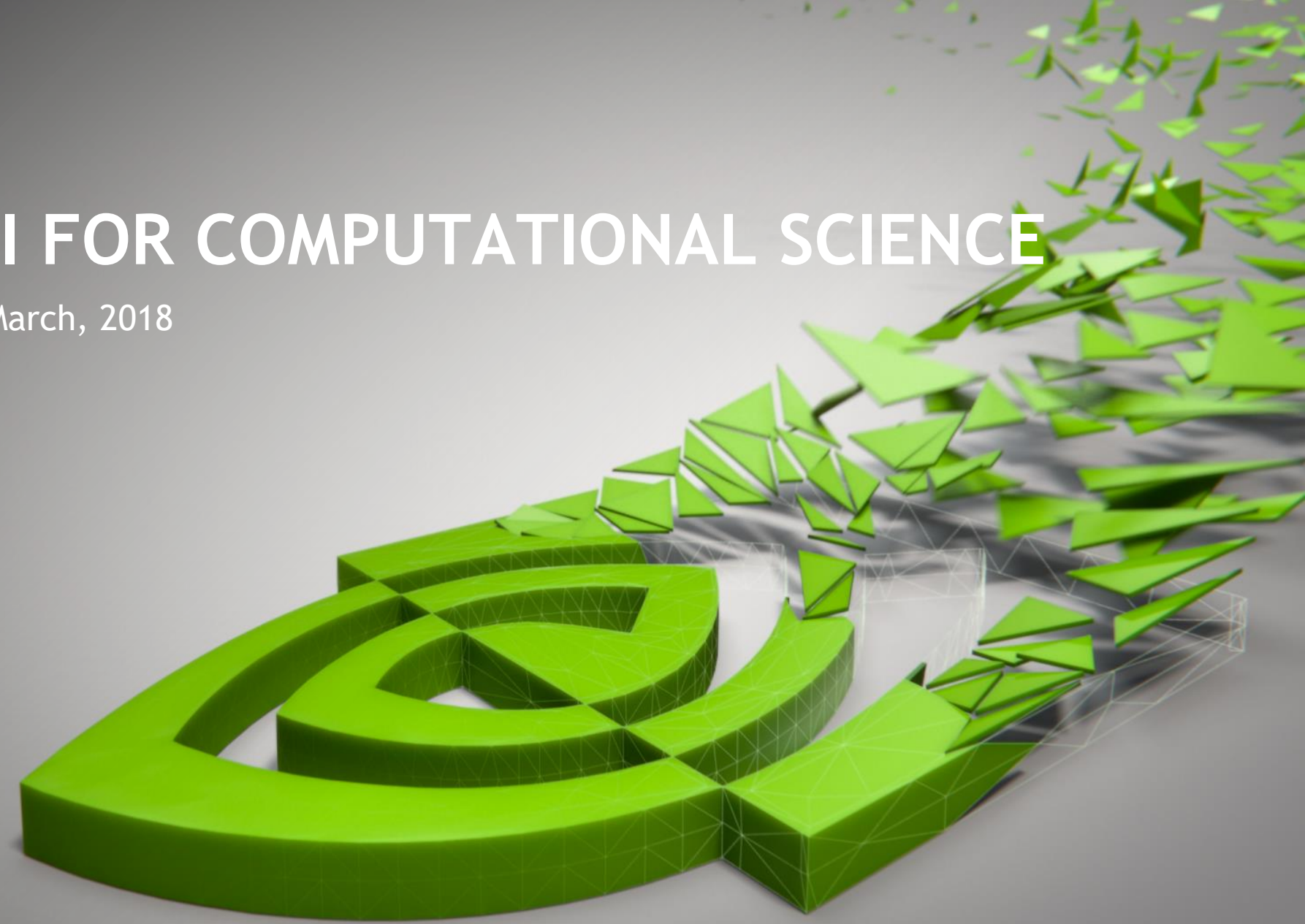
S8242 – AI FOR COMPUTATIONAL SCIENCE

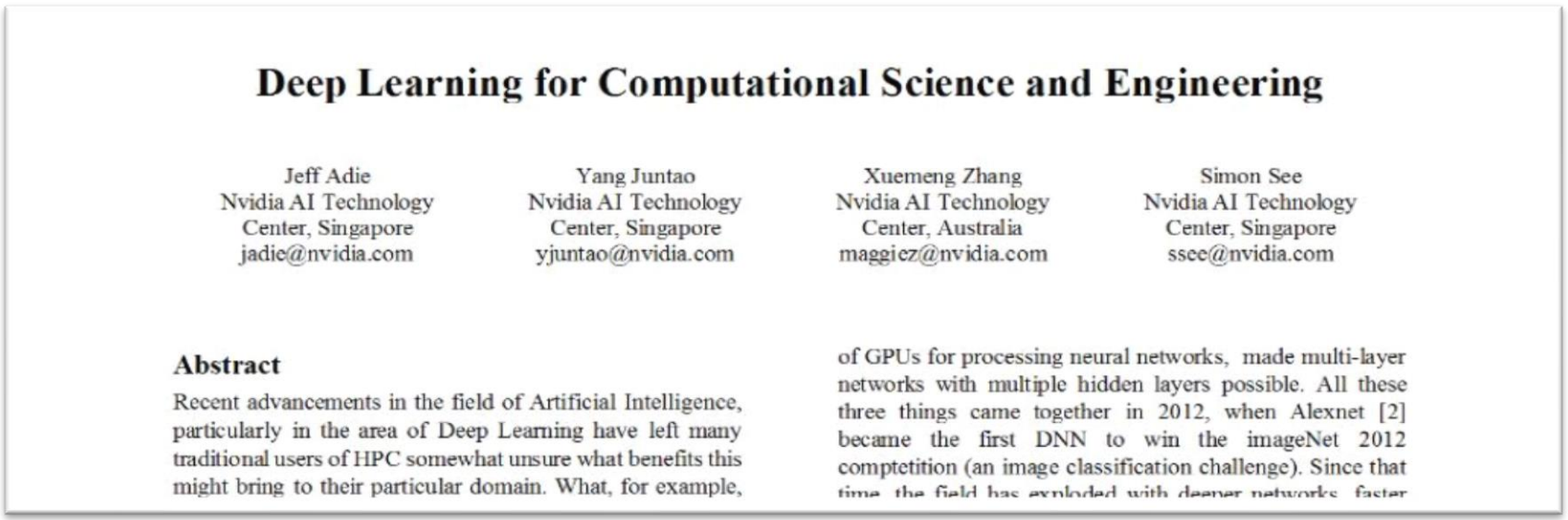
Yang Juntao, 26th March, 2018

NVIDIA



Introduction

- Nvidia AI Technology Center(NVAITC) carries out both core and applied research for various domains
- One core project is the study of the application of Deep Learning to traditional HPC
- We did a survey on the state-of-the-art for this project



Deep Learning for Computational Science and Engineering

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Abstract

Recent advancements in the field of Artificial Intelligence, particularly in the area of Deep Learning have left many traditional users of HPC somewhat unsure what benefits this might bring to their particular domain. What, for example, of GPUs for processing neural networks, made multi-layer networks with multiple hidden layers possible. All these three things came together in 2012, when Alexnet [2] became the first DNN to win the imageNet 2012 comptetition (an image classification challenge). Since that time, the field has exploded with deeper networks, faster

Domain Classification

Computational Mechanics	Earth Sciences	Life Sciences	Computational Physics	Computational Chemistry
Computational Fluid Mechanics	Climate Modeling	Genomics	Particle Science	Quantum Chemistry
Computational Solid Mechanics	Weather Modeling	Proteomics	Astrophysics	Molecular Dynamics
	Ocean Modeling			
	Seismic Interpretation			

Agenda

- Introduction
- Computational Mechanics
- Earth Sciences
- Computational Physics/Chemistry
- Life Sciences
- Conclusions

Computational Mechanics

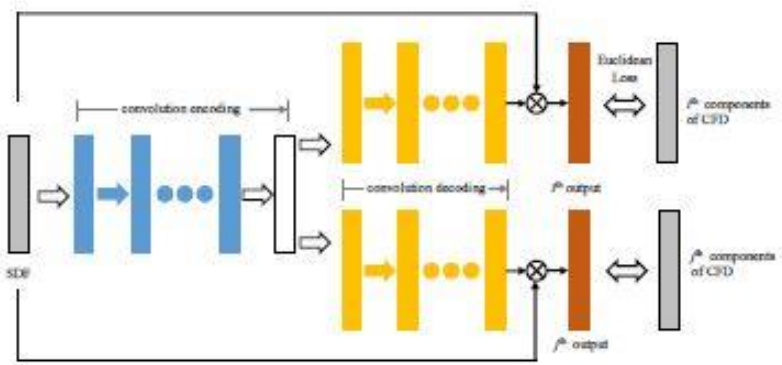
Convolutional Neural Networks for Steady Flow Approximation

A quick general CNN-based approximation model for predicting the velocity field of non-uniform steady laminar flow by Guo, et al. (2016)

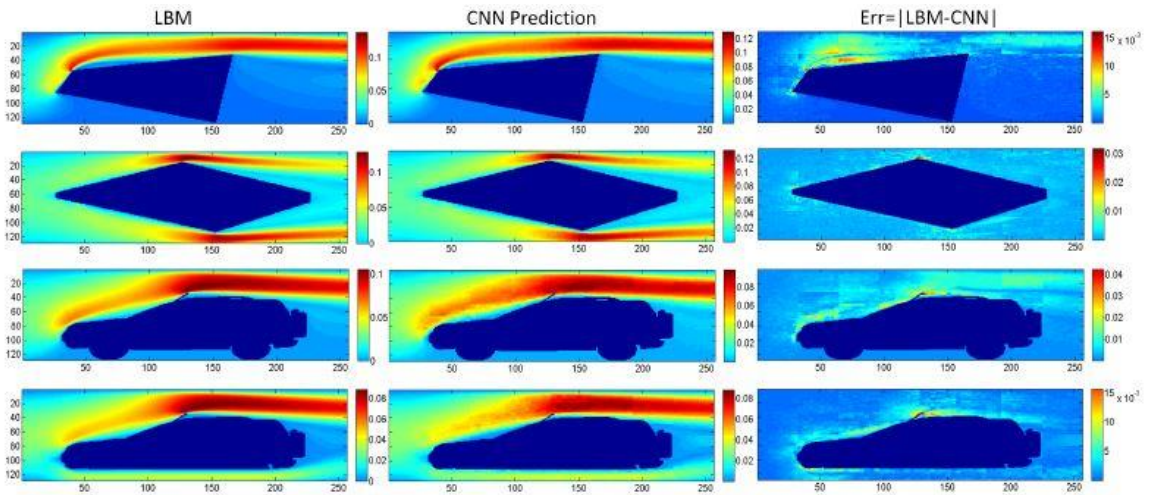
CNN-based approximation model trained by BLM simulation results

SFD data is used as import and error is used as lost function to train the convolutional neural networks.

82 seconds on a single core CPU to 7 milliseconds by leveraging both CNN and GPU at the cost of a low 1.98% to 2.69% error rate



CNN based CFD surrogate model architecture

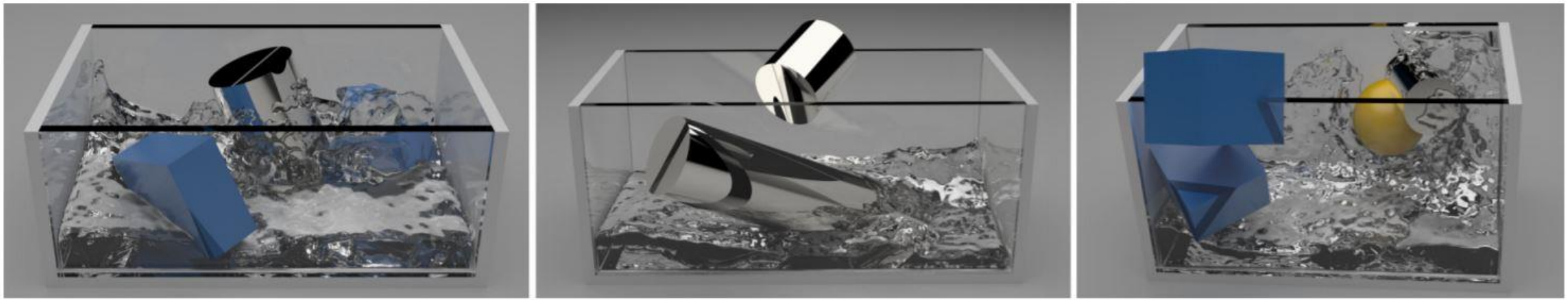


Results comparison between LBM model and CNN based surrogate model

Interactive Fluid Simulation With Regression Forest

Fluid Simulation with Trained Regression Forest [Ladicky et al, 2015]

- Regression Forested model trained with data generated with SPH method
- Realtime simulation generated by trained regression forest with GPU acceleration



Data driven fluid simulation using regression forests

Eulerian Fluid Simulation With Neural-Network

Accelerating Eulerian Fluid Simulation with Neuro-Networks

Acceleration of traditional Eulerian Fluid Simulation with Neuro-Network has been attempted by some researchers

The most computing costly pressure projection step is replaced with trained neuron-network

Convolutional Network has been tested and shown positive acceleration within reasonable error in the most recent publications.

Data Driven projection method in fluid simulation
[Cheng Yang et al. 2016]

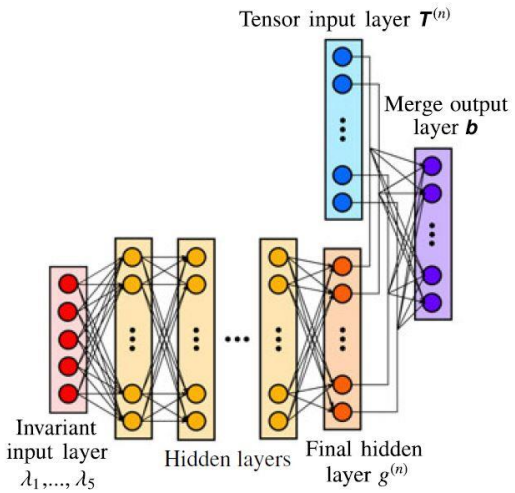
Accelerating Fluid Simulation with Convolutional Network [Tompson et al. ICML 2017]

Turbulence Modeling With Machine Learning Techniques

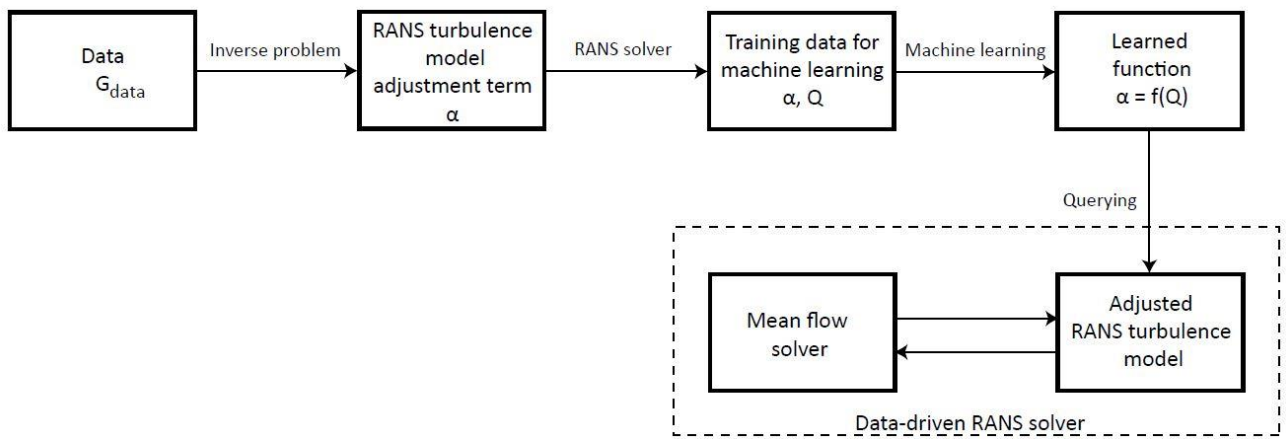
RANS method couple with machine learning techniques has been new frontier for turbulence modeling

The idea is to use machine learning techniques to learn from data generated by computational expensive DNS and add the term into RANS model to improve the accuracy of turbulence modeling

RANS results are used as import and DNS results are used as label to update the model.



