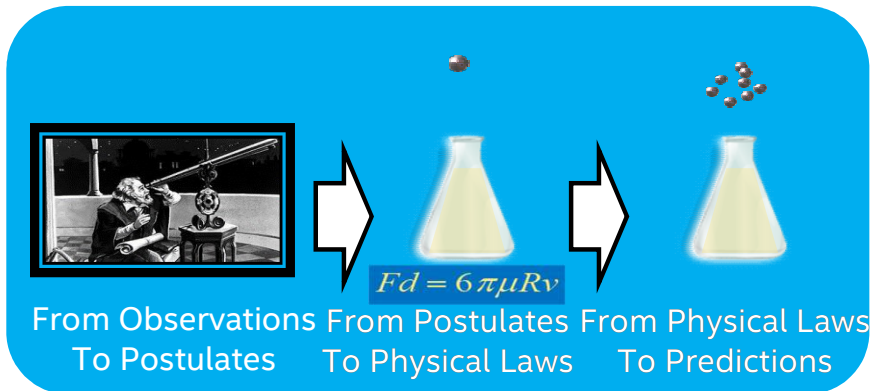


# EVOLUTION OF COMPUTER AS A TOOL



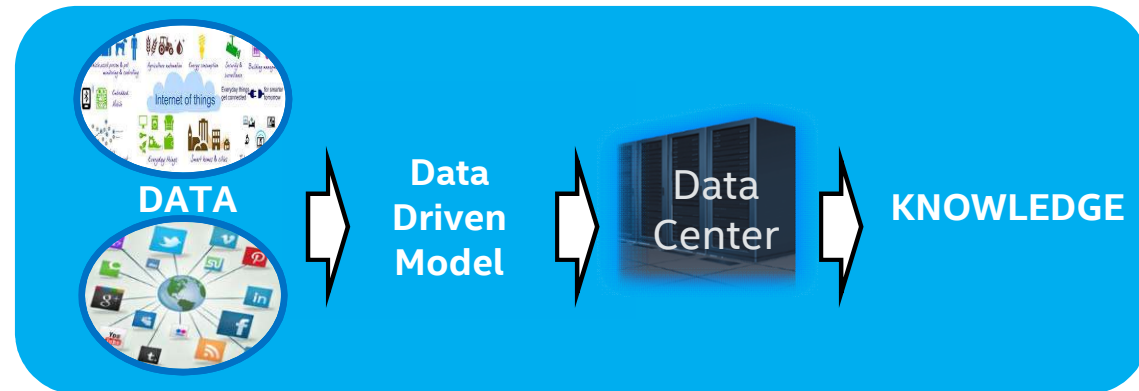
# DATA ANALYTICS SPEEDS SCIENTIFIC DISCOVERY

## Traditional



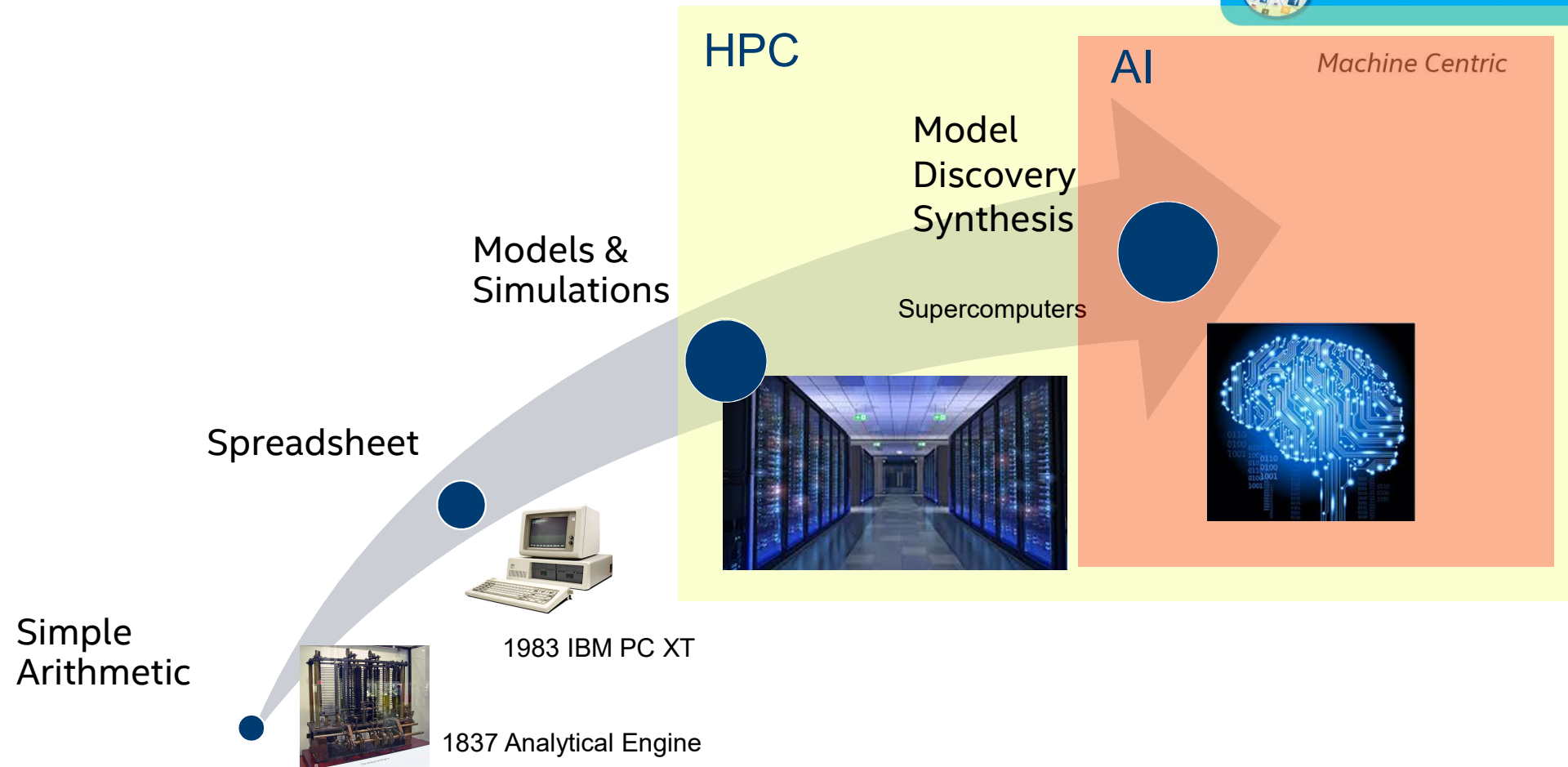
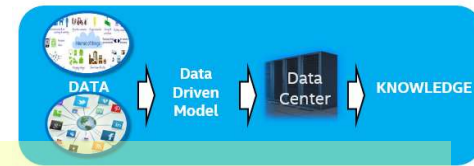
*Human Centric*

