Earth Science Technology Forum  
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Outline for talk

  (M. Halem)

• Describe the development, testing and machine learning neural net algorithmic tool for the
  D-Wave2X quantum annealing computer (QAC) at ARC.
  (J. Dorband, C. Pelissier, N. Tilak, S. Lomonaco, A. Shehab)

• Ingest and process 2 years of OCO-2 concentrations of CO2, collect ground truth ARM and
  Ameriflux data for 3 sites, assess accuracies of CO2, train QAC NN to infer collocated CO2 fluxes
  using D-Wave NN tool and ground truth data and then apply to non collocated OCO-2 observations.
  (M. Halem, P. Gentine, A. Radov, J. Dorband, R. Prouty)

• Incorporate NCAR photosynthetic parameterizations into the GSFC LIS land cover model and test
  Kalman filtering data assimilation of NEE by performing OSSEs and real CO2 fluxes.
  (K. Harrison, G. Nearing, P. Gentine, M. Halem, R. Prouty, C. Pelissier)

• Provide NDVI data coverage for 2 years for the 3 test sites employing QAC NN for image
  registration.
  (J. LeMoigne, D. Simpson, A. Shehab)
Problem Motivation: Are seasonal amplitudes of CO2 growing?

Fig. 1. Observed peak-to-trough seasonal amplitude (A) and phase (B), given by the day of year of downward zero crossing, of CO2 concentration at Barrow (71°N, blue) and Mauna Loa (20°N, black) measured by the Scripps CO2 Program (7, 8) and the NOAA Global Monitoring Division (9). Growth rate of amplitude is given in percent change per year, with one-sigma uncertainty of ±0.05-0.07% year⁻¹. Seasonal CO2 cycles observed at Barrow (C) and Mauna Loa (D) for the 1961-63 or 1958-63 and 2009-11 time periods. The first six months of the year are repeated.

Can we predict the Hyperventilating Biosphere? - Inez Fung Science vol 341

Why is biological breathing showing annual increasing net carbon oscillations and will it continue?
Will satellite observations of surface CO2 improve hydrological predictions of net ecosystem exchange?
Can quantum annealing computers effectively and efficiently answer the above two science problems?

ORBITING CARBON

LAND SURFACE MODEL

D-Wave Quantum Annealing

OBSERVATORY

CARBON UPTAKE

Boltzmann Machine

Measures surface CO2 from space
Vegetation model assimilates CO2 fluxes for photosynthesis
NN trains CO2 to infer CO2 Fluxes from Station Data
History of Simulated and Quantum Annealing

Annealing, is a heat and cooling process that alters the physical and chemical properties of a material by the diffusion of atoms within a solid material towards its equilibrium state (to increase ductility, reduce hardness and relieve internal stresses by minimizing the amount of Gibbs free energy). Heat increases the rate of diffusion by providing the energy needed to break bonds. Controlled cooling strengthens material by reducing to a lattice crystal structure ground state with minimum energy.


- The Metropolis algorithm is among the ten algorithms that have had the greatest influence on the development and practice of science and engineering in the 20th century (Beichl& Sullivan, 2000).


## DWAVE Quantum Computer

### Trait Comparison

<table>
<thead>
<tr>
<th>Trait</th>
<th>Classical bit</th>
<th>Quantum bit</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Binary system</strong></td>
<td></td>
<td><img src="image" alt="Superconducting qbits" /></td>
</tr>
<tr>
<td><strong>State</strong></td>
<td>Simultaneous superposition. [\psi = \frac{1}{\sqrt{2}} (</td>
<td>\uparrow\rangle +</td>
</tr>
<tr>
<td><strong>Measurement</strong></td>
<td>Probabilistic.</td>
<td>Deterministic.</td>
</tr>
<tr>
<td><strong>Interaction between bits</strong></td>
<td>“Chimera graph”</td>
<td>None.</td>
</tr>
</tbody>
</table>
Computing on the DWAVE

Quadratic Unconstrained Binary Optimizations (QUBOs)

**Numerical Task:**

\[
\min \mathcal{O}(\mathbf{q}) , \quad \mathcal{O} = \sum_{ij} \alpha_{ij} q_i q_j , \quad q_i \in (0, 1)
\]

\(\alpha_{ij} = \text{user specified "couplings".}\)

**Results:** collect statistics and take the **BEST** solution.

DWAVE searches the entire space and returns potential candidates for the global minimum.