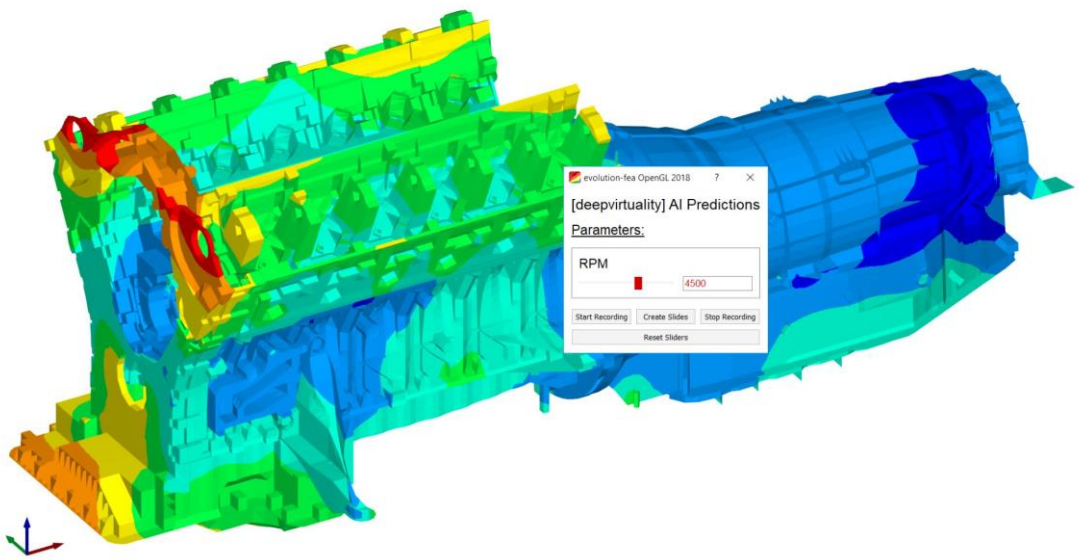
Tensor Basis Neural Network(TBNN) is proposed by Julia Ling and et al. (J.Fluid Mech 2016)



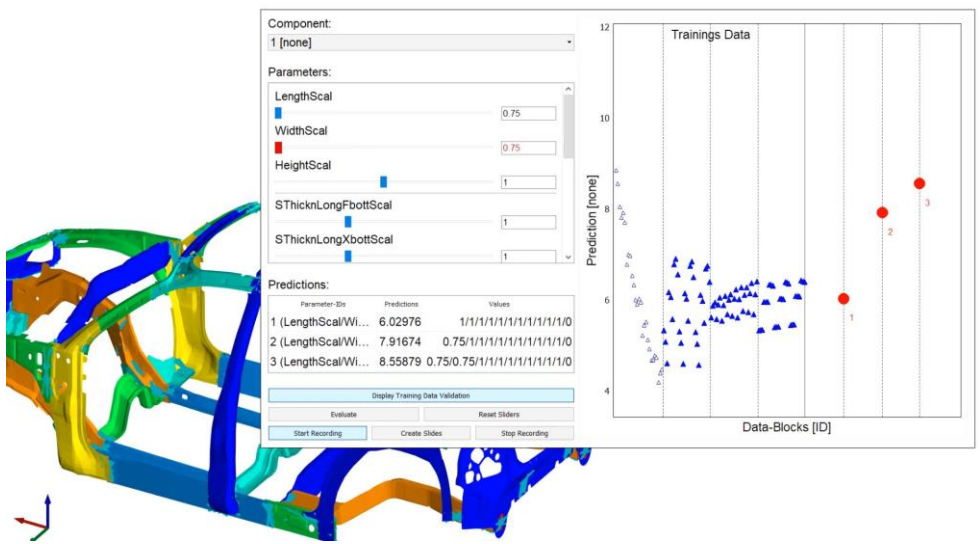
Inverse Modeling Framework propsed by Universrity Michigan from “Machine Learning Methods for Data-driven turbulence modeling”, Zhang and Duraisamy (2015)

FEA trained neural network

FEA trained deep neural network for surrogate modelling of estimated stress distribution. Deepvirtuality, a spinoff from Volkswagen Data:Lab under Nvidia Inception Program has demonstrate with their software aimed for a quicker prediction of structural data.



An demonstration of Structure Born Noise of a V12 Engine with Deepvirtuality



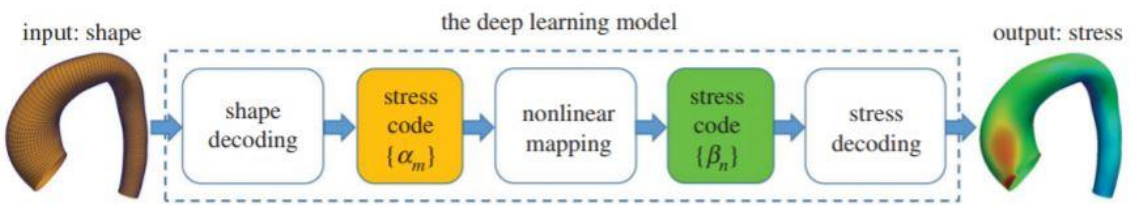
Torsional Frequencies of a Car Body by Deepvirtuallity

FEA Updated with neural network in Bio-tissue

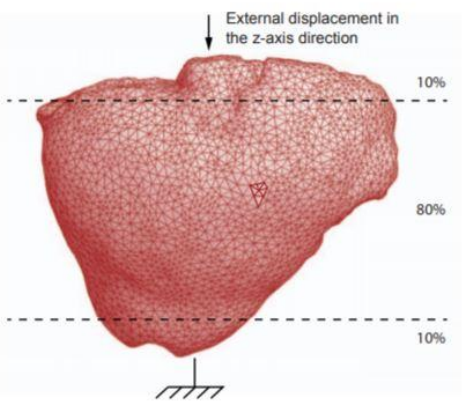
FEA trained deep neural network for surrogate modelling of estimated stress distribution. Traditional machine learning method has been used before, now deep learning techniques has been attempted for such model.

FEA generated stress distribution data is feed into neural network to train the neural network for fast stress distribution estimation. (Liang et al, 2018)

Ensembled decision tree model has also been applied for FEA update in “Machine Learning for modeling the biomechanical behavior of human soft tissue”. Data driven simulation has been done on Liver and Breast tissue. (Martin-Guerrereo, 2016)



Neural Network used for stress mapping by Liang Liang et al (2018)

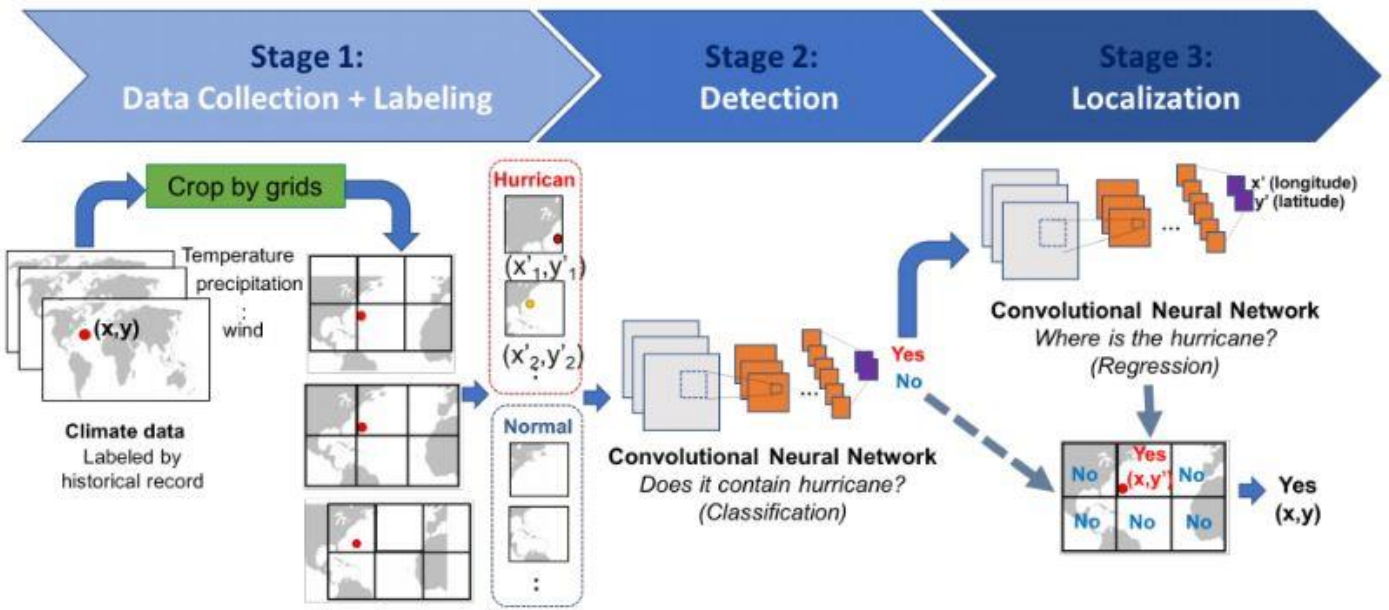


FEA model for Liver from “Machine Learning for modelling the biomechanical behavior of human soft tissue” (Martin-Guerrereo, 2016)

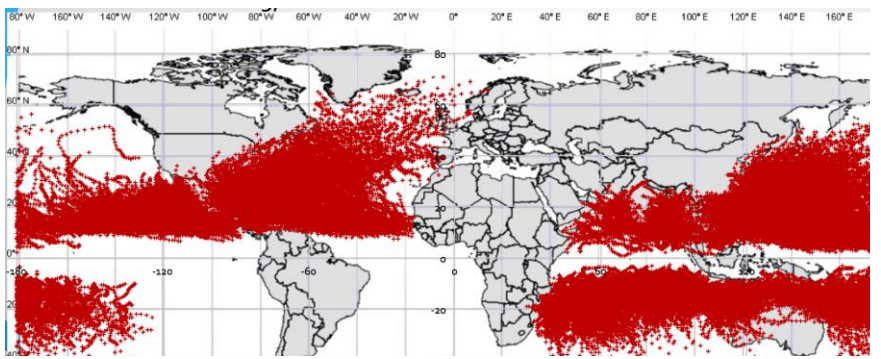
Earth Science

Anomaly detection in climate data

Identifying “extreme” weather events in multi-decadal datasets with 5-layered Convolutional Neural Network. Reaching 99.98% of detection accuracy. (Kim et al, 2017)



Systemic framework for detection and localization of extreme climate event

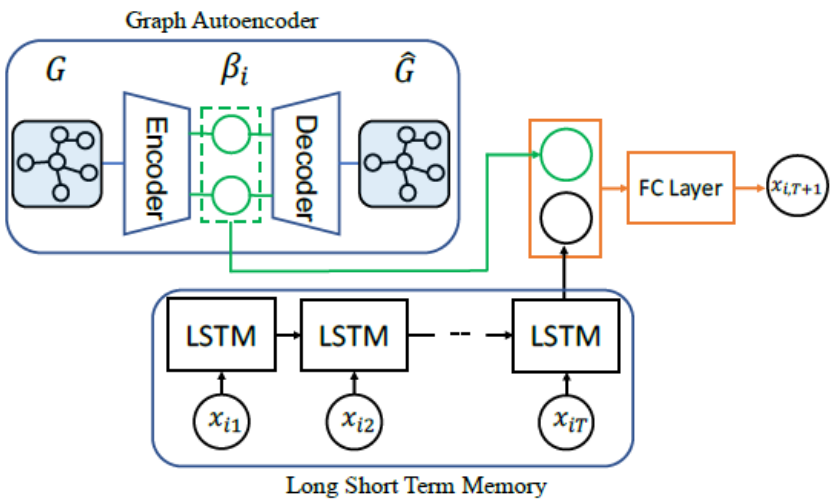


Dataset: Visualization of historic cyclones from JWTC hurricane report from 1979 to 2016

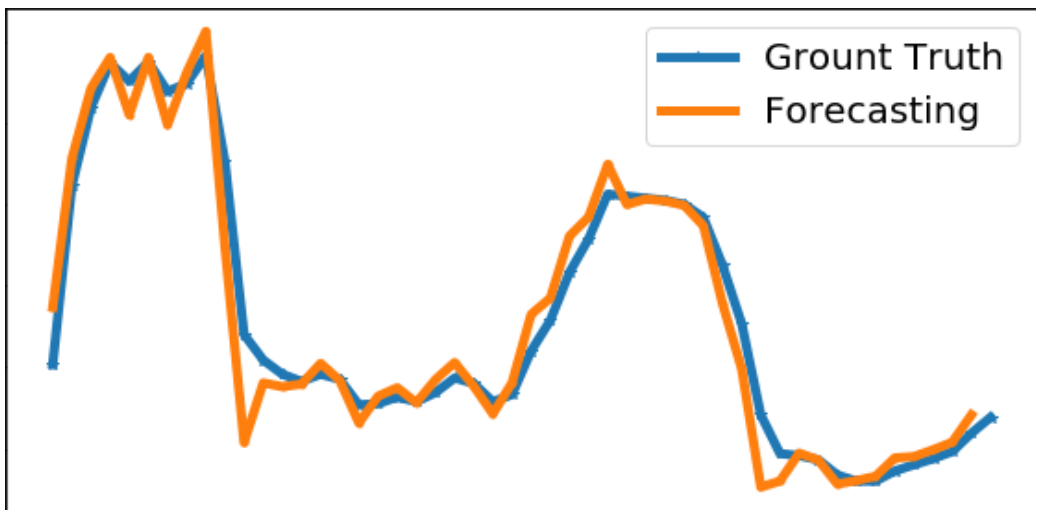
GAE + RNN for improved spatiotemporal data

Multiple climate sets covering different places and time: Combining them is a huge challenge (Seo et al, 2017)

New network handles both spatial and temporal properties together to solve this problem.



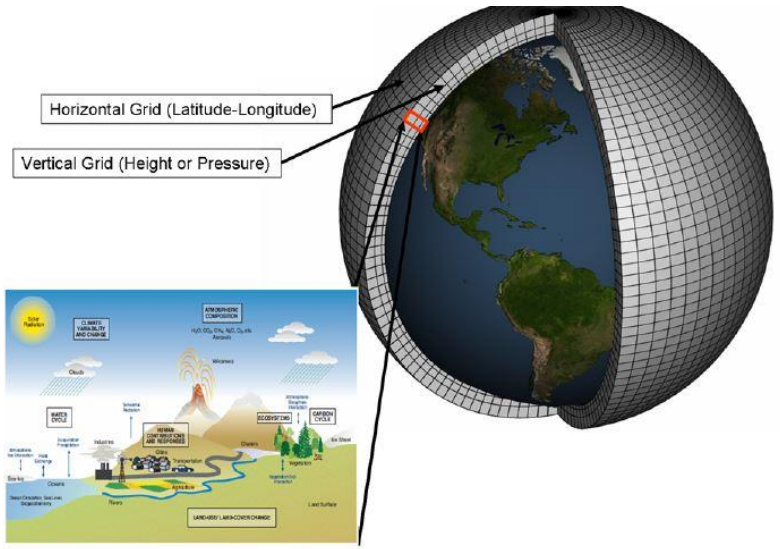
GAE-RNN model architecture



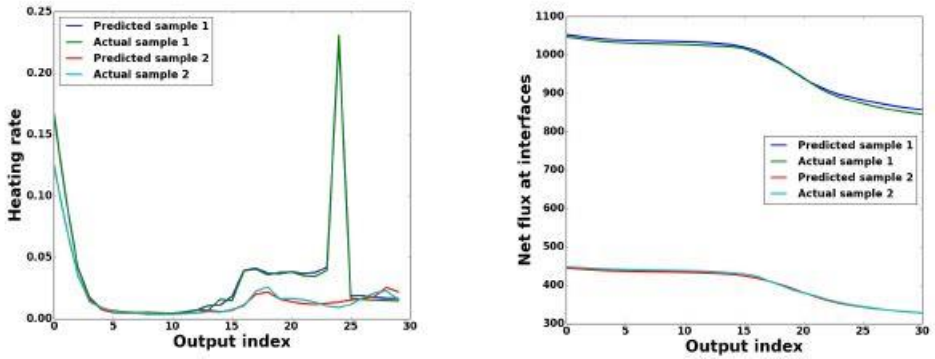
Forecasting of temperature

Emulating RRTMG with Deep Neural Networks for the Energy Exascale Earth System Model

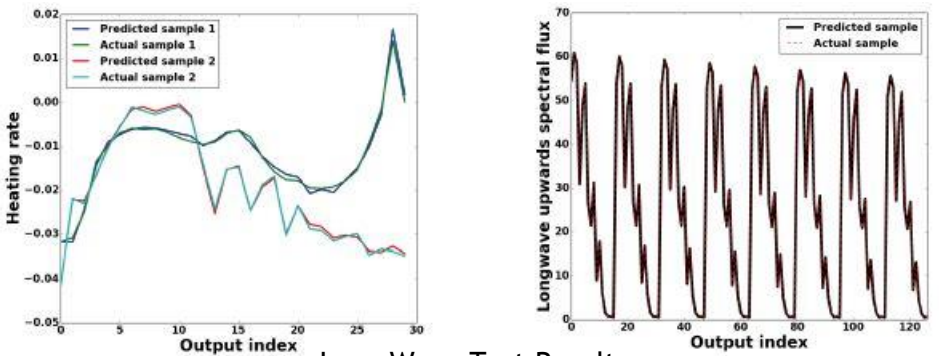
- Rapid Radiation Transfer Model for GCMs(RRTMG) is the most time consuming component of General Circulation Models(GCMs)
- Oak Ridge National Laboratory made use of Deep Neural Network to learn from RRTMG model.