## Emerging



*Machine Centric*

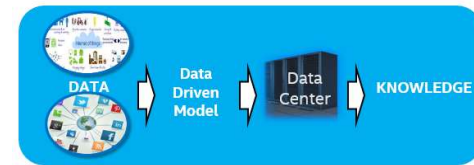
# EVOLUTION OF COMPUTER AS A TOOL (NEW FRONTIER)



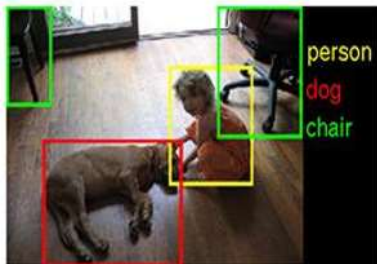
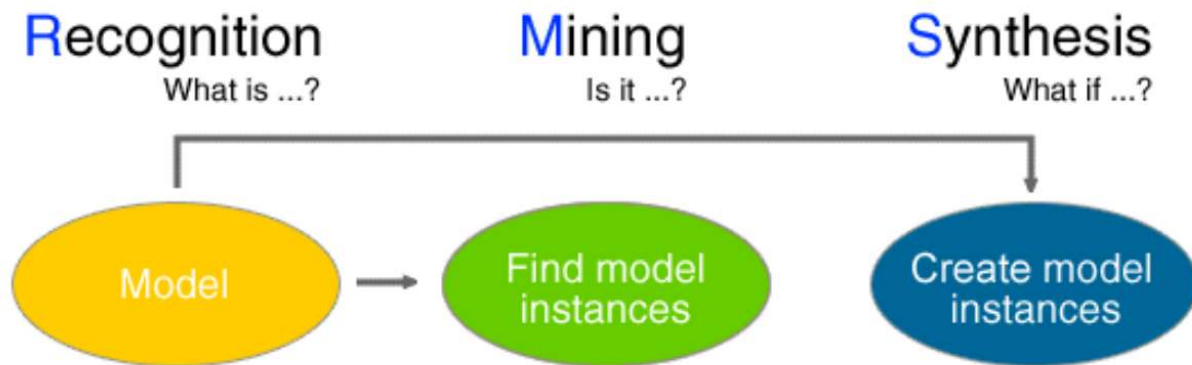


# ARTIFICIAL INTELLIGENCE (AI)

AI (especially in the form of automatic model construction) is being adopted to replace human for tedious manual tasks.



*Machine Centric*



# HPDA / HPC + AI = NEW GROWTH FOR HPC

Latest round of AI revolution driven by affordable/ubiquitous compute and vast amount of data.