Restricted Boltzmann Machines (RBM)

**Numerical Task:** train a RBM neural network using “contrastive divergence”.

\[
E(\mathbf{q}) \sim \sum_{ij} \alpha_{ij} q_i q_j
\]

\[
P \propto e^{\frac{\Delta E}{T}}
\]

**Stochastic Binary Neural Network**

\[
\alpha_{ij}^k \rightarrow \alpha_{ij}^{k+1}
\]

Generate Boltzmann statistics

**Solution Statistics**

Energy/solutions

**DWAVE is a physical realization of a RBM!**
Quantum Annealing Studies

• Implemented a quantum-based RBM on the D-Wave as a general tool for applications of neural nets.
• Evaluate the RBM tool by employing same C Code for RBM evaluations on classical computer.
• Tested a purely RBM tool (no connections between neurons/qubits) using MNIST data for 100 training cases, 100 test cases.
• Both classical and quantum version of RBM attained an accuracy on or near 100% for MNIST training data.
• Classical attained 70% on test data while quantum attained near 60%.
• Implemented Deep Learning on D-Wave; 1 to 3 hidden layers partially connected BM.
• Virtual qubits allow for more connected cost functions. Studied behavior of virtual qubits, conducted stochastic measurements of qubit chains, compared to theoretical qubit chain behavior, appears to be stable.
A Prototype RBM Evaluation using MNIST

• Classifying hand-written digits from the MNIST dataset into 10 classes.
• Each sample is a 28x28 gray-scale image.
• We used 100 samples for training and 100 samples for testing our RBM model.
• RBM used had 794 input nodes and 1100 hidden nodes.
Classic vs Quantum RBMs
Learning Profiles

100 training cases
100 test cases
• 3 primary regions selected for observations:
  • Barrow, (69.0,-162.0) (71.4,-152.0), Oklahoma City, (34.5,-99.5)(36.5,-96.5), K34, Brazil (-3.6, -61.5) (-1.6, -59.0)
  • OCO2 – Orbiting Carbon Observatory 2 Launched July of 2014. Level 2 lite data has been collected and processed since September of 2014 and still being collected daily.
  • DOE – Atmospheric Radiation Measurement (ARM) Carbon Dioxide measurements collected for all 3 sites from 2001 until July of 2015.
  • ONRL Fluxnet/Ameriflux (NASA DAAC) A "network of regional networks," coordinates regional and global analysis of observations from micrometeorological tower sites
The satellite tracks, along with CO2 values have been mapped using http://www.hamstermap.com/ a google maps tool, to help visualize the data. This technique allows for interactive zoom options, as well as CO2 level, point by point comparisons.
All OCO-2 targeted samples fall within 10 mile radius of the ARM tower
On this particular case, there are over 4300 targeted samples taken during the OCO-2 overpass
OCO2 vs ARM Comparison near Oklahoma City