GCM for climate modeling



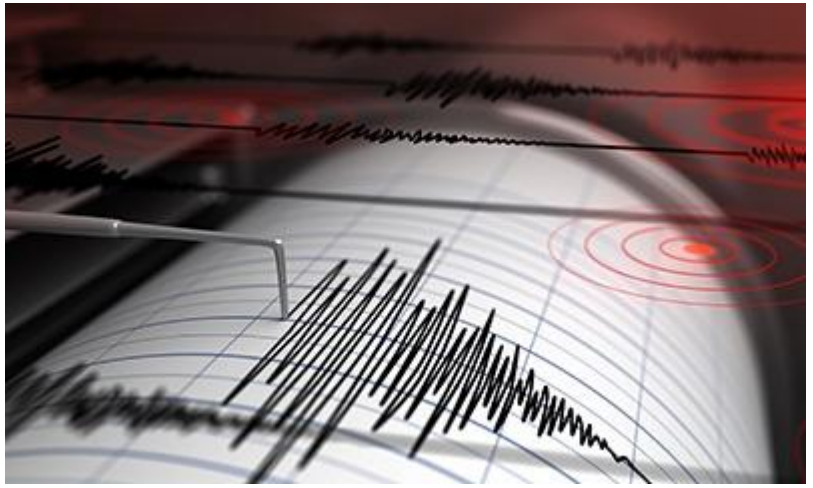
Short Wave Test Results

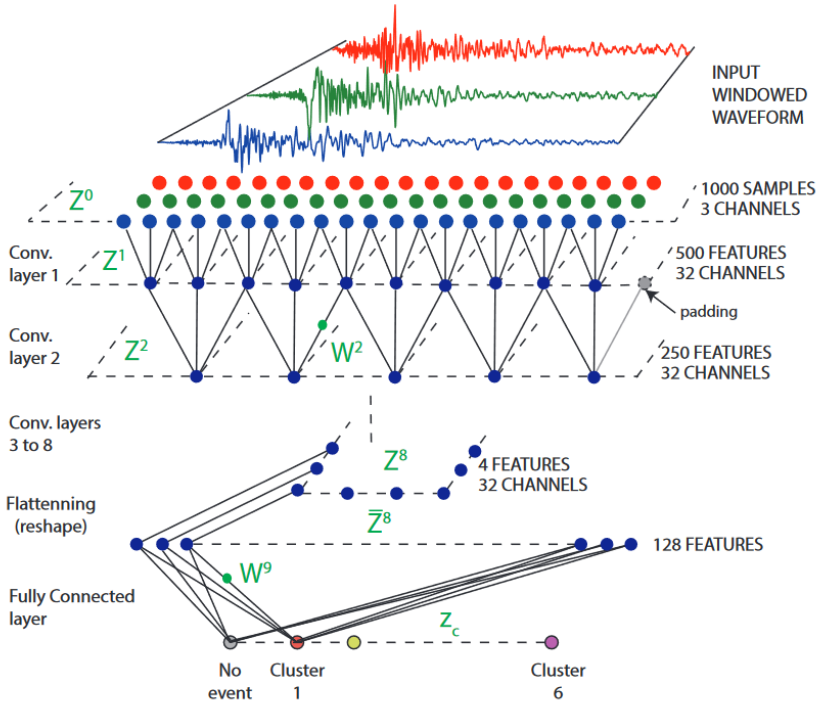


Long Wave Test Results

Deep Learning for Seismic Events

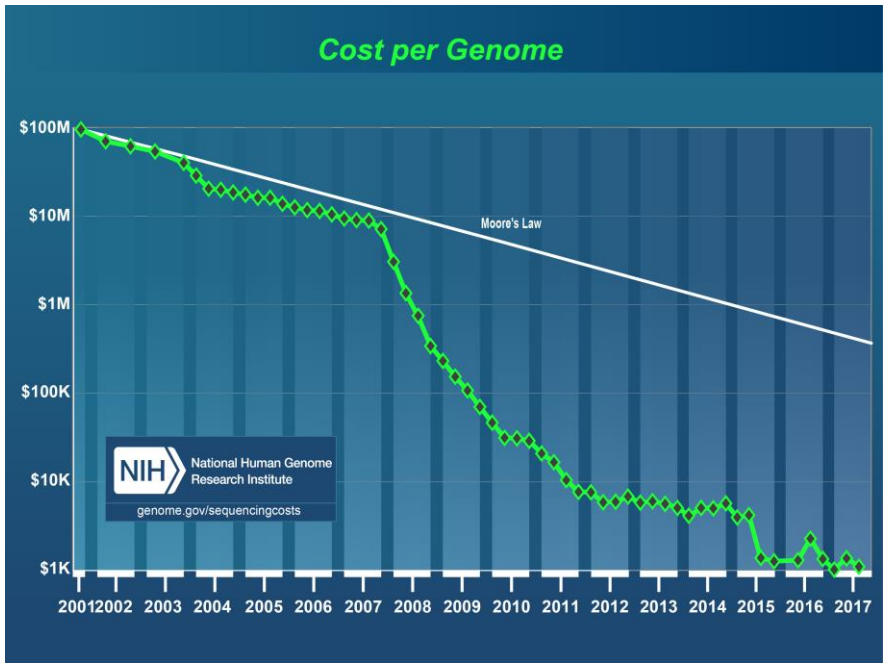
- Detecting earthquakes from seismic data [Perol, et al]
- 20x improvement in detection vs manual.
- Orders of magnitude faster

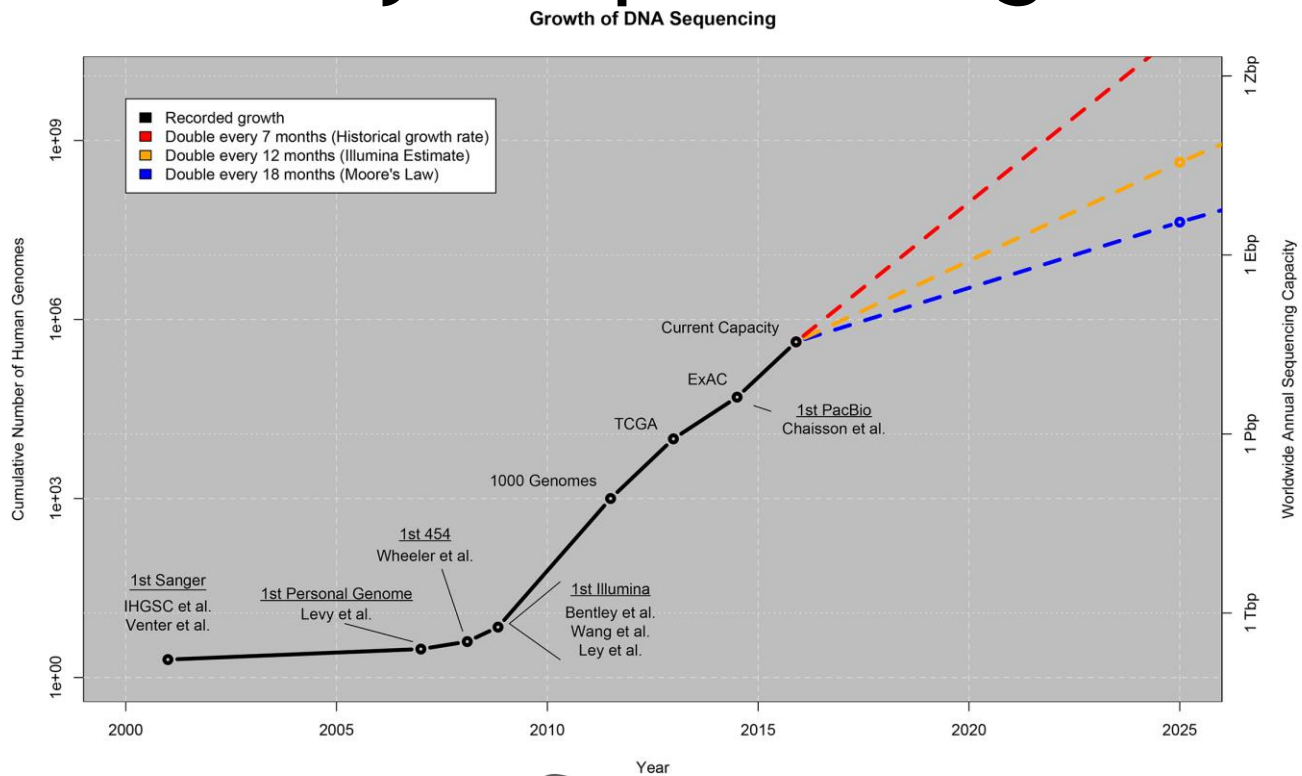




Life Science

Decode the human genome by deep learning





GA II
1.6 billion bp per day
(2008)

GA IIx
5 billion bp per day
(2009)

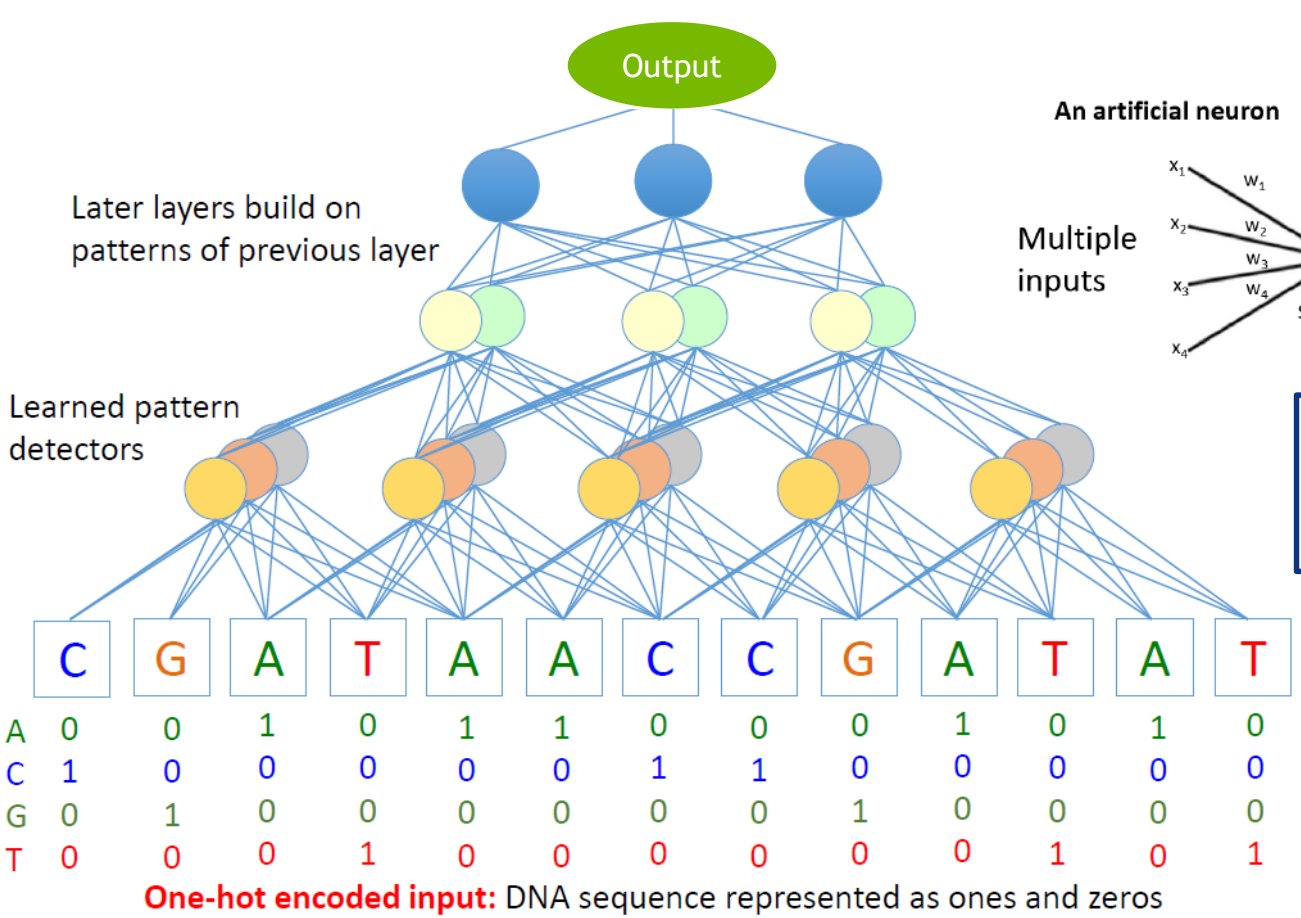
HiSeq 2500
60 billion bp per day
(2012)