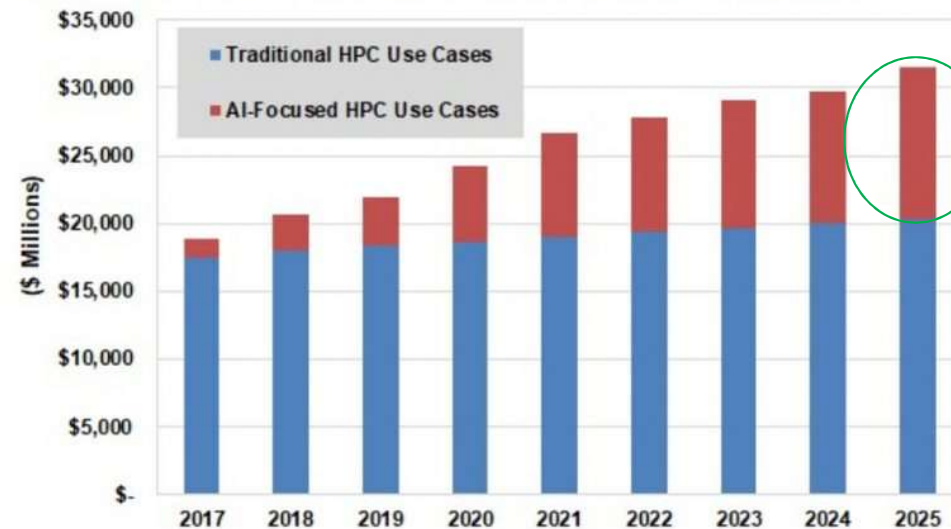
AI is being adopted by all business.



WAYMO



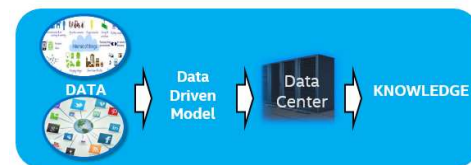
Total Enterprise HPC Revenue by Market Segment, World Markets: 2017-2025



HPC+AI is becoming the driving-force for HPC growth (~40% HPC market by 2025)

World HPC Revenue (2017-2025) (Source: Tractica)

# AI FOR SCIENCE



*Machine Centric*

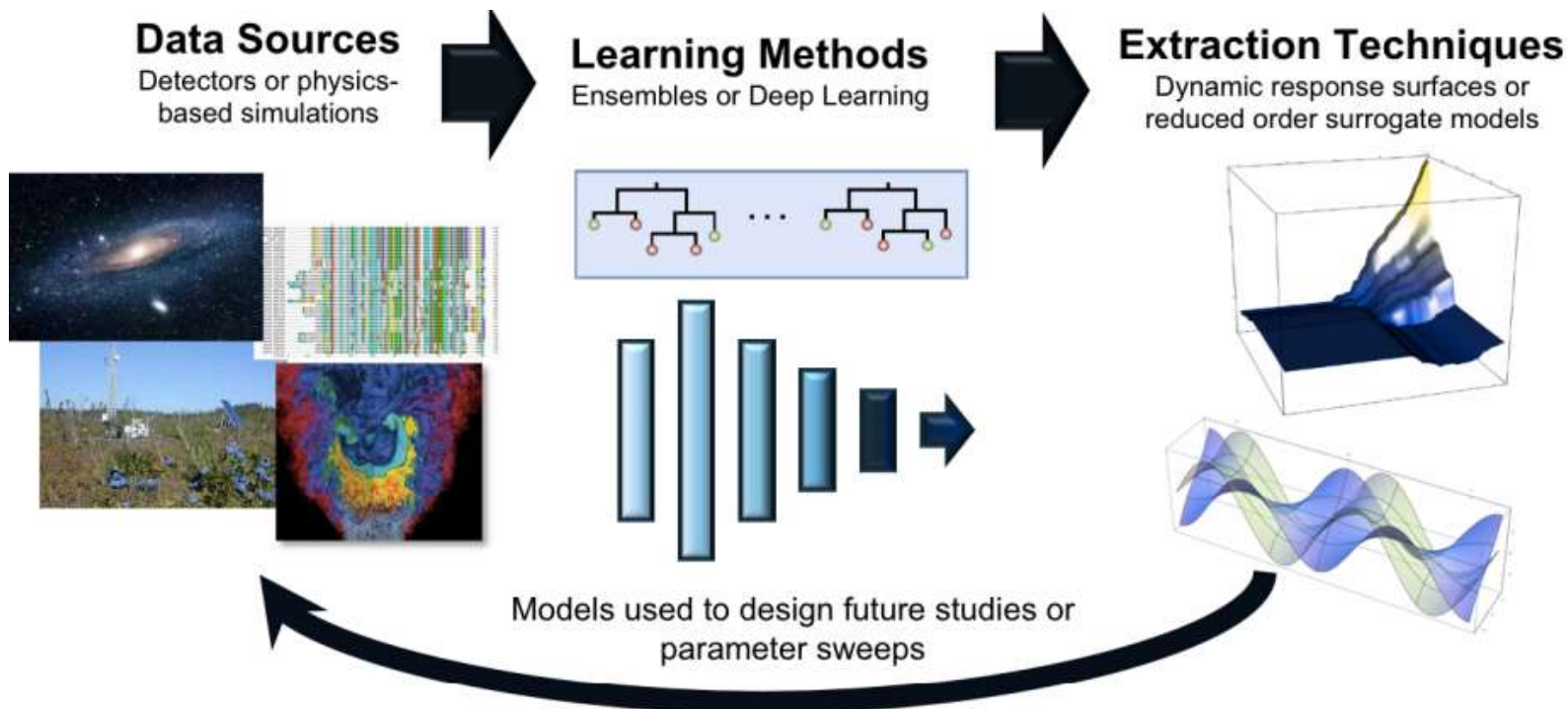
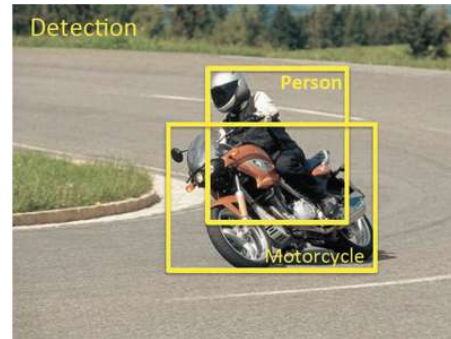