<table>
<thead>
<tr>
<th>Date</th>
<th>4m</th>
<th>25m</th>
<th>60m</th>
<th>OCO2</th>
</tr>
</thead>
<tbody>
<tr>
<td>10/3/14</td>
<td>386.3332819</td>
<td>394.6344485</td>
<td>390.9355092</td>
<td>395.4361724</td>
</tr>
<tr>
<td>10/30/14</td>
<td>401.2256545</td>
<td>404.8536971</td>
<td>396.3650433</td>
<td>395.7083233</td>
</tr>
<tr>
<td>11/24/14</td>
<td>398.1087561</td>
<td>398.2196341</td>
<td>429.9921762</td>
<td>398.0109639</td>
</tr>
<tr>
<td>1/25/15</td>
<td>413.8416835</td>
<td>410.2235257</td>
<td>400.0879616</td>
<td>397.398894</td>
</tr>
<tr>
<td>2/10/15</td>
<td>397.7759594</td>
<td>396.5604284</td>
<td>399.970837</td>
<td>400.9904037</td>
</tr>
<tr>
<td>2/19/15</td>
<td>403.7240008</td>
<td>397.6349329</td>
<td>394.4884016</td>
<td>400.0255873</td>
</tr>
<tr>
<td>6/20/15</td>
<td>403.1288341</td>
<td>391.7279216</td>
<td>390.7480839</td>
<td>401.5713586</td>
</tr>
<tr>
<td>7/11/15</td>
<td>397.7759594</td>
<td>397.6349329</td>
<td>394.4884016</td>
<td>404.4339711</td>
</tr>
</tbody>
</table>
Surface carbon fluxes using neural network

Pierre Gentine, Bin Fang, Filipe Aires, Catherine Prigent, Jana Kolassa
Training Data Set: Atmospheric Radiation Measurement (ARM)

**Measured quantities:**
1. CO2 concentration
2. H2O concentration
3. Temperature
4. Pressure
5. Wind Speed
6. Horizontal Wind Direction
7. Rotation to zero w
8. Rotation to zero v
9. CO2 Flux

**Measured at heights:**
1. 4 meters
2. 16 meters
3. 25 meters

**Data samples:**
30 minutes apart
Dec 2002 – Oct 2014
Around 180k samples.
### ARM Data Attributes (At 4m) and Volume

<table>
<thead>
<tr>
<th>Value</th>
<th>CO2 Flux(umol m-2 s-1)</th>
<th>CO2(m mol m-3)</th>
<th>H2O(m mol m-3)</th>
<th>Temperature(degree C)</th>
<th>Pressure (kPa)</th>
<th>Wind Speed(m s-1)</th>
<th>horizontal wind direction</th>
<th>rotation to zero w(theta)</th>
<th>rotation to zero v(phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min</td>
<td>-140.5</td>
<td>0.0792</td>
<td>0</td>
<td>-17.31</td>
<td>0.38</td>
<td>0.158</td>
<td>0.0087</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Max</td>
<td>69.271</td>
<td>139.33</td>
<td>2108.7</td>
<td>40.55</td>
<td>100.95</td>
<td>15.314</td>
<td>359.99</td>
<td>61.592</td>
<td>180.00</td>
</tr>
<tr>
<td>Average</td>
<td>-0.626</td>
<td>16.092</td>
<td>688.89</td>
<td>21.8193</td>
<td>97.7852</td>
<td>4.6211</td>
<td>173.368</td>
<td>1.416</td>
<td>73.327</td>
</tr>
<tr>
<td>Standard Deviation</td>
<td>4.4978</td>
<td>1.7935</td>
<td>384.35</td>
<td>9.57815</td>
<td>1.6441</td>
<td>2.5330</td>
<td>94.668</td>
<td>1.1683</td>
<td>60.240</td>
</tr>
</tbody>
</table>

10 years of ½ hour ARM measurements : 48 * 365* 10 =175,200

2 years of OCO-2 CO2 at ARM station: 5 * 26 * 2 * 4000 = 1,040,000

3 Sites: Barrows, Oklahoma City, K34 Amazon

Obtain Attributes from MERRA and repeat calculations with measured and observed CO2.
Prediction Accuracy of Feed-forward Neural Network

1. Error for complete test data

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Mean Error</td>
<td>0.065</td>
</tr>
<tr>
<td>Error standard deviation</td>
<td>3.936</td>
</tr>
<tr>
<td>Root Mean Squared Error</td>
<td>3.939</td>
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</tbody>
</table>

2. Error for test data after removing outliers

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<table>
<thead>
<tr>
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<tbody>
<tr>
<td>Mean Error</td>
<td>1.133</td>
</tr>
<tr>
<td>Error standard deviation</td>
<td>4.43</td>
</tr>
<tr>
<td>Root Mean Squared Error</td>
<td>4.58</td>
</tr>
</tbody>
</table>
# Prediction Accuracy of RBM

