

Earth Science Technology Forum

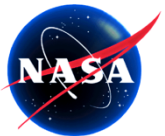
June 14-16, 2016

Feasibility Studies of Quantum Enabled Annealing Algorithms for Estimating Terrestrial Carbon Fluxes

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J. LeMoigne, K. Harrison, C. Pellisier, D. Simpson **GSFC**, P. Gentine, **CU**.

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Outline for talk

- Overview. Science motivation. Annealing History.
(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?

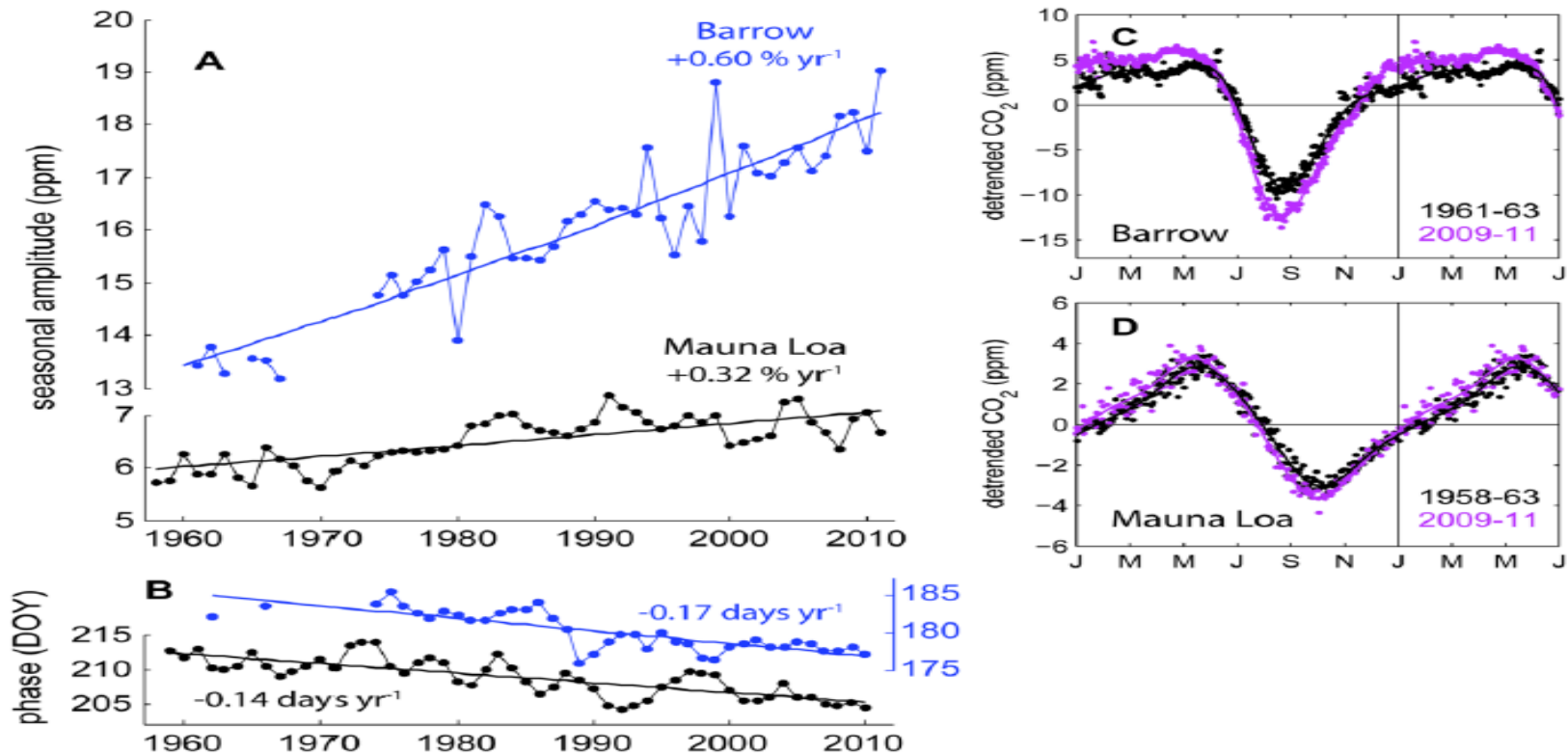


Fig. 1. Observed peak-to-trough seasonal amplitude (A) and phase (B), given by the day of year of downward zero crossing, of CO₂ concentration at Barrow (71°N, blue) and Mauna Loa (20°N, black) measured by the Scripps CO₂ Program (7, 8) and the NOAA Global Monitoring Division (9). Growth rate of amplitude is given in percent change per year, with one-sigma uncertainty of $\pm 0.05\text{--}0.07\%$ 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.