Diagram from J. Brown presentation, AI at Scale in Biology, AI for Science, September 2019



# WHAT DOES HPC+AI CONVERGED WORKLOAD LOOK LIKE



# TWO PATHS OF HPC + AI: HPDA VS. AI IN MOD/SIM

## High Perf. Data Analytics:

Harvest patterns / insights from data



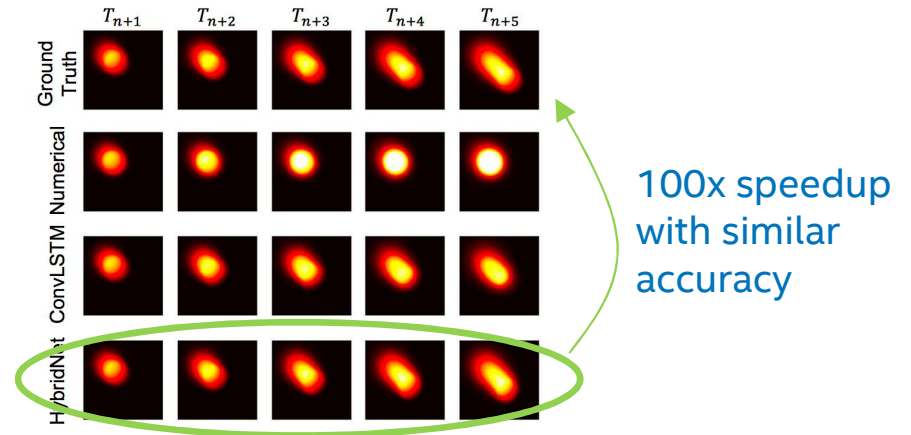
Statistical methods /  
ML model

Abnormality Detection (e.g. frauds)  
Recognition (e.g. face, voice, tumor, terrorist, etc.)  
Recommendations (e.g. what movies you may like)

## AI in Mod/Sim:

Use of ML models to speedup modeling / simulation

Example: Heat diffusion for manufacturing

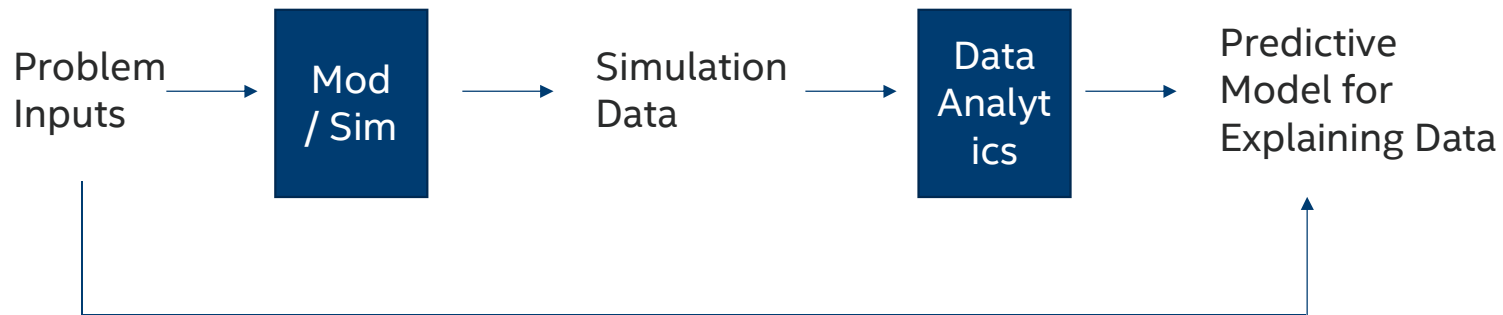


$$\frac{\partial T_{xy}}{\partial t} = C \cdot (T_{external} - T_{xy}) + K \cdot \Delta T_{xy},$$

\* "HybridNet: Integrating Model-based and Data-driven Learning to Predict Evolution of Dynamical Systems" <https://arxiv.org/pdf/1806.07439.pdf>

\* Majority of HPC+AI today

## WAYS IN COMBINING HPC AND ML (1: HPDA)



- Machine Learning is applied in **TANDEM** to model / simulation to **IDENTIFY** underlying data patterns
  - Mod/Sim and Data Analytics run separately and use different software stacks
- Train on observed / simulation data (e.g. weather, molecular simulation, etc.)
  - Data is stored in IO. Potentially an IO problem.