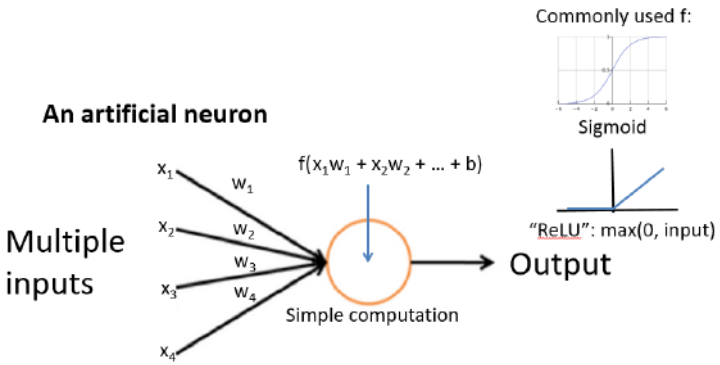
MinIon

SmidgION

Deep CNN on DNA sequence inputs

Anshul Kundaje team, Stanford University



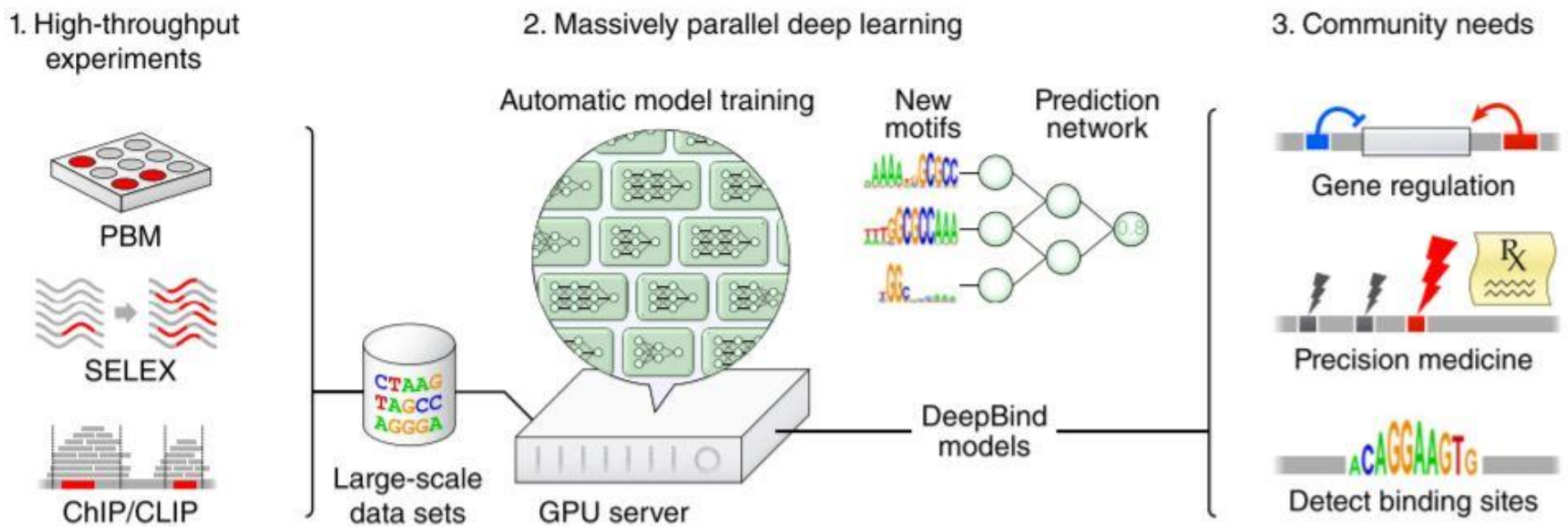


Johnny Israeli
Deep Learning for shallow sequencing
Thursday, 3pm, Room 210D

source from Anshul Kundaje's presentation online

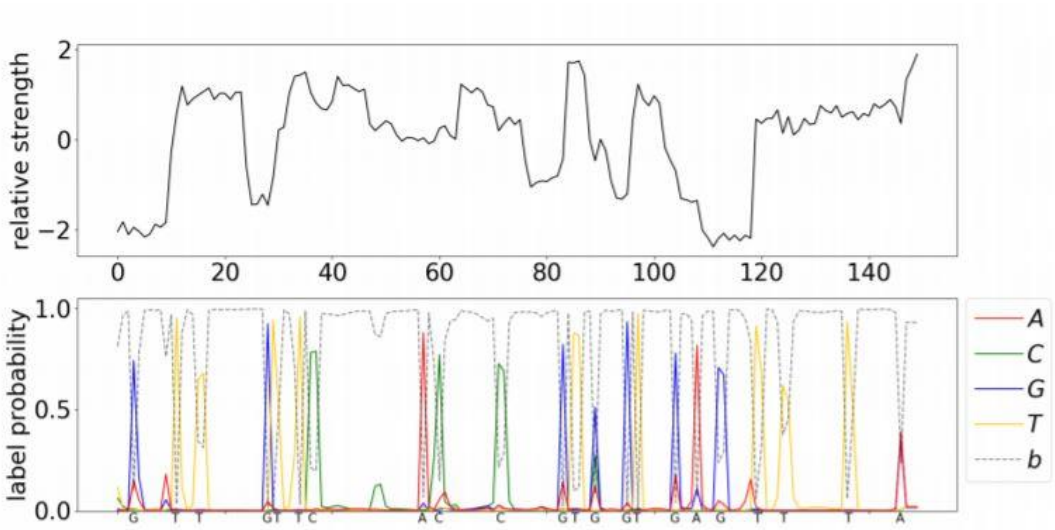
Predicting of sequence specifies of DNA- and RNA binding proteins

- DeepBind was proposed and build by [Babak et al, Nature Biotechnology] for predicting of sequence specifies of DNA- and RNA-binding proteins.

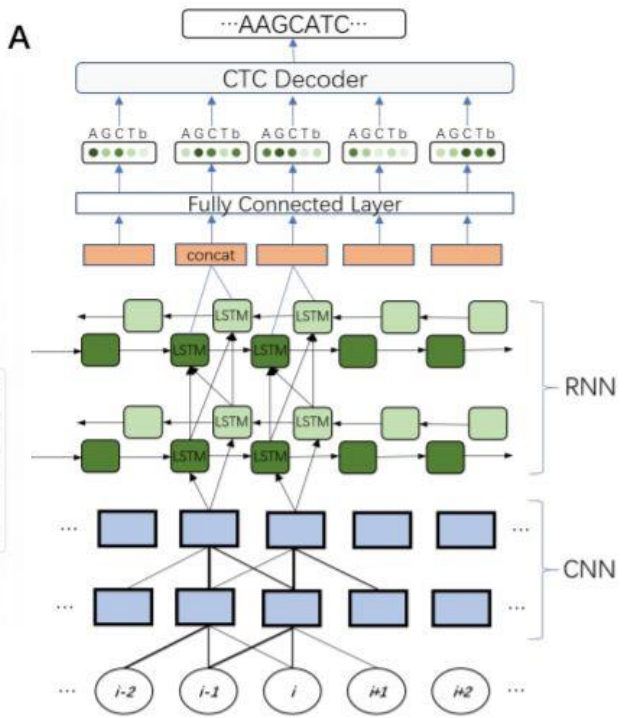


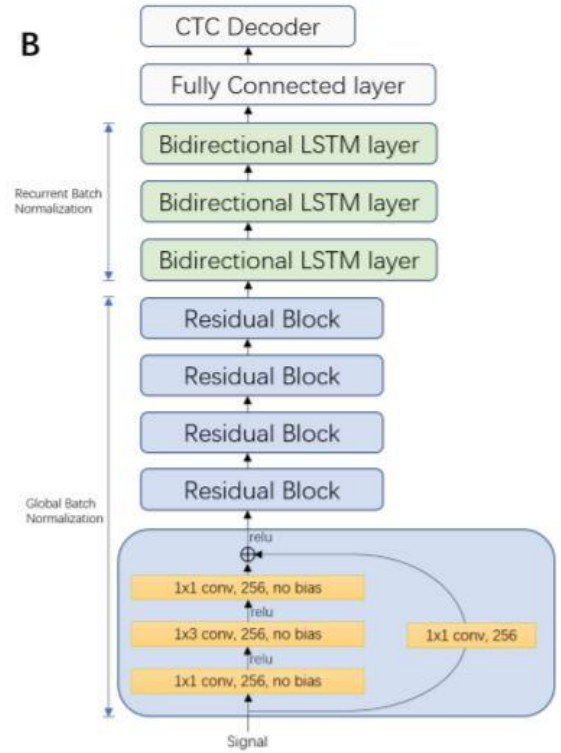
DeepBind's input data, training procedure and applications

Translating nanopore raw signal directly into nucleotide sequence using deep learning



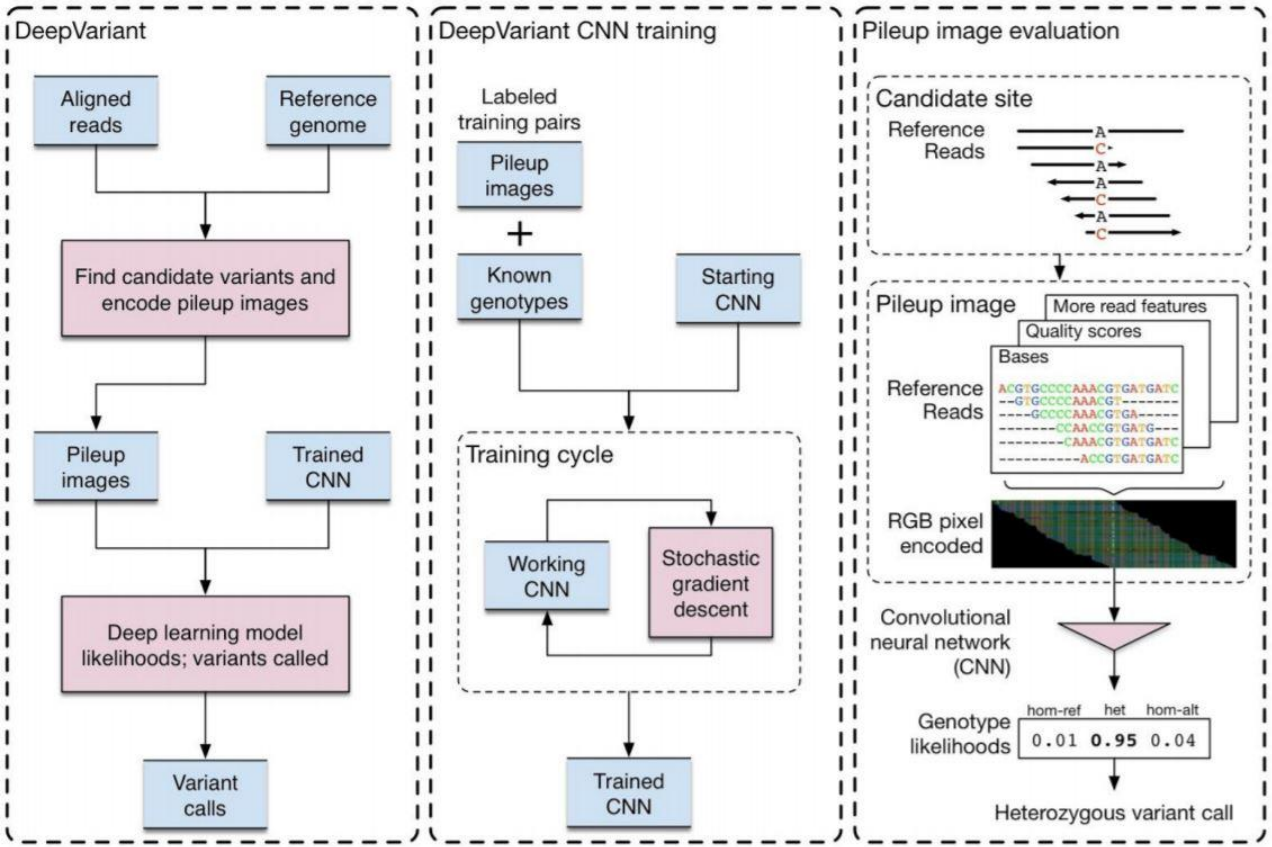
SmidgION





Creating a universal SNP and small indel variant caller with deep neural networks

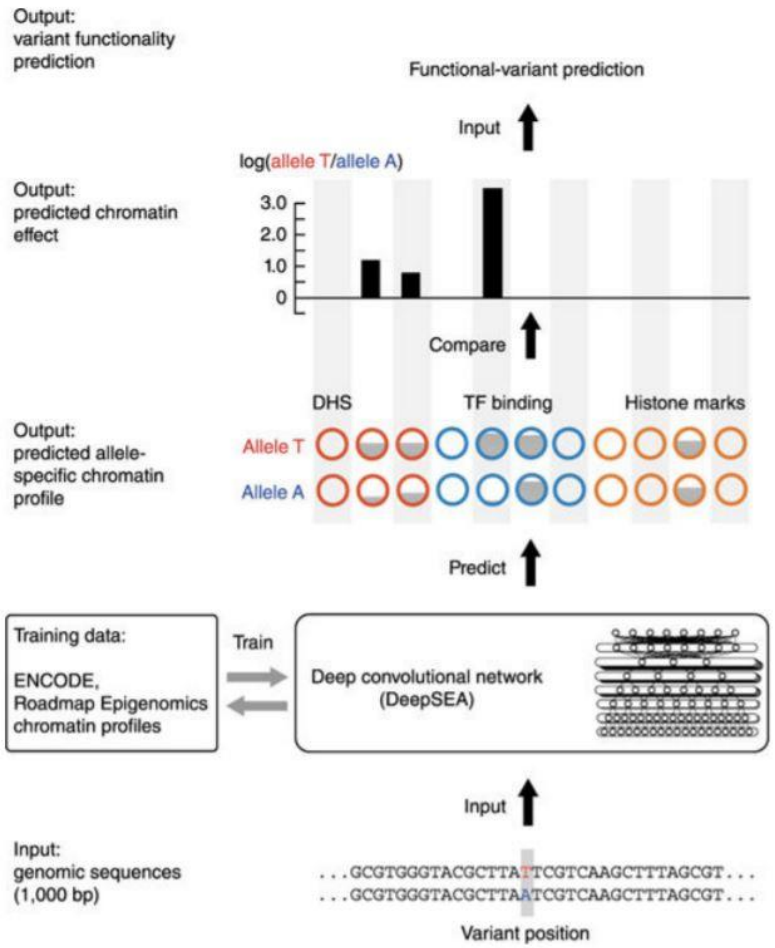
- DeepVariant is proposed and build by Ryan, et al for rapid determination of genetic variants in an individual's genome with billions of short and errorful sequence reads.
- It out performed statistical models handcrafted by thousands of researchers in decades.



DeepVariant Framework

Creating a universal SNP and small indel variant caller with deep neural networks

- [Zhou, et al, Nature Methods] proposed another deep learning based model for predicting effects of noncoding variants named DeepSEA.
- The core of DeepSEA is a typical convolutional neural network trained with ENCODE, Roadmap Epigenomics chromatin profiles



DeepSEA framework

Computational Physics

Deep Learning in High Energy Physics - CERN

Challenges:

- HL-LHC (High-Luminosity Large Hadron Collider) project, the ever increasing event complexity
- Model Independent Searches

Deep Learning Solutions for:

- Triggering on rare signals
- Faster data processing and simulation
- Pattern recognition to extract physics content
- Lower Energy Computation
- Unsupervised Learning to Search for New Physics

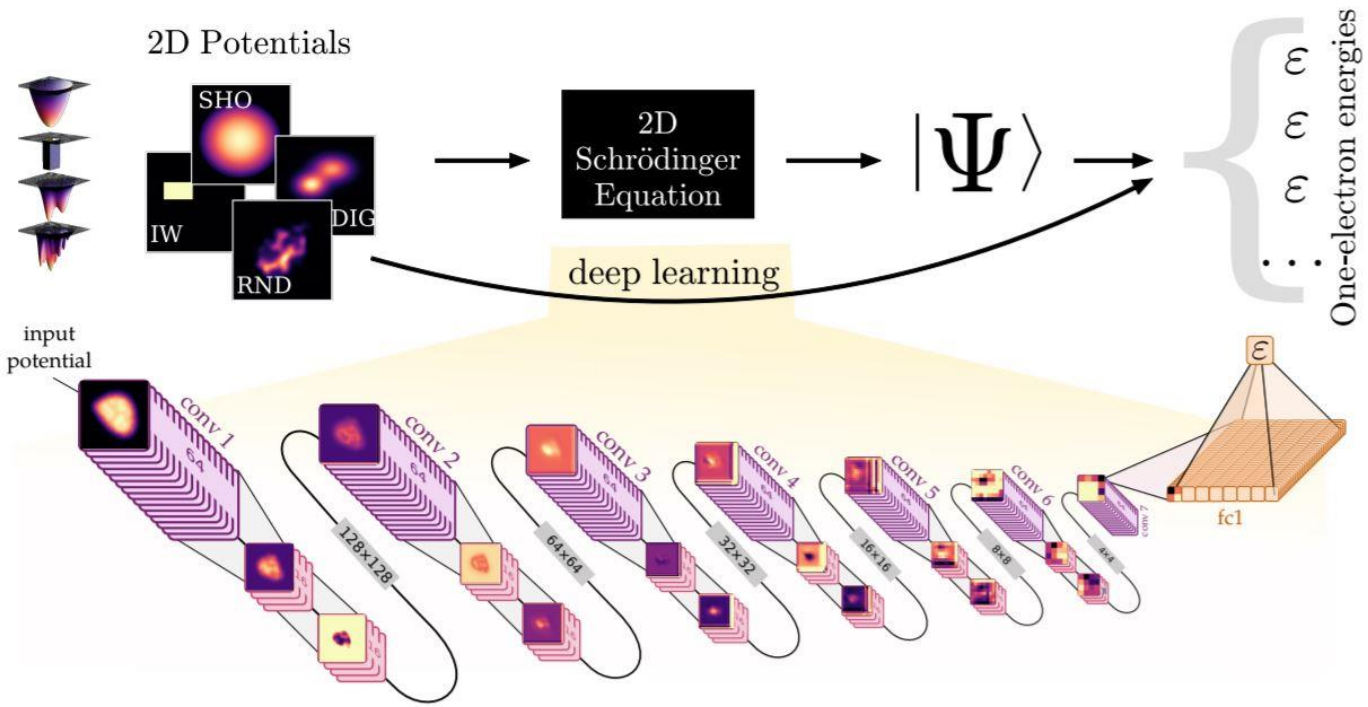
IML LHC

Inter-Experimental LHC Machine Learning Working Group

Deep Learning and the Schrodinger equation

ConvNN is used to be trained for solving Schrodinger equation.