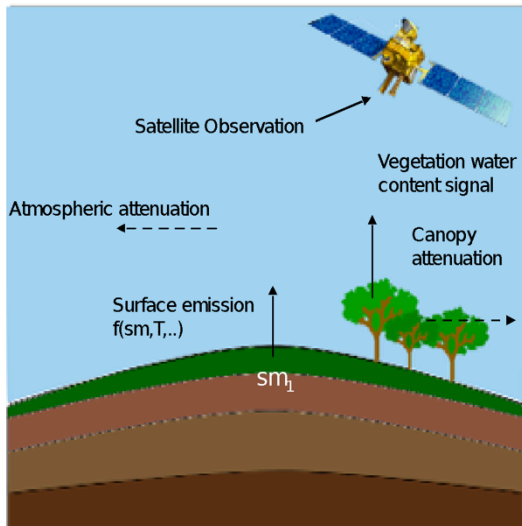
Graven, H.D. Enhanced seasonal exchange of CO₂ by northern ecosystems since 1960. *Science* **341**, 1085-1089 (2013).

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

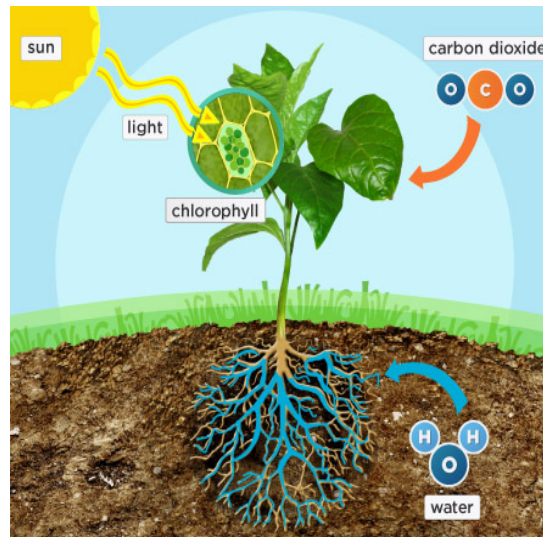
OBSERVATORY



Measures surface CO2 from space

LAND SURFACE MODEL

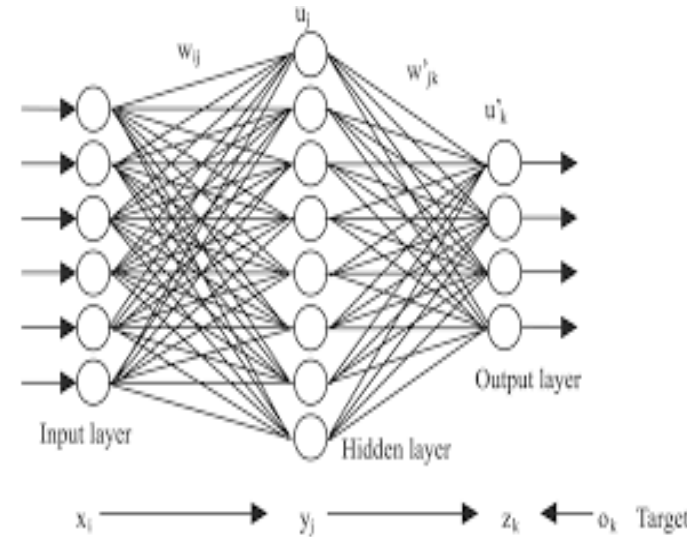
CARBON UPTAKE



Vegetation model assimilates CO2 fluxes for photosynthesis

D-Wave Quantum Annealing

Boltzmann Machine



NN trains CO2 to infer CO2 Fluxes from Station Data

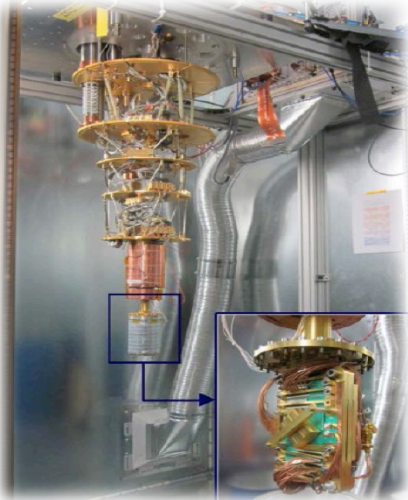
History of Simulated and Quantum Annealing