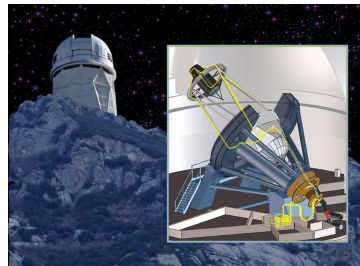
**Key Challenges: different management stack,  
Data Management / IO**

# HPDA EXAMPLE IN COSMOLOGY (COSMOFLOW @ SC'18)

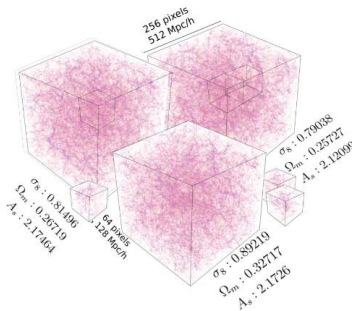
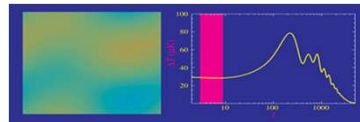
Problem: Finding the parameters that govern the universe expansion from the Big Bang

Traditional HPC approach

- 1) Scientists build universal models.
- 2) Models are simulated and correlated w/ observations.



↓ Reduced Statistics

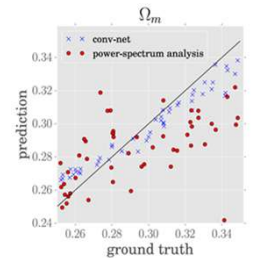
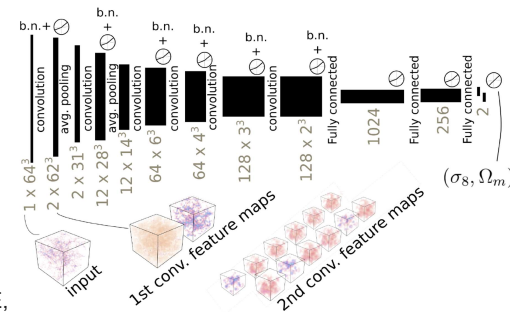


HPDA approach

- 1) Train 3D CNN to create a model correlates parameters and the generated models.
- 2) Apply model to infer observations.

Performance:

~1000x speedup on optimized IA framework  
~6M times speedup with 8192 nodes



Mathuriya, Amrita, et al. "CosmoFlow: using deep learning to learn the universe at scale." SC18: International Conference for High Performance Computing, Networking, Storage and Analysis. IEEE, 2018.

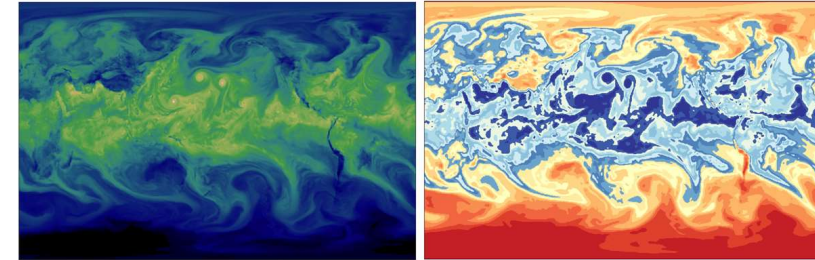
# HPDA EXAMPLE IN WEATHER (DISCO @ SC'19)

DisCo – Unsupervised Detection of Spatiotemporal Structure  
Collaboration w/ UC Davis and NERSC (2018-2019)

- Target spatio-temporal data
- Requires much higher dimensions (10s to 100s)
- First distributed-memory implementation w/ scikit-learn API using daal4py

Performance:

- 30x single node speedup (via. Intel® Data Analytics Acceleration Library (Intel® DAAL))
- 20,000x to 30,000x speedup with 1024-node Cori supercomputer



(f) Water vapor field of CAM5.1 climate model simulation

(g) Climate local causal state field



(a) Turbulence vorticity field

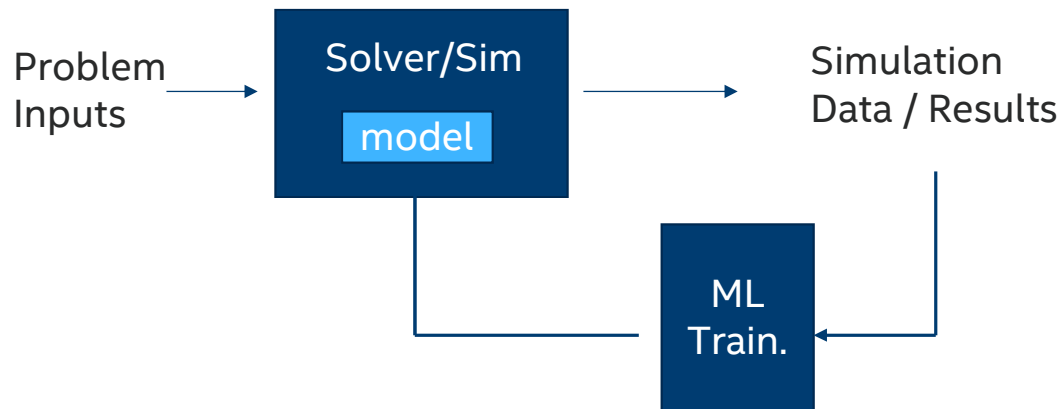
(b) Turbulence state field, fine structure