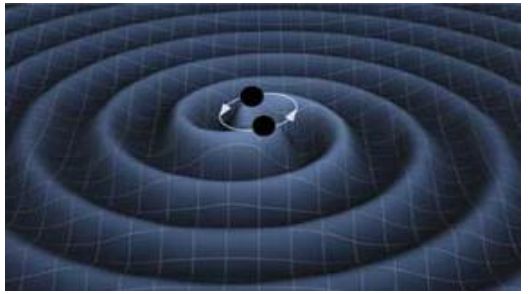
ConvNN is trained with simulation data to predict the ground-state energy of an electron in four classes of confining two-dimentional electrostatic potential



Deep learning and the Schrodinger equation

Deep Learning for Gravitational Wave Detection

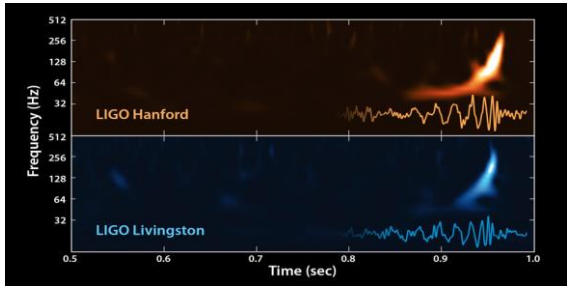
Deep learning method named deep filtering was used in the first detection of gravitational wave. Numerical simulated data was used for training deep filtering, a convolutional neural network to replace matched filtering. It provided 20X speed up on single core and potential to be accelerated further with GPU.



Gravitational wave due to black hole collide and merge

To be observed

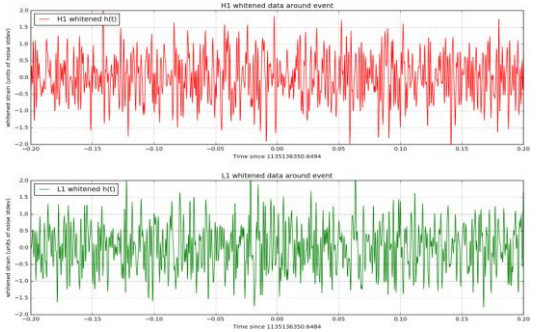
LIGO facility



Actual Signal Caused by Gravitational Wave

How to find The signal???

Deep Learning

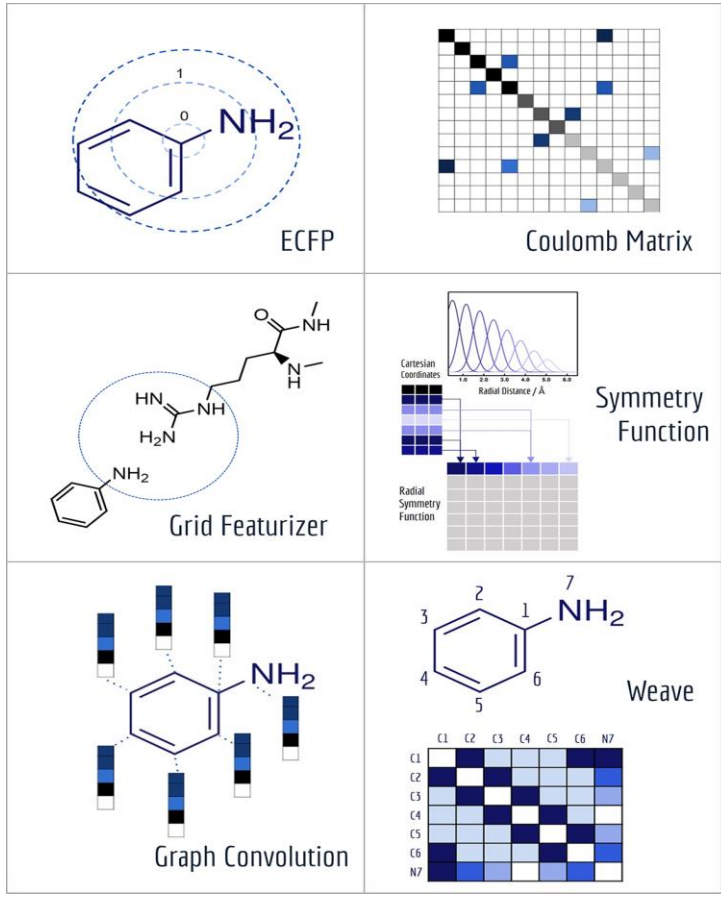


Actual observed data

Computational Chemistry

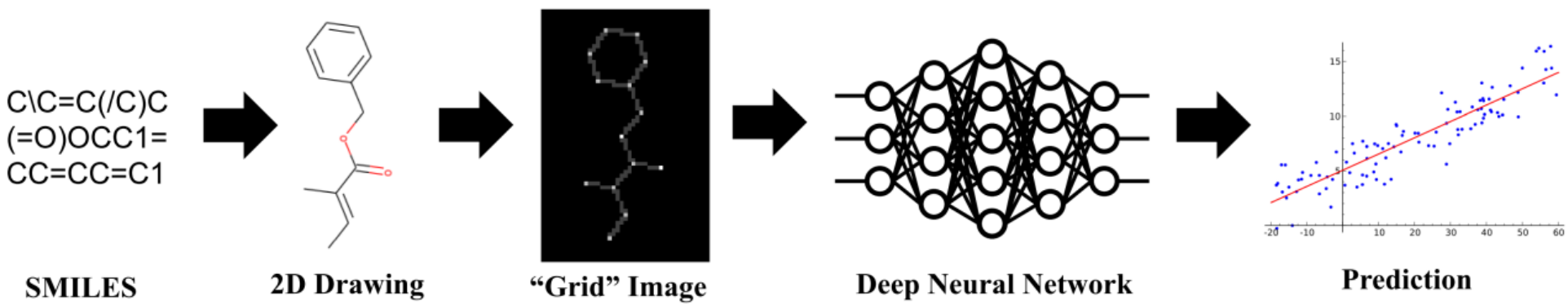
Sharing and using datasets for drug discovery

- DeepChem: Open Source framework for drug discovery using deep learning
- MoleculeNet: System for using/benchmarking using DeepChem – The “ImageNet” of Chemistry
  - “Smart” splitters for training/validation/testing
  - 17 curated datasets containing > 700,000 compounds
  - Selection of featurizers and models



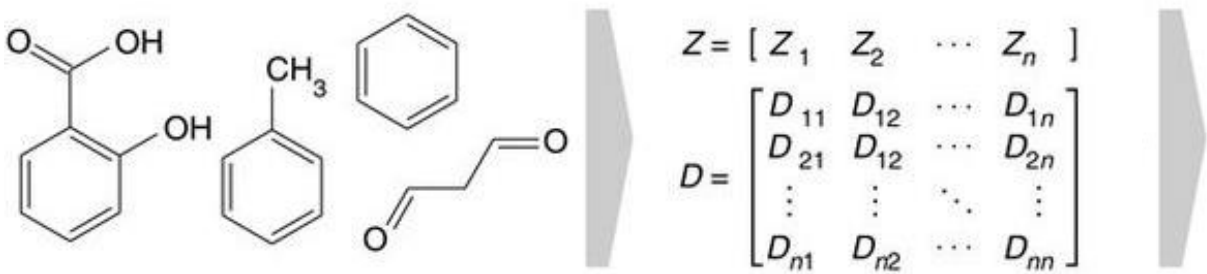
Chemception: The QC version of Inception

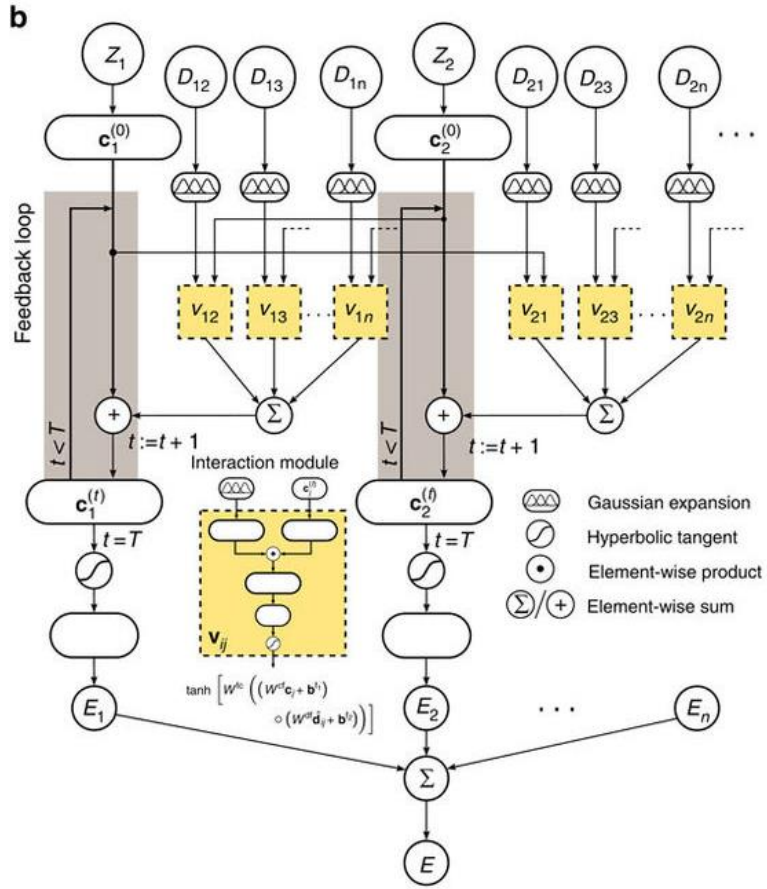
- Goh, et al. devised a CNN called Chemception that can perform all predictive requirements (toxicity, activity, solvation) as well as current expert QSAR/QSPR for a complex molecule (HIV) after being trained for only 24 hours on a single GTX 1080



Predicting MD energies (1)

- Schutt, et al. devised a DTNN that can calculate the chemical space for a medium-sized molecule with an max error of 1 kcal/mol.





Thank You

Acknowledgement

Jeff Adie
Principal Solution Architect
Singapore

Maggie Zhang
Solution Architect
Australia

Simon See
Director,
Solution Architect

Backup Slides

Backup Slides for Computational Mechanics

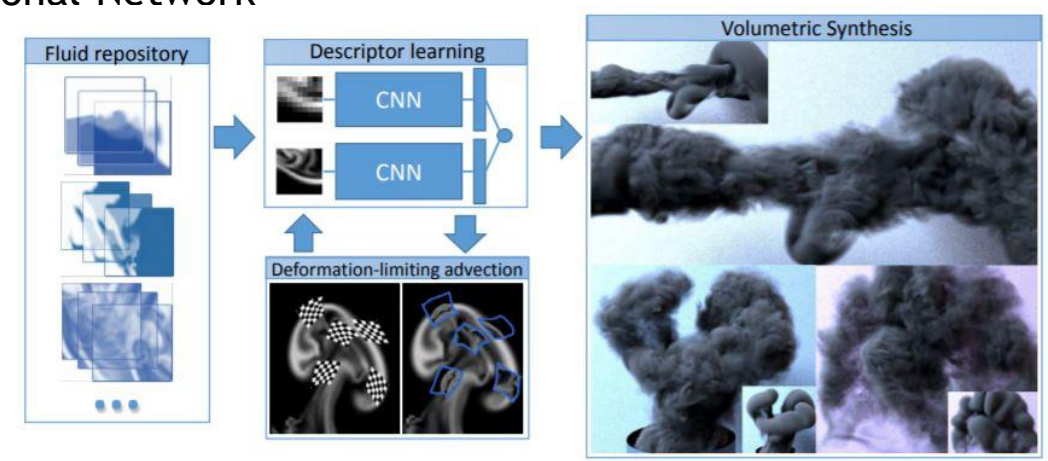
mantaflow – simulation package work with deep learning

Mantaflow is an open-source framework targeted at fluid simulation research. It allows coupling and import/export with deep learning frameworks. It is currently being developed and maintained by Technical University of Munich. Below are some publications used manta flow for research on deep learning coupled fluid simulation reserach

Data-driven Synthesis of Smoke Flows with CNN-based Feature Descriptor

Accelerating Fluid Simulation with Convolutional Network

Mantaflow framework for fluid simulation



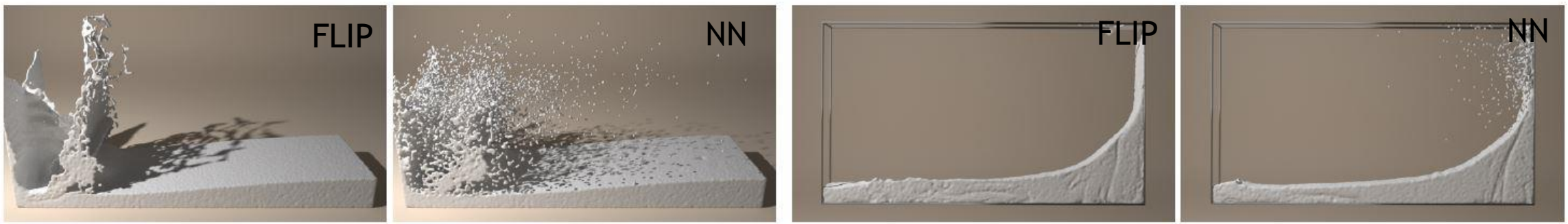
Framework from data-driven synthesis of smoke flows with CNN-based feature descriptor [Chen, et al, 2016]

Liquid Splash Modeling with Neural Networks

Improved FLIP simulation on Splash Modeling with neural networks. (Um et al, 2017)

Classical FLIP method is used for major body of the fluid simulation. Trained Neural Networks is used to identify regions that splash took place. The network will also provide initial condition for droplets leave the main body. Droplets will not be computed with FLIP methods until rejoin the main body of the fluid.

High-resolution FLIP simulation results are used as input data for training the neural network. And the neural network could be coupled with low resolution FLIP to generate high accurate results in a faster way.