1. Error for complete test data

<p>| | |</p>
<table>
<thead>
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<tbody>
<tr>
<td>Mean Error</td>
<td>12.67</td>
</tr>
<tr>
<td>Error standard deviation</td>
<td>4.30</td>
</tr>
<tr>
<td>Root Mean Squared Error</td>
<td>13.38</td>
</tr>
</tbody>
</table>

2. Error for test data after removing outliers

<p>| | |</p>
<table>
<thead>
<tr>
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<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean Error</td>
<td>6.60</td>
</tr>
<tr>
<td>Error standard deviation</td>
<td>2.62</td>
</tr>
<tr>
<td>Root Mean Squared Error</td>
<td>7.10</td>
</tr>
</tbody>
</table>
Current Studies

• It was pointed out that NN need net surface radiation as critical input for inferring CO2 fluxes.
• The prediction accuracy for RBMs also suffers due to noise in the data. Comparatively, feed-forward neural networks are more tolerant to noise.
• Implementing an alternative training algorithm for RBM regression application other than contrastive divergence.
• We observed that the ARM data is noisy and contains a number of outliers. We need to carefully curate this data or use multiple sources of measurements.
Main role of LIS in QAC project

1. Introduce NCAR photosynthetic parameterization into LIS model.
2. To use as the baseline for measuring the added value of data assimilation
3. As training data for a machine-learning observation operator

   We have completed a 10-year CONUS run and a 5-year global run.

1. Noah-MP is NCEP’s newest version of the WRF with lower boundary condition. It is 1\textsuperscript{st} version with dynamic carbon partitioning and fluxes.
2. About 1350 hours of CPU time per year of simulation at 1/8 degree spatial resolution, 15 minute temporal resolution.
3. NLDAS parameters and forcing data for the CONUS run.
4. GLDAS parameters and Princeton forcing for global run.
NASA Land Information System (LIS)

Uncoupled or Analysis Mode

LIS - OPT/UE
Optimization and Uncertainty Estimation (LM, GA, RW-MCMC, DEMC)

LIS - DA
EnKF

States (Soil Moisture, Carbon pools)

LIS - LSM
Noah-MP

Parameters
AVHRR landcover, STATSGO-FAO soils, NCEP albedo

Meteorological Boundary Conditions (Forcings)
MERRA2

Dynamic veg (Dickinson et al., 1998)

Observations (Soil Moisture, Snow, Skin Temperature)

OCO-2

Water and Energy Fluxes, Soil Moisture and Temperature profiles, Land surface states

NEE

Coupled or Forecast Mode

Weather

Agriculture

Hydrologic Forecasts

WRF

Noah MP: Global run: NEE seasonal cycle
The basic finding is that even the “best-case” scenario (i.e., assimilation of relatively accurate in situ observations) is difficult because of the highly-nonlinear relationship between vegetation and soil carbon stores and NEE (net ecosystem exchange).

Thus, this is a perfect candidate for nonlinear DA like what we are proposing to do with Boltzmann Machines.

We used Kalman-type (locally linear) DA schemes at 10 heavily instrumented FluxNet sites over different biomes and found three major types of results (examples of each in following slides):

1. DA worked. In these cases the model had some ability for realistic NEE.
2. Predictions had some bias in more than half of the test cases
3. Both prior and posterior DA results were nonsense. NEE is hard to predict without accurate model parameterization. Model predictions in some locations were unrelated to observations.
4. Assimilation strategy worked in 1 out of 31 cases.
Noah MP: Site runs

Showing daily min and max as there are large fluctuations within and across days.
Preliminary DA Results: Sensitivity Analysis

Sensitivity of $Q_a$ to Plant Mass Perturbations

Sensitivity of $Q_a$ to Soil Moisture Perturbations

Compare Sensitivity of $Q_a$ to SM and PM Perturbations
Retrieval Results
(2011)
Retrieval Results (2011)
LIS model needs Vegetation Land Cover

• Image Registration Challenge: given two Earth remotely sensed images, determine the transformation (e.g., composition of translation and rotation) that transforms one image into the other.