(c) Turbulence state field, coarse structure

A. Rupe, et. al, "DisCo: Physics-based Unsupervised Discovery of Coherent Structures in Spatiotemporal System", submitted for SC'19 workshop



## WAYS IN COMBINING HPC AND ML (2: AI IN MOD/SIM)

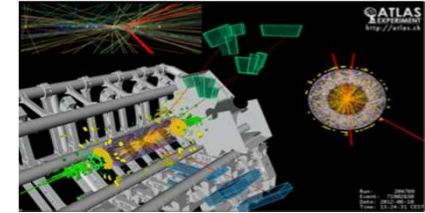


- Machine learning model can be trained separately, but it is **USED** with the solver / simulator
  - Implies ML models need to be usable in native solver / simulator programming environment (C/C++ or FORTRAN)
- Data used to train ML models are still pre-generated and stored in IO subsystem

**Key Challenge: Data management / IO as well as model integration**

# HPC + AI IN PARTICLE PHYSICS (ETALUMIS @ SC'19)

Problem: Infer properties of particles and interactions from LHC at CERN



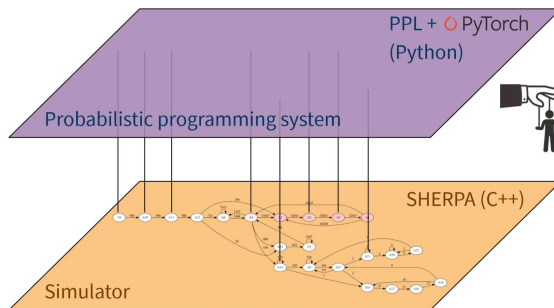
## Traditional HPC approach

- Particle types are determined by tracing the path of particles inside the detectors. It is then validated using physical model.

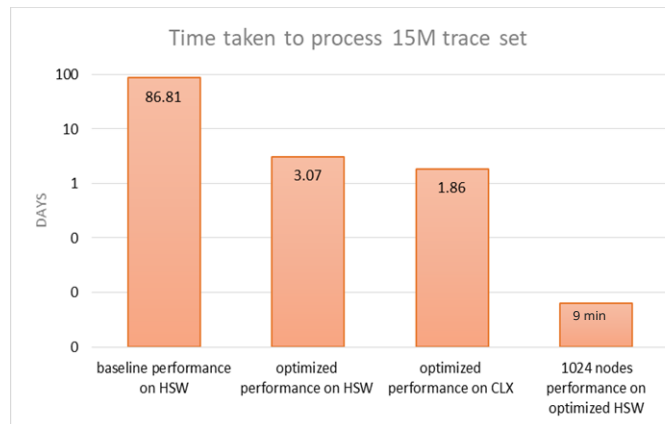
## HPC + ML approach

- 1) Use forward simulation traces to train a Probabilistic Programming model to correlate possible particle types and interactions to detection.
- 2) Apply model to infer observations directly from detector.

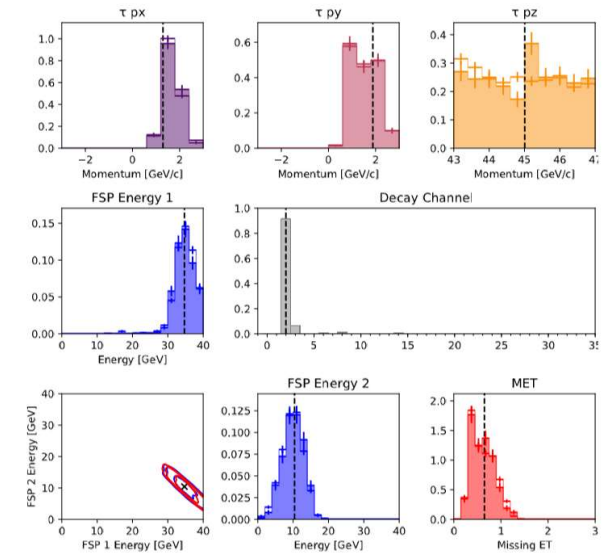
## Etalumis Integration of PPX w/ SIM



A. Bayden, et. al. "Etalumis: Bringing Probabilistic Programming to Scientific Simulators at Scale", to appear at SC'19



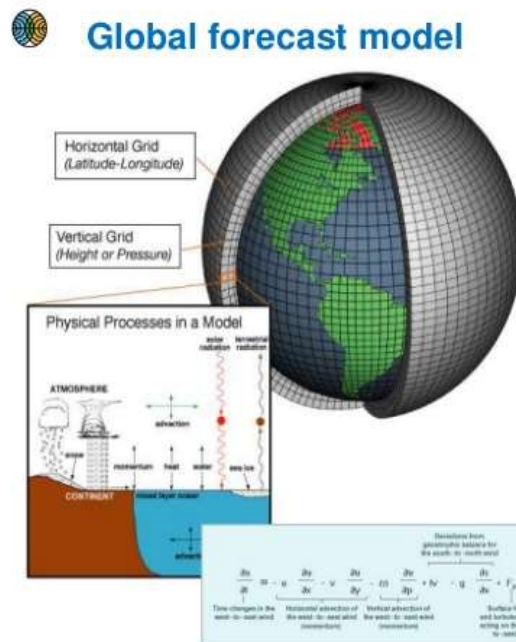
Achieved: 28x speedup on single node,  
14,000x speedup w/ 1024 nodes;  
230x speedup on inference