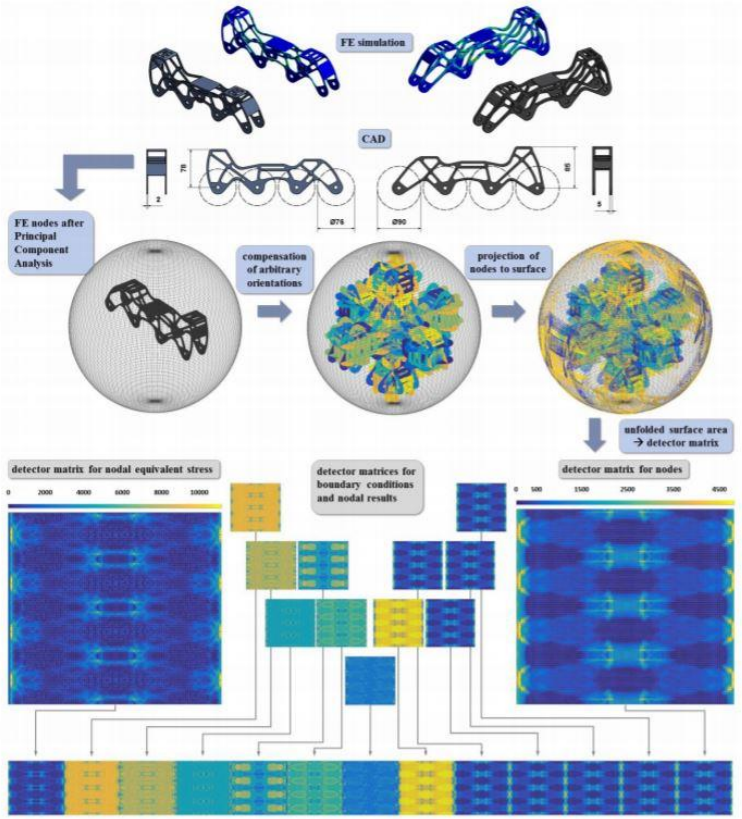
Liquid Splash Modeling with Neural Networks

Plausibility checks for structural mechanics with deep learning

AlexNet is trained to classify plausibility of FEA simulation results to facilitate design engineers for faster design. (Spruegel, 2017)

The FEA model is transformed to a constant array of numerical values by spherical detector surface techniques

The trained AlexNet reached a precision of 86.11%

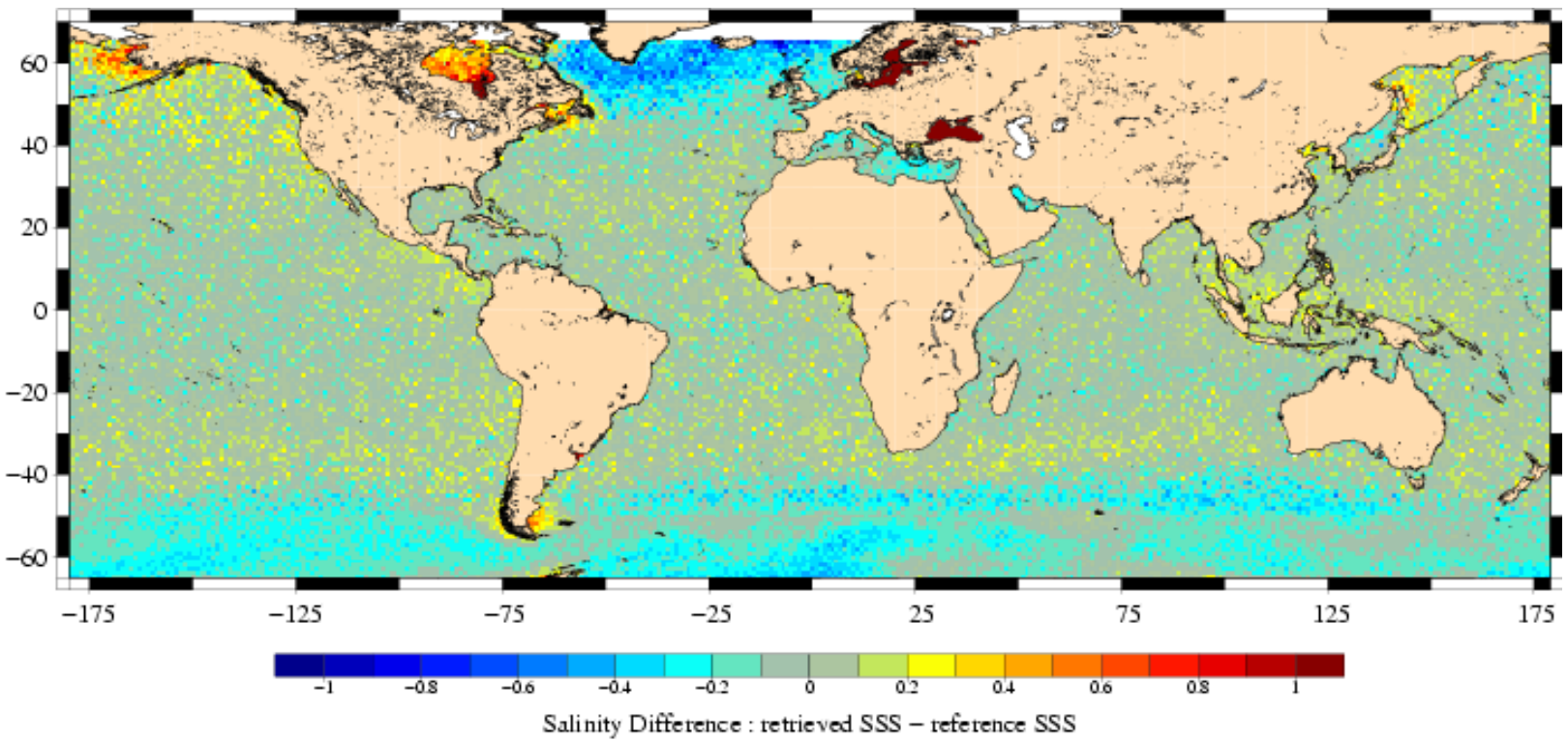


One example from “Generic Approach to Plausibility checks for structural mechanics with deep learning”

Backup Slides for Earth Science

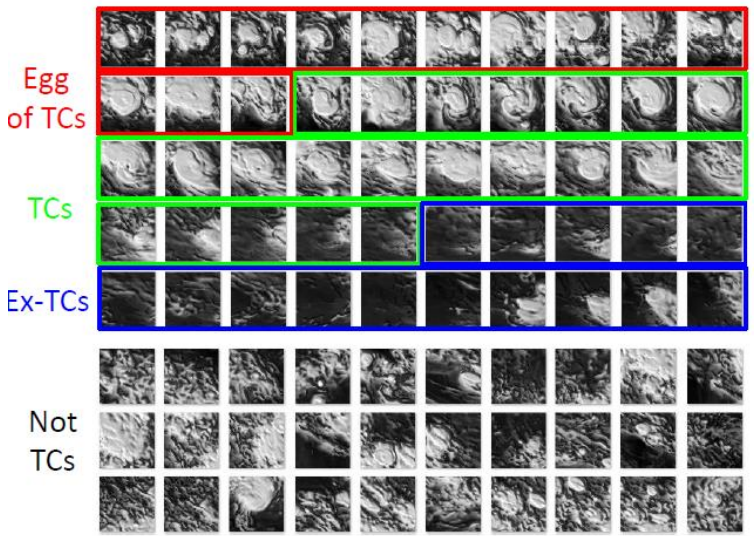
Predicting Ocean Salinity

- Bharaskin, et al using a simple MLP with low resolution data
- Later work by Amman, et al uses surface brightness from Satellite images and ensembles to combine multiple DNNS - achieved > 97% accuracy

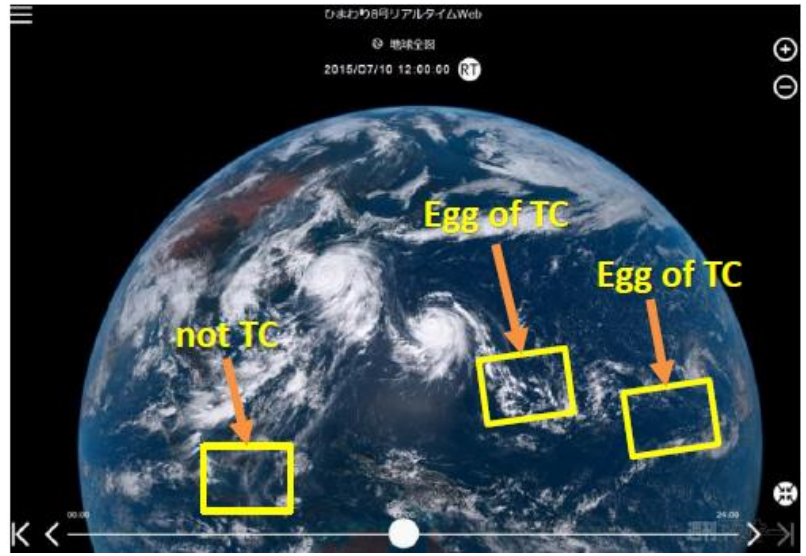


Predicting Tropical Cyclones

- Trained with over 10 million images and 2,500 tropical Cyclone (TC) tracks with ensemble learning.(Matsuoka et al, 2017)
- Can predict 2 days faster than model and observational data



Training Data Examples



Prediction Results

Spatial Downscaling of climate data

DNN combining low resolution reanalysis data with local station data to spatial downscaling of climate variables. (Mouatadid et al, 2017)

Method is suitable for stations with or without historical data
Study over 56 years of NCEP reanalysis data + 12 local stations
Results show excellent correlation for air temperature and precipitation values

Station	Neurons in layers	Air temperature		Precipitation	
		$RMSE$	R^2	$RMSE$	R^2
s1	(144-17-1)	1.119	0.991	0.576	0.860
s2	(144-7-1)	0.327	0.980	1.299	0.827
s3	(144-17-1)	1.814	0.987	0.538	0.749
s4	(144-17-1)	1.949	0.997	0.199	0.856
s5	(144-17-1)	0.494	0.994	0.673	0.616
s6	(144-7-1)	0.498	0.995	0.625	0.619
s7	(144-17-1)	0.725	0.994	0.335	0.893
s8	(144-17-1)	0.945	0.998	0.160	0.807
s9	(144-7-1)	0.427	0.995	0.647	0.624
s10	(144-7-1)	0.848	0.988	0.896	0.649
s11	(144-7-1)	0.810	0.997	0.299	0.888
s12	(144-7-1)	0.329	0.992	0.750	0.829

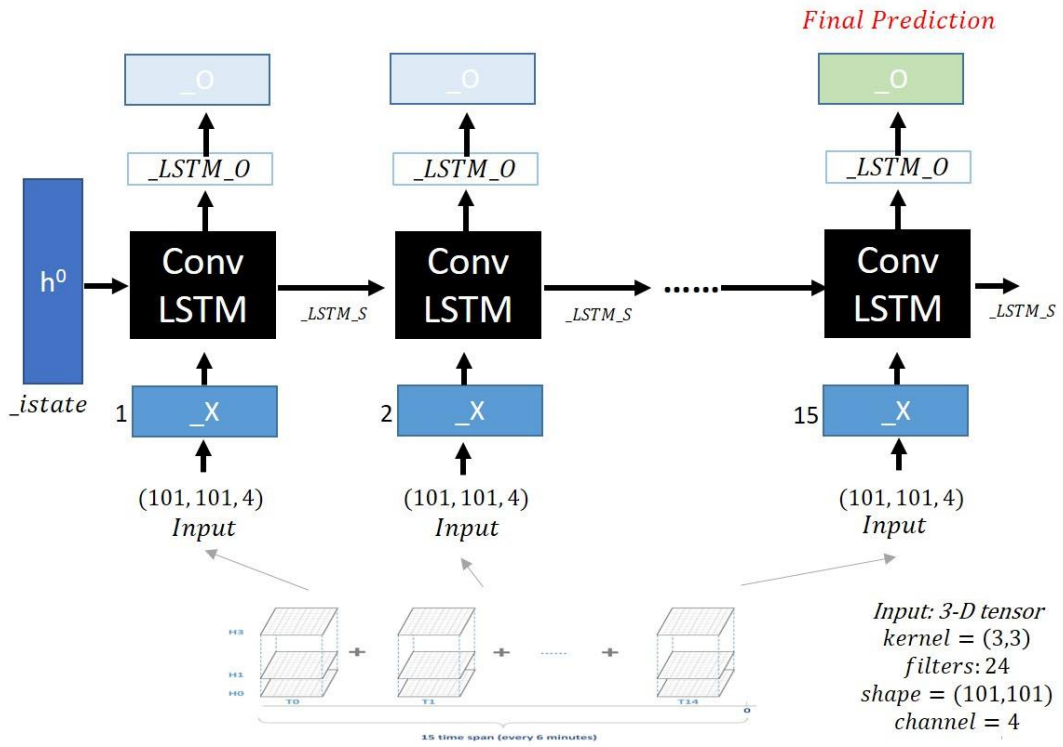
Results of the best models at test time

Predicting Precipitation from radar data

- Uses conv LSTM nodes to take 101x101x4 input data from weather radar
- Trained with 2 years of data
- Final result shows RSME of 11.31%, lower than results with linear regression or FCN

Model	RMSE	Drop(%)
Linear Regression	14.69	-
DeepRain: FC-LSTM[7]	14.46	1.6
DeepRain: Conv-LSTM(one-Stacked)	11.51	21.6
DeepRain: Conv-LSTM(two-Stacked)	11.31	23.0

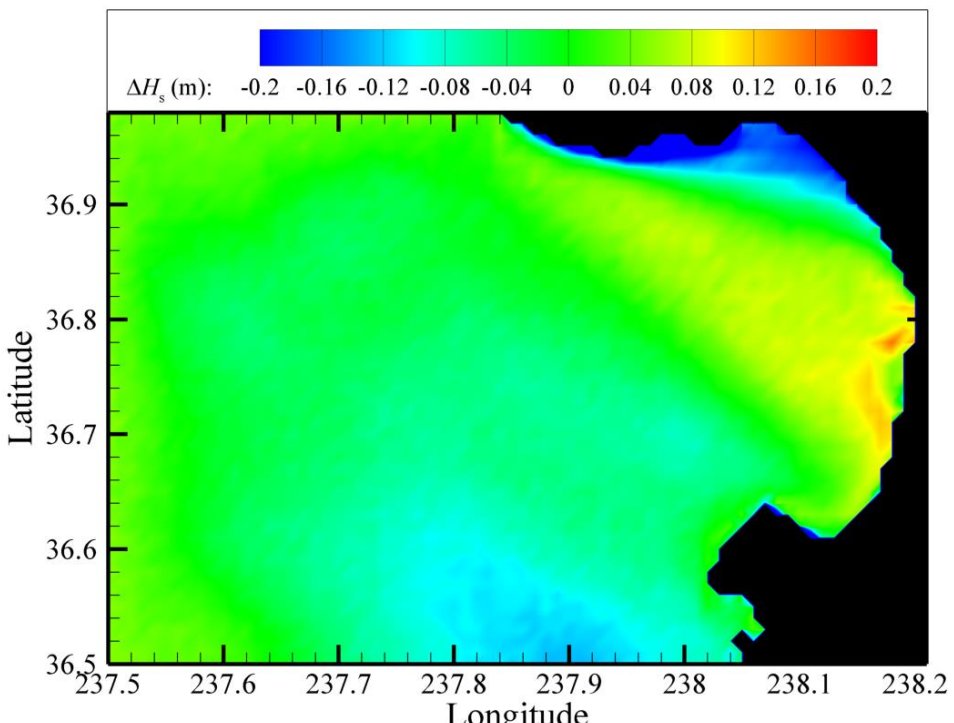
Precipitation Prediction Comparison Results



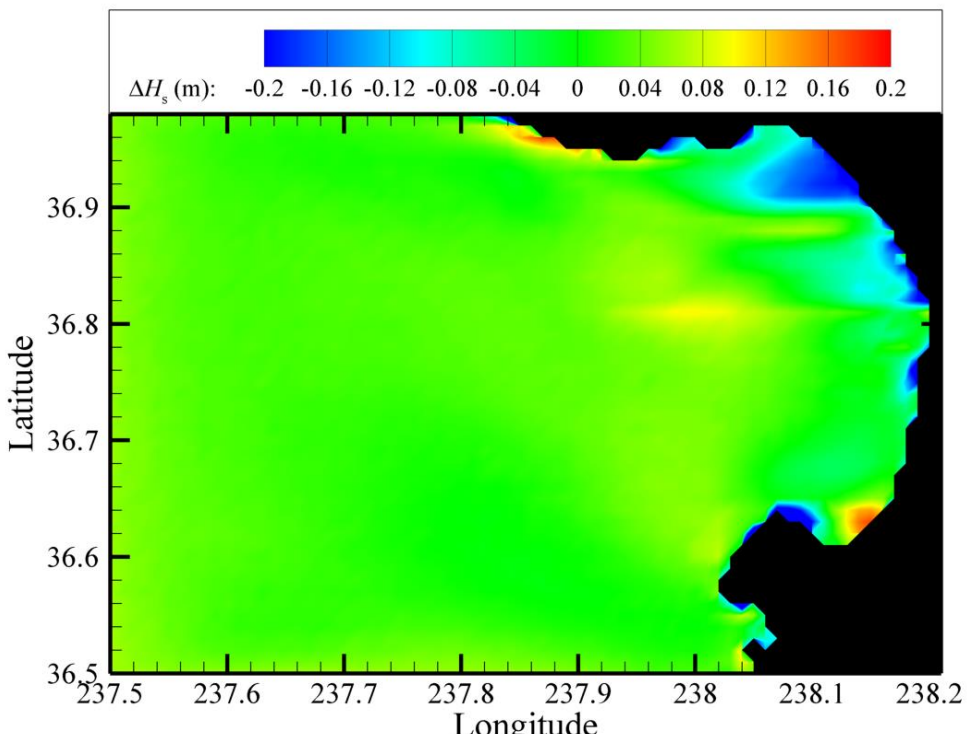
LSTM Architecture

Predicting Coastal Waves

- James, et al. devised a DNN that is 1,000 times faster than numerical methods for modeling waves with and RSME < 7 cm.