• Efforts in implementing image registration on the D-Wave have focused on using neural networks.

• Other methods have been considered, but neural networks seem to be most suited for the D-Wave computation model.
A Restricted Boltzmann Machine (RBM) has been implemented on a conventional computer. Test images used for the network:
- Ohio River (ground-based radar with artificial translations)
- Landsat images (with real translations and rotations)

RBM “votes” on what translations it thinks it sees in a test image

Results were met with some success, but RBM often does not find the correct transformation.

RBM has so far been implemented entirely on a conventional computer. Implementation entirely on the D-Wave is limited by D-Wave qubit capacity: images are larger than can be stored on the D-Wave.
Feed-forward Neural Network

• The most promising approach to date appears to be using the D-Wave to compute weights for either a conventional feed-forward artificial neural network or an RBM. This would use the D-Wave as a kind of co-processor to a conventional computer:
  – Weights would be computed on the D-Wave
  – Actual feed-forward or RBM network would be implemented on a conventional computer.

• Computing weights through training is the most time-consuming part of a neural network implementation, so this is a good place to leverage the D-Wave capabilities.
NASA has acquired the D-Wave 2X system at ARC in collaboration with Google with more than 1,000 working qubits that realizes quantum annealing at the hardware level. Papers seem to indicate that quantum annealing is indeed realized in the machine.

IARPA has issued a solicitation for a Quantum-Enhanced Optimization program. The goal is to build a prototype quantum annealer of about 100 qubits with high-performance superconducting qubits with more complex connectivity between qubits.

DOE has acquired the Dwave 2X system at LANL and set up a forum Quantum for Quants to discuss and present issues related to the perspective of quantum annealing.

NSF, Director France Cordova, has unveiled a 9 point research agenda to shape the agency's next few decades. The next quantum revolution is one of 6 research areas.

Google has announced they are developing a gate-model quantum computation platform to simulate quantum annealing. It is not yet known that they have constructed a large-scale systems that can supersede the D-Wave machines with error-correcting codes fully implemented which can support large numbers of qubits.

NIST maintains an archive of more than 200 quantum algorithms for Gate and Annealing systems and still growing.
Projected Quantum Annealing Computers: TRL

- D-Wave 2X June 1, 2016 TRL = 3
- D-Wave 3X June 1, 2017 TRL = 4
- Google Group: quantum annealing architectural primitives not available Est. TRL = 4/5
- Lincoln Labs June 1, 2017 TRL = 4
- Lincoln Labs June 1, 2018 TRL = 5
- Lincoln Labs June 1, 2020 TRL = 6/7
Thanks
<table>
<thead>
<tr>
<th></th>
<th>Gate model</th>
<th>Quantum annealing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Target</td>
<td>Universal computation</td>
<td>Combinatorial optimization</td>
</tr>
<tr>
<td>Strengths</td>
<td>A few algorithms are proven to be exponentially faster than their classical counterparts.</td>
<td>Many problems of practical importance, such as machine learning, can be represented as combinatorial optimization. Resilient against noise.</td>
</tr>
<tr>
<td>Weaknesses</td>
<td>Very susceptible to decoherence, i.e. easily destroyed by noise. Faster than conventional machines only for a few tasks.</td>
<td>Problems are yet to be found that can be solved exponentially more efficiently than by classical methods and are of practical significance.</td>
</tr>
<tr>
<td>Current Status of Implementation</td>
<td>About 10 qubits (ions, photons, quantum dots, superconductors,..)</td>
<td>More than 1,000 qubits (superconducting circuits)</td>
</tr>
<tr>
<td>Prospects</td>
<td>Needs extremely many qubits, millions or more, if one implements error corrections. Will take decades to realize.</td>
<td>Will need tens of thousands of qubits. May be realized within a decade.</td>
</tr>
</tbody>
</table>
Links to Data

- [http://www.arm.gov/sites](http://www.arm.gov/sites)
- [http://www.archive.arm.gov/discovery/#v/results/s/fcat::carbon](http://www.archive.arm.gov/discovery/#v/results/s/fcat::carbon)
References


• M. Halem et. al., “A Restricted Boltzmann Neural Net to Infer Carbon Uptake from OCO-2 Satellite Data” American Geophysical Union, Fall meeting Dec. 2015 San Francisco.