# AI IN MOD/SIM EXAMPLE IN CLIMATE / WEATHER FORECAST

Forecast model has an insatiable compute demand (EF is not enough)

- ML model is accurate enough to replace part of the simulation to improve resolution



Physical laws are presented in a form that a computer can compute the future state of atmosphere from the present state of atmosphere.

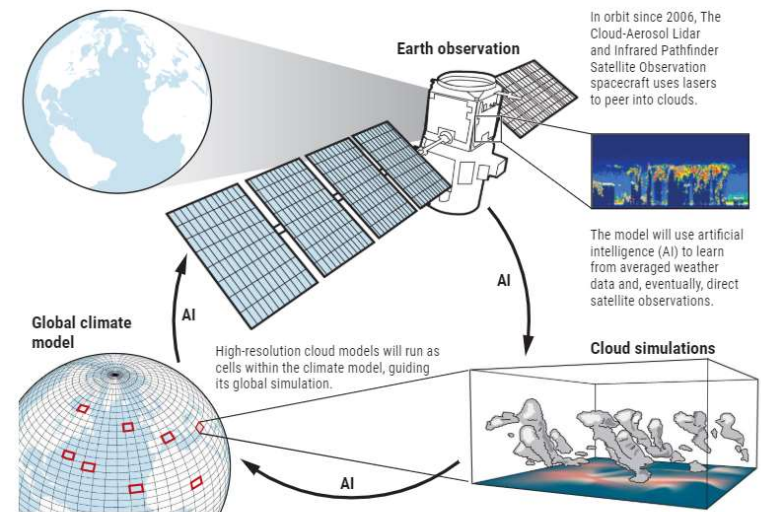
All physical variables (temperature, pressure, humidity, ...) are presented in a grid with several layers.

The typical distance between grid points is 3-15 km. The number of vertical levels varies typically between 50 and 150.

## Limitations:

- Update cycle (3-) 6-12 h
- NWP not good in predicting the proper time and place of convective rain storms

## ML tackle the limitation (clouds simulation)

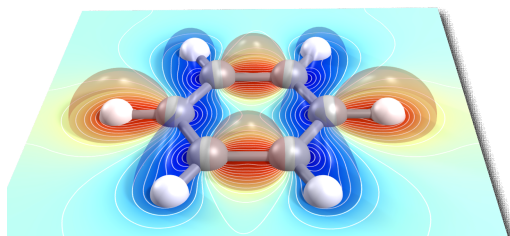


T. SCHNEIDER ET AL., GEOPHYSICAL RESEARCH LETTERS 44, 12,396 (2017), ADAPTED BY N. DESAI/SCIENCE

Methods described in <https://www.sciencemag.org/news/2018/07/science-insurgents-plot-climate-model-driven-artificial-intelligence>

# AI IN MOD/SIM EXAMPLE DL GUIDED MONTE CARLO SIMULATION

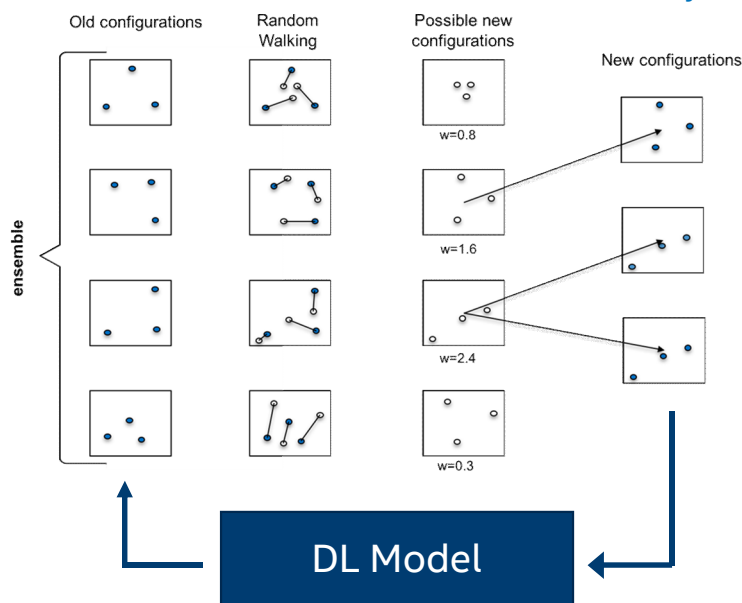
Quantum Molecular Simulations (QMS) are commonly used to study material properties



Traditional method is iterative and the amount of computation grows exponentially with number of atoms. One can quickly require EF of compute with  $\sim 1000$  atoms.