RMSE heat map for Machine Learning Model

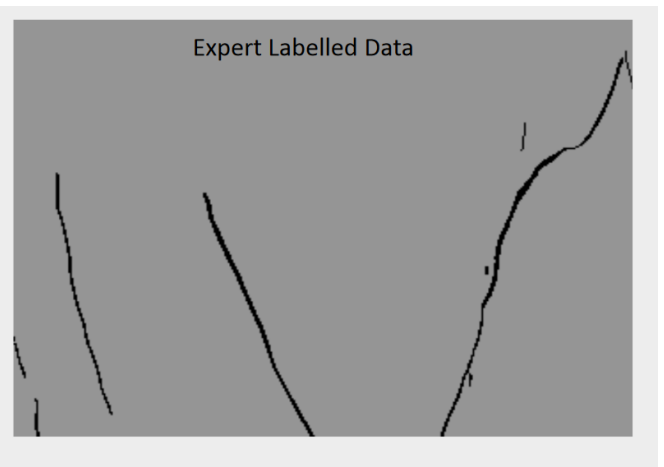


RMSE heat map for SWAN numerical model

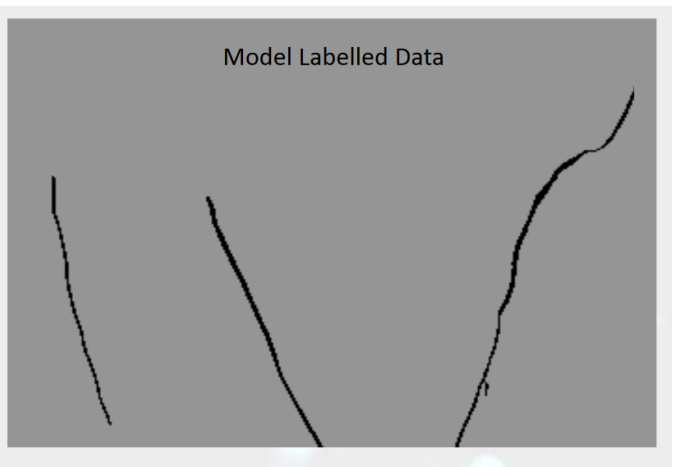
Deep Learning for Upstream O&G

- Automatic fault interpretation from seismic data [Bhaskar & Mao]

Slice of Seismic Volume



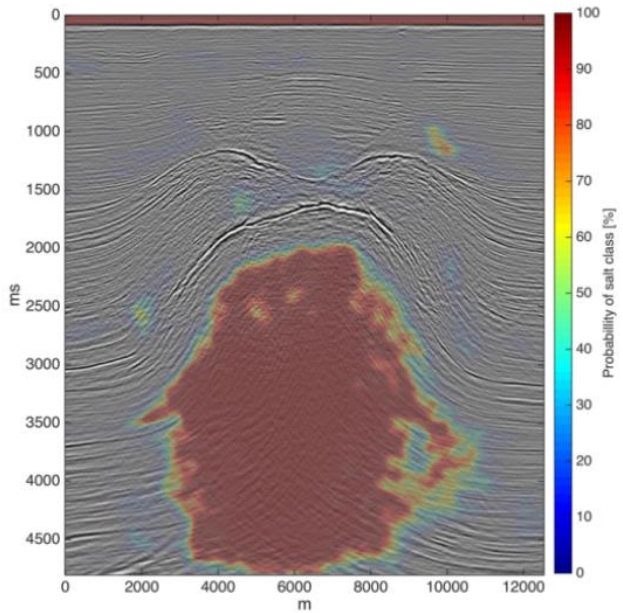
Ground Truth



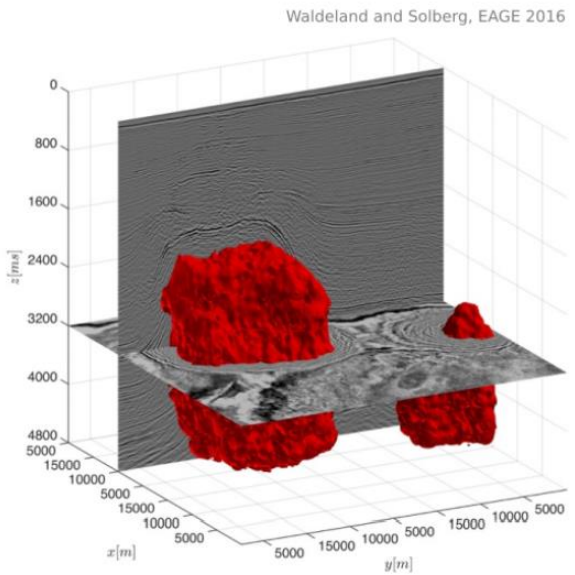
Model Output

Deep Learning for Upstream O&G

- 3D reconstruction of salt deposits [Waldeland & Solberg]



Slice of Labelled training data



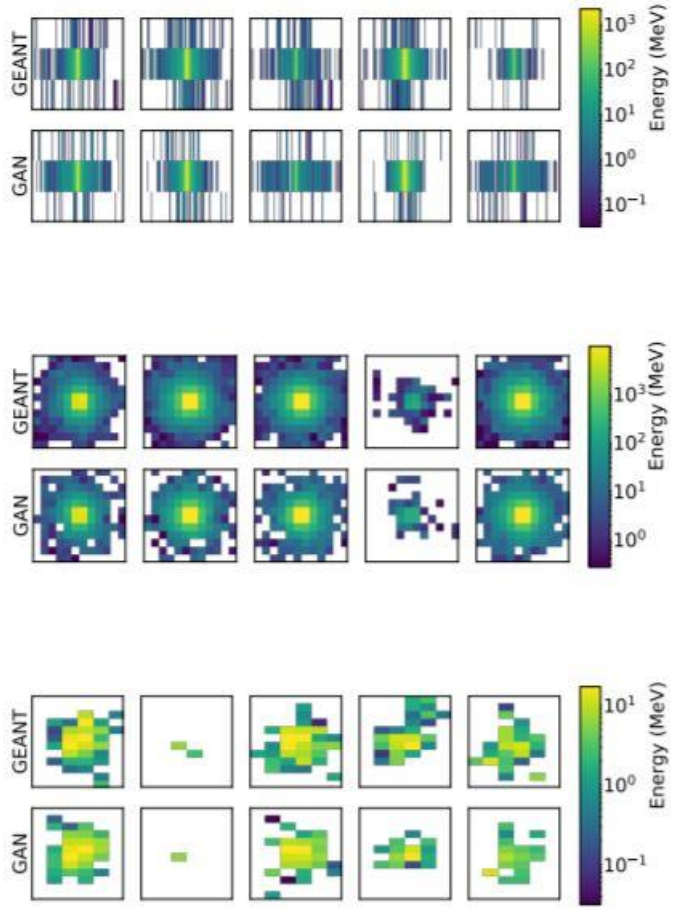
Reconstruction with Deep Learning model

Backup Slides for Physics/Chemistry/Biology

Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multi-Laver Calorimeters

Deep Neural Network-based generative model is introduced to enable high-fidelity, fast, electromagnetic calorimeter simulation

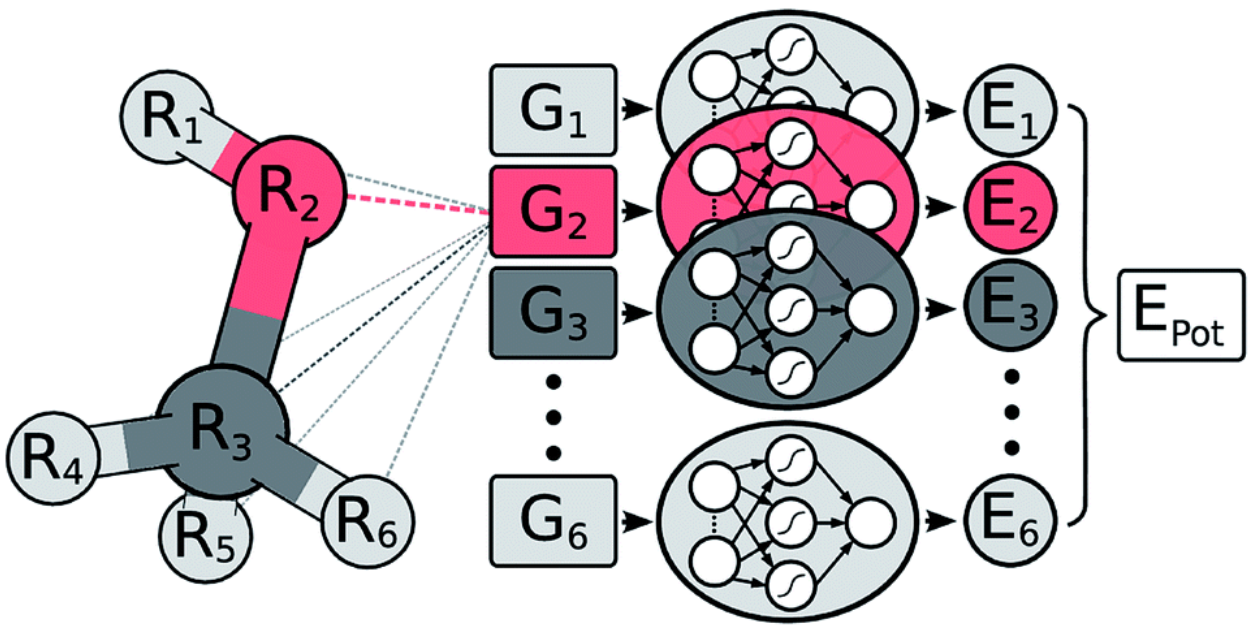
- GAN-based methods are used , named CALOGAN to model the physical sequential dependence among the calorimeter layers
- The new methods achieved speed-up factors of up to 100,000X not considering the challenges of precision



Simulation Results Comparison

Predicting MD energies (2)

- Gastegger, et al. devised a DNN called HDNNP that can perform *ab-initio* MD with both a very low error (MAE = 0.048 kcal/mol) and much faster than traditional techniques (3 hours vs 7 days)

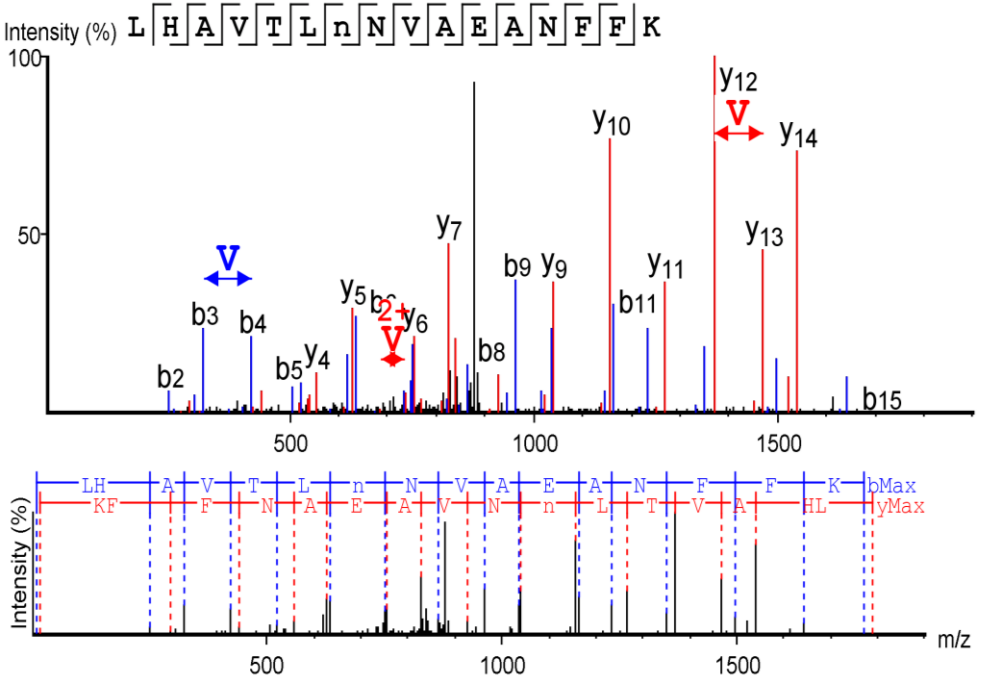


De novo Peptide Sequencing by Deep Learning

Ngoc Hieu Tran, Xianglilan Zhang, Lei Xin, Baozhen Shan, Ming Li, University of Waterloo, 2017.

"two young girls are playing with lego toy."

source provided by Xianglilan Zhang



Spectrum Captioning?

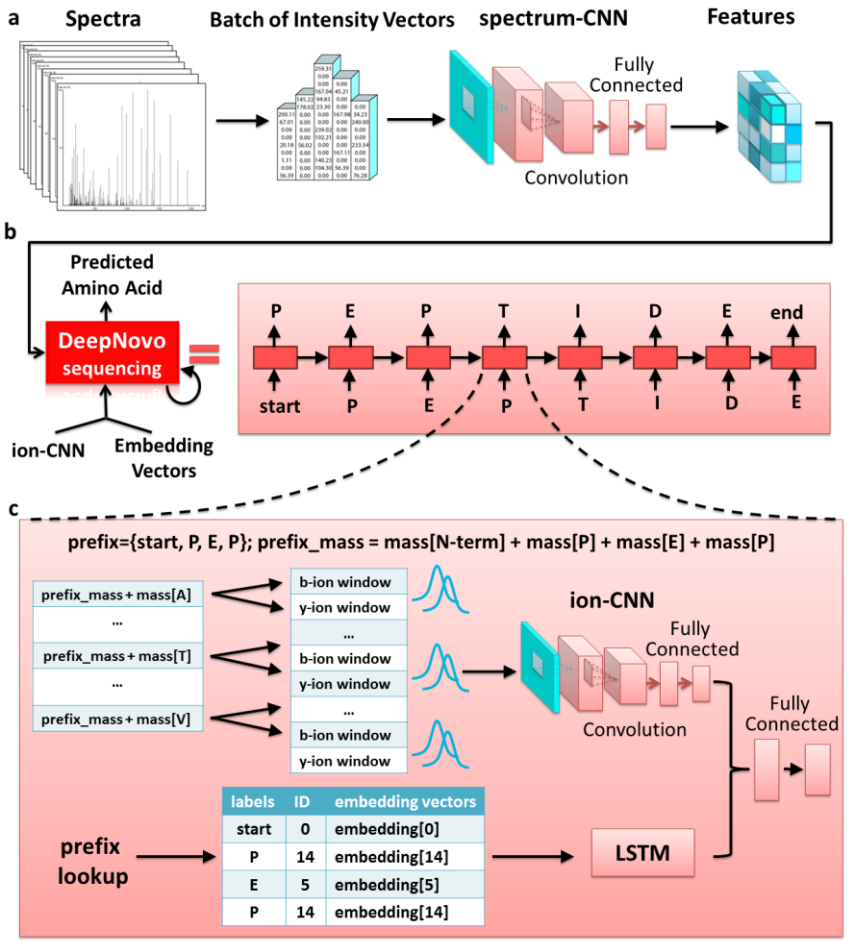
L H A V T L n N V A E A N F F K

De novo Peptide Sequencing by Deep Learning

Ngoc Hieu Tran, Xianglilan Zhang, Lei Xin, Baozhen Shan, Ming Li, University of Waterloo, 2017.