• M. Halem, T. Lee, R. Biswas, “Quantum Annealing Computing for earth and Space Science” Session submitted ESSI, American Geophysical Union, Fall meeting, 2016


• L.H. Kauffman, S.J. Lomonaco Jr., “Braiding With Majorana Fermions” Int’l Society for Optics and Photonics, 2016

• S.J. Lomonaco Jr.,” How to build a device that cannot be built” Quantum Information Processing, Volume 15 Number 3 ISSN 1570-0755

• G. Nearing, “Data Assimilation & Dynamic Vegetation Models”; American Geophysical Union, Fall Meeting; San Francisco, CA, December 2015.
• C. Pelissier, “Quantum Annealing in Earth Science : image registration and data assimilation in predicting annual net anthropogenic CO$_2$ uptake in land vegetation" Presented at Supercomputing ’15 , Austin, TX
• A.M.O.Shehab, S. Lomonaco, M. Halem, “An overview of the quantum wavelet transform, focused on earth science applications”, (Poster) , American Geophysical Union, Fall Meeting, December 2015, San Francisco, California.
• M. Halem et. al., “A Quantum Annealing Computer Team Addresses Climate Change Predictability.“ Earth Science Technology Forum: Annapolis,MD. June 14-16


QAC Accomplishments on D-Wave To Date (CONT.)

• Implemented Noah MP model of photosynthesis into GSFC LIS model and conducted a 10 year global OSSE LIS-Noah model run including Alaska and Amazon of an OSSE to evaluate land surface model predictions from OCO-2 data assimilation. (G. Nearing, K. Harrison)

• Testing solution of observation cost function blending of a 3-D variational or Kalman filter formulation of the LIS-Noah model CO2 flux prediction with the derived CO2 flux from OCO-2 using the BM NN algorithm. (G. Nearing, C. Pelissier, K. Harrison, P. Gentine).

• Performed monthly sun induced Fluorescence calculation from Gome-2, ERA-Land, FLUXNET-MTE on a classical feed forward perceptron NN with cross entropy cost function to eliminate outliers. (P. Gentine, Columbia U)

• Performed image registration of MODIS EVI data vegetation Indices for 3 sites initially using classical neural nets. (J. LeMoigne, D. Simpson, GSFC)

• Developing HAAR wavelet algorithm for image registration implementation with full adder on D-Wave. (A. Shehab, S. Lomonaco, J. LeMoigne)

• Simulation Studies for comparison of time continuous CO2 flux assimilation with D-Wave and classical computer BM implementation. (G. Nearing, K. Harrison, R. Prouty, M. Halem, GSFC, UMBC)

• Established strong collaboration with AMES Quantum AI Lab. Held several face to face meetings with their staff and exchanged progress on D-Wave algorithms and quantum performance. Submitted AGU session on “QAC for ESS Applications” with T. Lee, R. Biswas, M. Halem, A. Ortiz
Simulated Annealing and Quantum Annealing

- The phenomena of quantum superposition and tunneling imply that certain types of energy landscapes can be more efficiently explored by quantum annealing than classical simulated annealing [1].
- Comparison of quantum annealing and simulated annealing- H. Nishimori
Team Presentations


2. J. Dorband - Deep Learning Boltzman Machine, Characterization of Qubit Chain on D-Wave;


4. N. Talik-CO2 Flux Prediction Using Restricted Boltzmann Machines

5. K. Harrison- 10 year Global LIS-Noah CO2 flux predictions and NEE.

6. P. Gentine – Classical NN prediction of Sun Fluorescence from GOME-2

7. D. Simpson- MODIS image registration using NN

8. O. Shehab –Implementation of full adder on Dwave for HAAR Wavelets

9. M. Halem- Next 6 Months Activities