Goal: determine the best wave functions to describe the molecule energy

## QMCPACK: One of DoE Exascale Projects



Deep learning model is used to guide selection of “New Configurations” and allow skipping of critical simulation steps.

# HPC + AI CONVERGENCE CHALLENGES

Significant increase in compute demands

- 300,000x increase in ML training demand (compare to only 10x increase in HPC demands)
- Few optimized networks outside of image / speech domains.

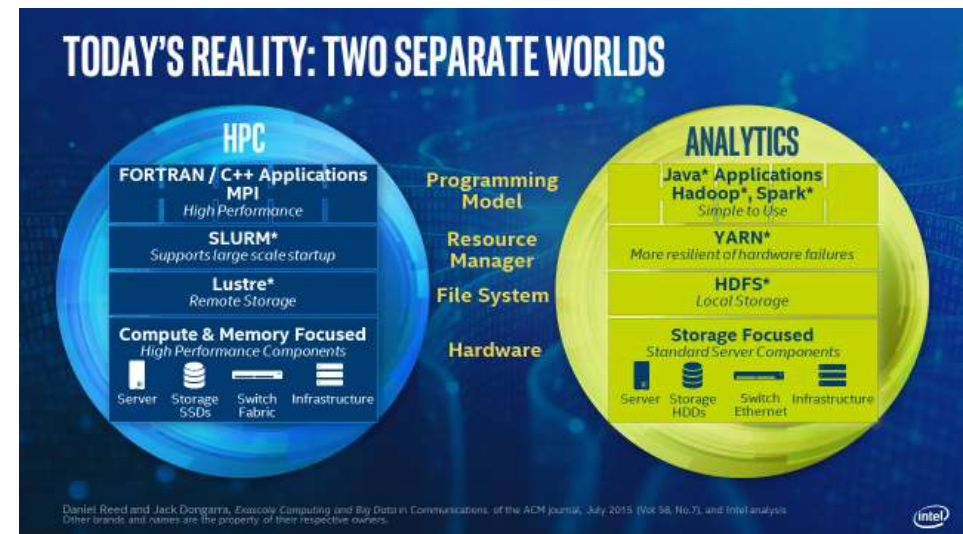
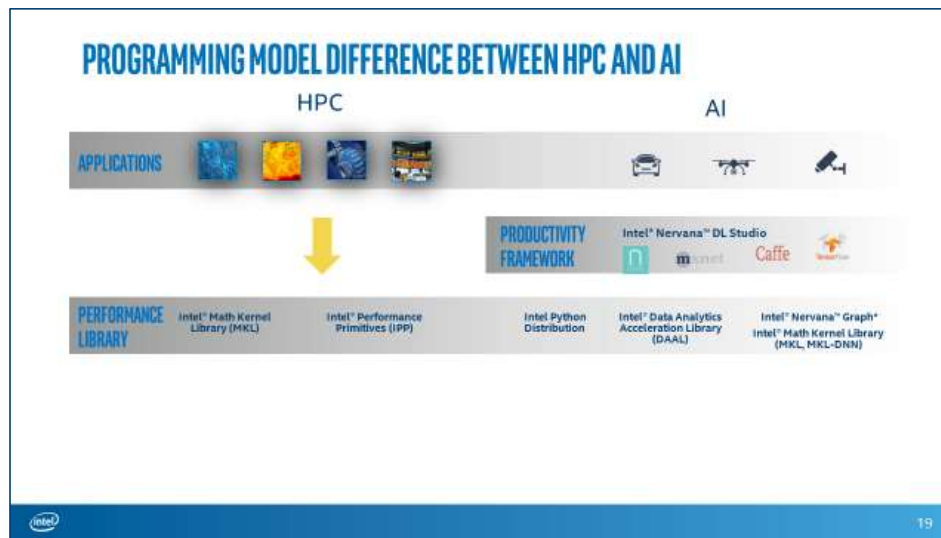
Not enough labelled data. Currently available labeled datasets:

- Government: 8
- Economics: 6
- Images: 25
- Sentiments: 5
- Language: 13
- Medical: 1



# HPC + AI CONVERGENCE CHALLENGES

- Different programming models / tools
- Different resource management stacks
- Different data formats, file systems



# GAPS

## Integration of ML model to mod/sim code:

- ML models are described and coded at higher level frameworks (TF, Pytorch, etc.)
- Trend: Community is working on more interchangeable format (ONNX, etc.)
- Still far from plug-n-play into HPC model / simulation codes
- **Need:** framework to embed ML model to model / simulation codes

## Custom layers:

- Most commercial customers embed their IPs in customer layers/ops
- These layers are often not optimal for CPU, GPU, ACC, etc.
- **Need:** optimizer to generate high performance code for CPU, GPU, ACC, etc.

# SUMMARY

HPC + AI is one of the most critical emerging workloads

Challenges exist for HPC + AI convergence:

- Programming model difference
- Resource management difference
- Data management requirements / file system differences

Solutions are WIP to address resource management / IO issues

Gaps exist in lack of tools to (1) integrate ML models with Mod/Sim code as well as (2) generate optimal implementation for custom layers

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