DeepNovo Architecture

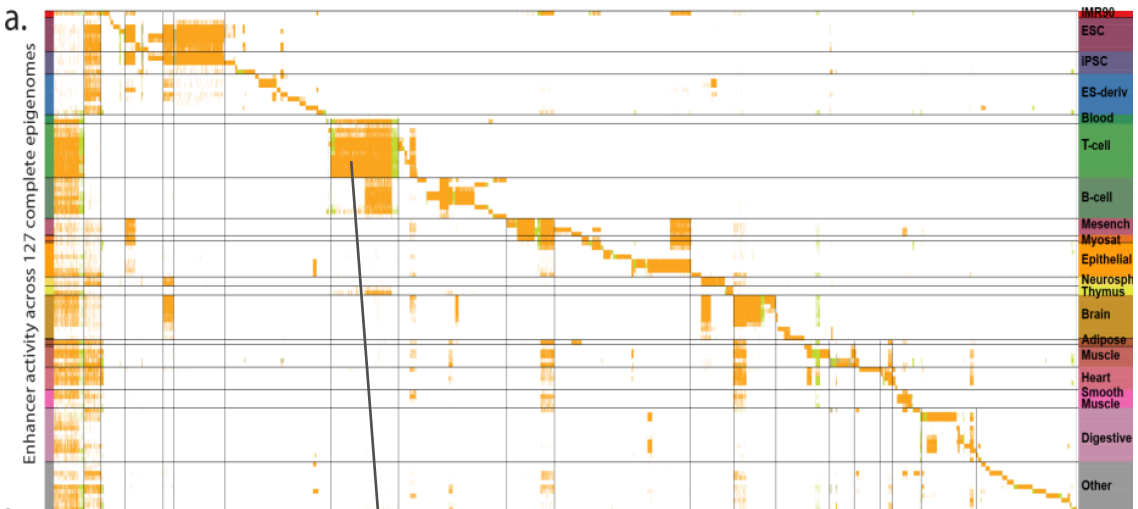
- ion-CNN, spectrum-CNN, LSTM
- *Knapsack* Dynamic Programming
  - Peptide mass, prefix mass, suffix mass
  - All amino acid combinations for a given total mass
  - Filter out amino acids with unsuitable mass
- Beam Search: explore a fixed number of top candidate sequences at each iteration.
- Bi-directional Sequencing



source provided by Xianglilan Zhang

Decode the human genome by deep learning

Anshul Kundaje team, Stanford University



Decoding DNA words and grammars that specify tissue-specific control elements

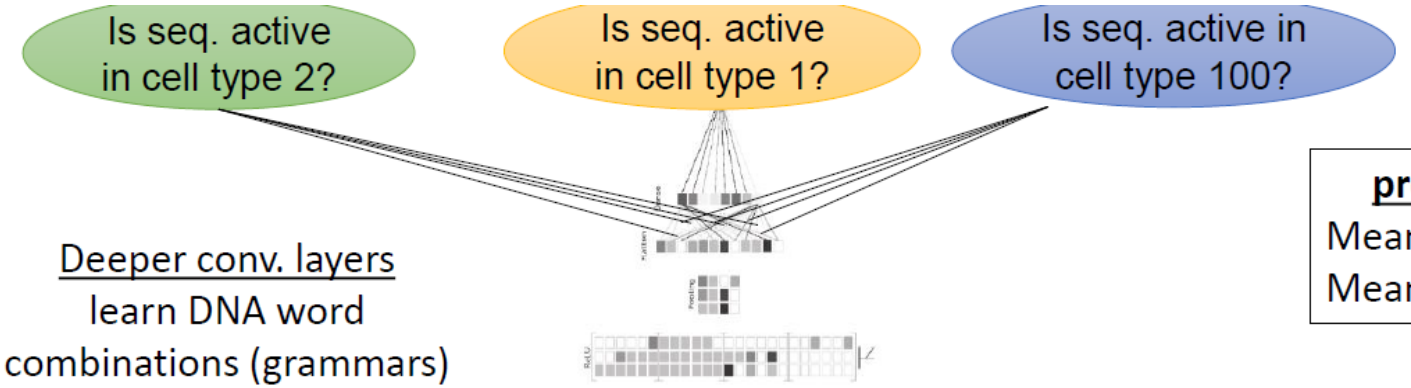
'Motif Discovery'

Regulatory proteins bind **DNA words** (landing pads) in control elements!

source from Anshul Kundaje's presentation online

Multi-task deep CNNs learn discriminative DNA word pattern detectors

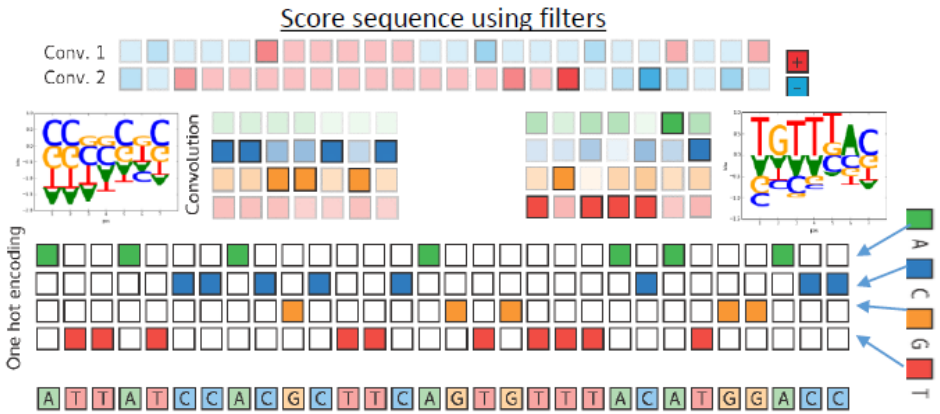
Anshul Kundaje team, Stanford University



Multi-task learning

Deeper conv. layers learn DNA word combinations (grammars)

prediction accuracy
Mean auROC = 0.82
Mean auPRC = 0.65



Millions of input sequences of control elements

Convolutional layers
Neurons learn DNA word pattern detectors

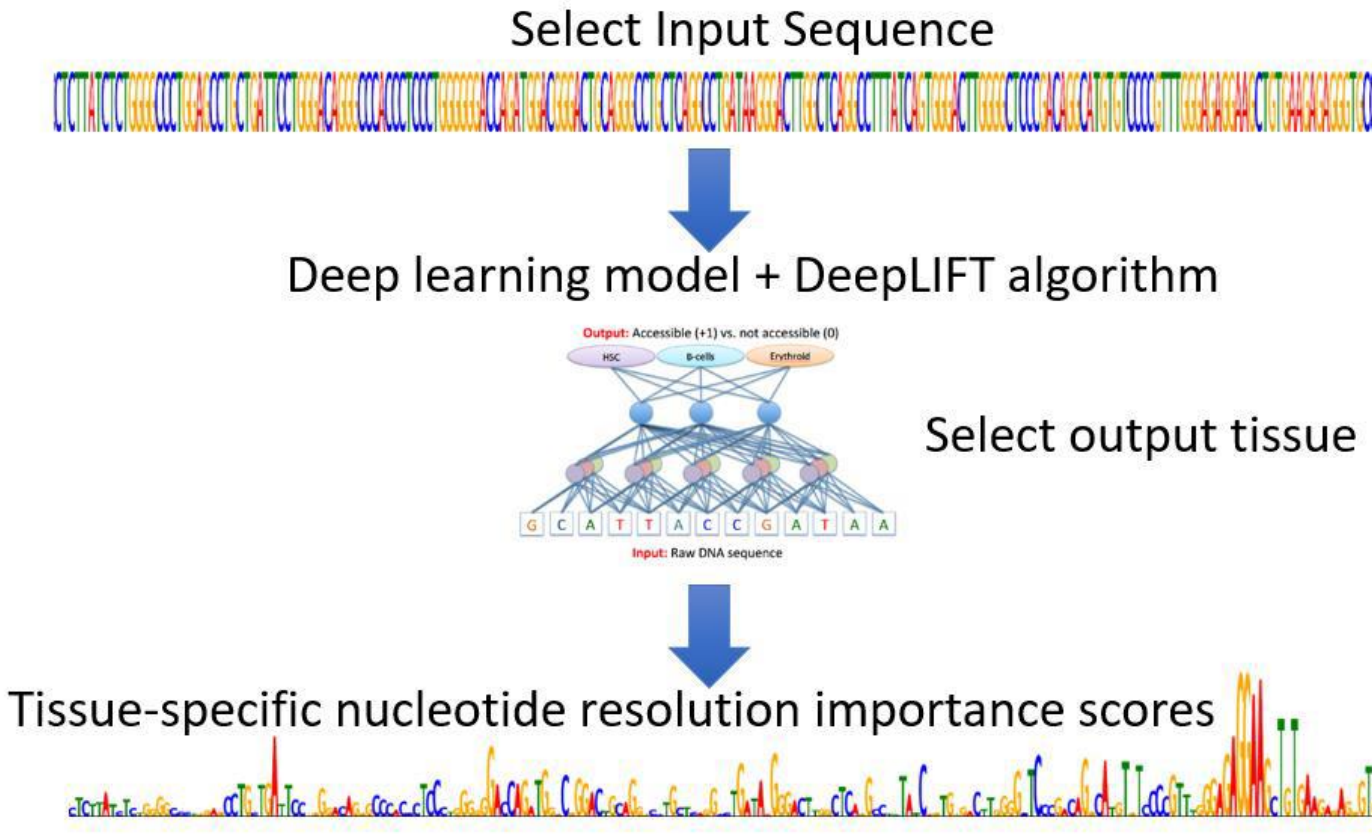
Similar to
Kelley et al. 2016 (Basset)
Zhou et al. 2015 (DeepSEA)

source from Anshul Kundaje's presentation online

Identify important parts of the input sequences

Efficient “Backpropagation” based approaches

DeepLIFT identifies combinatorial grammars of DNA words defining tissue-specific control elements!



Shrikumar et al.
https://arxiv.org/abs/1704.02685
CODE:
https://github.com/kundajelab/deeplift

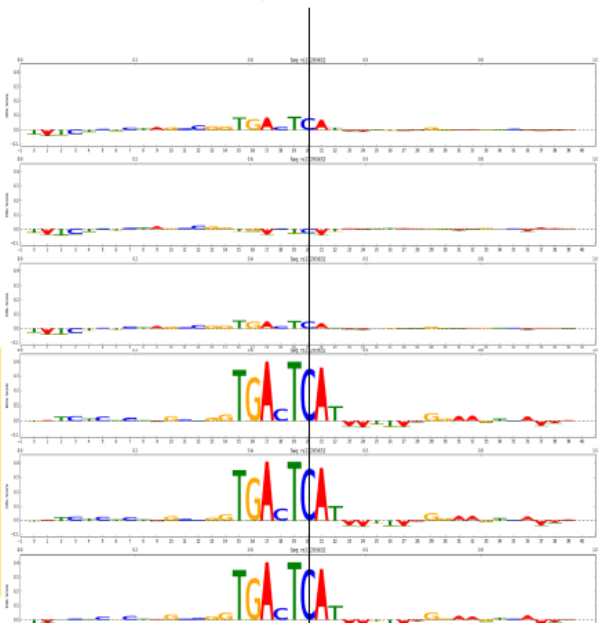
source from Anshul Kundaje’s presentation online

Deep CNNs can predict and interpret effects of disease-associated genetic variants in relevant tissue context

A genetic variant C -> T strongly associated with **coronary heart disease**

Unstimulated coronary smooth muscle cells

Stimulated coronary smooth muscle cells from patients



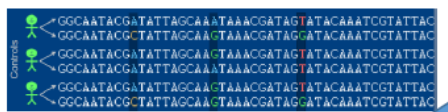
Original prediction:	Mutated prediction:	Difference (Percent):
0.558	0.543	**-1.5%**
0.528	0.583	**+5.4%**
0.554	0.557	**0.3%**
0.969	0.926	**-4.3%**
0.960	0.900	**-5.9%**
0.889	0.756	**-13.2%**

- Breaks the 'C' in TGACTCA DNA word which is binding site for an important protein (AP1).
- Variant specifically manifests in stimulated cells

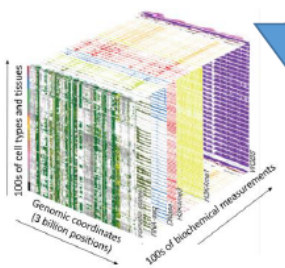
Breaking the 'C' results in significant drop in probability of active control element!

source from Anshul Kundaje's presentation online

Future of personalized medicine



Personal genome sequenc



Personal functional genomic data

Electronic medical records / Clinical data / biometrics / Literature mining

Longitudinal data

Domain-specific machine learning + AI

Rapid interpretation of personal genomes

Data-driven personal diagnosis (cause rather than symptoms)

Drug target identification and design

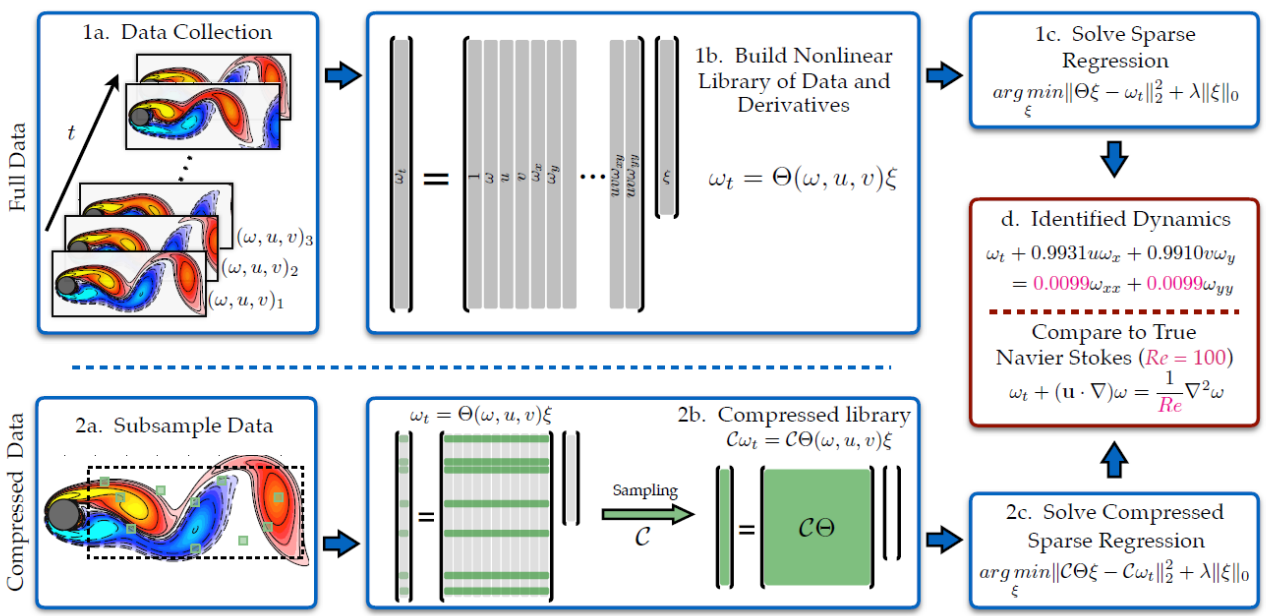
Optimal treatment regimens

source from Anshul Kundaje's presentation online

General Numerical Methods

PDE-FIND: Data-driven discovery of partial differential equations

- Rudy, et al. Create a large internal library from data and derivatives and a sparse regression method capable of discovering the governing partial differential equations of a given system by time series measurements in the spatial domain.



Deep Learning for Monte Carlo

- Improving SLMC via DNN for effective model [Shen, et al]
- Generalizing Hamiltonian Monte Carlo through efficient MCMC with DNN mixed sampler [Levy, et al]
- Applying Deep CNNs to MCST for improved move prediction strength in computer games [Graf & Platzner]