- 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.
- N. Metropolis, et.al., "Equation of State Calculations by Fast Computers." J. Chem. Phys. 21, (1953).
- 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).
- W.K. Hastings, "Monte Carlo Sampling Methods Using Markov Chains and Their Applications" Biometrika 57 (1970).
- S. Kirkpatrick et. al., "Optimization by Simulated Annealing" Science 220 (1983). A method for efficient techniques for finding minimum or maximum values of a function of very many independent variables, usually called the cost function.
- T.Kadowaki, H. Nishimori. "Quantum annealing in the Transverse Ising Model" Phys. Rev. 58 (1998). They proposed theory of quantum annealing; that quantum fluctuations cause transitions between states and play the same role as thermal fluctuations in simulated annealing for finding the minimum of a multivariable objective (cost) function.

DWAVE Quantum Computer



DWAVE 2X at NASA AMES.



Quantum chip with 1097 "qubits"

Trait	Classical bit	Quantum bit
Binary system		
State	Simultaneous superposition. $\psi = \frac{1}{\sqrt{2}} (\uparrow\rangle + \downarrow\rangle)$	Either 0 or 1. $\Delta V = 0$ or $\Delta V \neq 0$
Measurement	Probabilistic.	Deterministic.
Interaction between bits	"Chimera graph" bits 	None.

Computing on the DWAVE

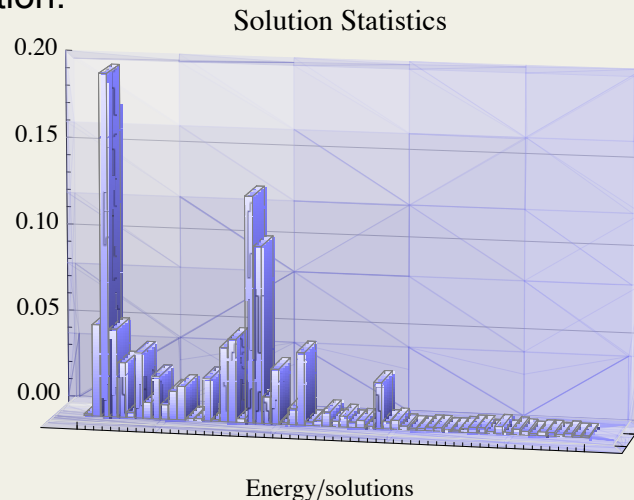
Quadratic Unconstrained Binary Optimizations (QUBOs)

Numerical Task:

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

α_{ij} = user specified “couplings”.

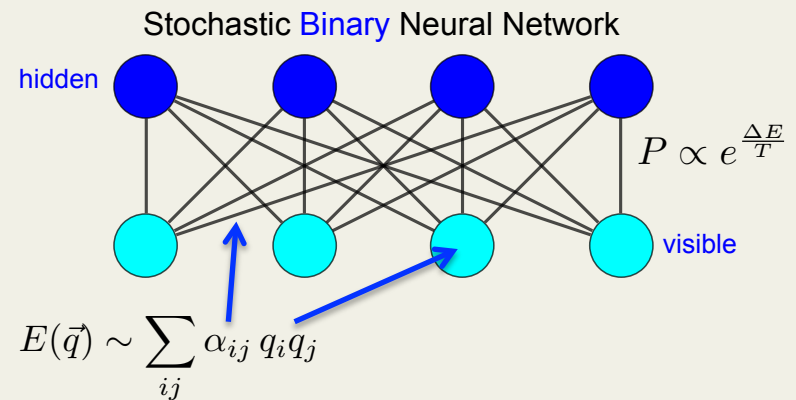
Results: collect statistics and take the **BEST** solution.



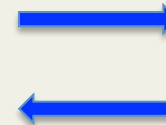
DWAVE searches the entire space and returns potential candidates for the global minimum.

Restricted Boltzmann Machines (RBM)

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



$\alpha_{ij}^k \rightarrow \alpha_{ij}^{k+1}$
update coefficients



Generate Boltzmann statistics

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.

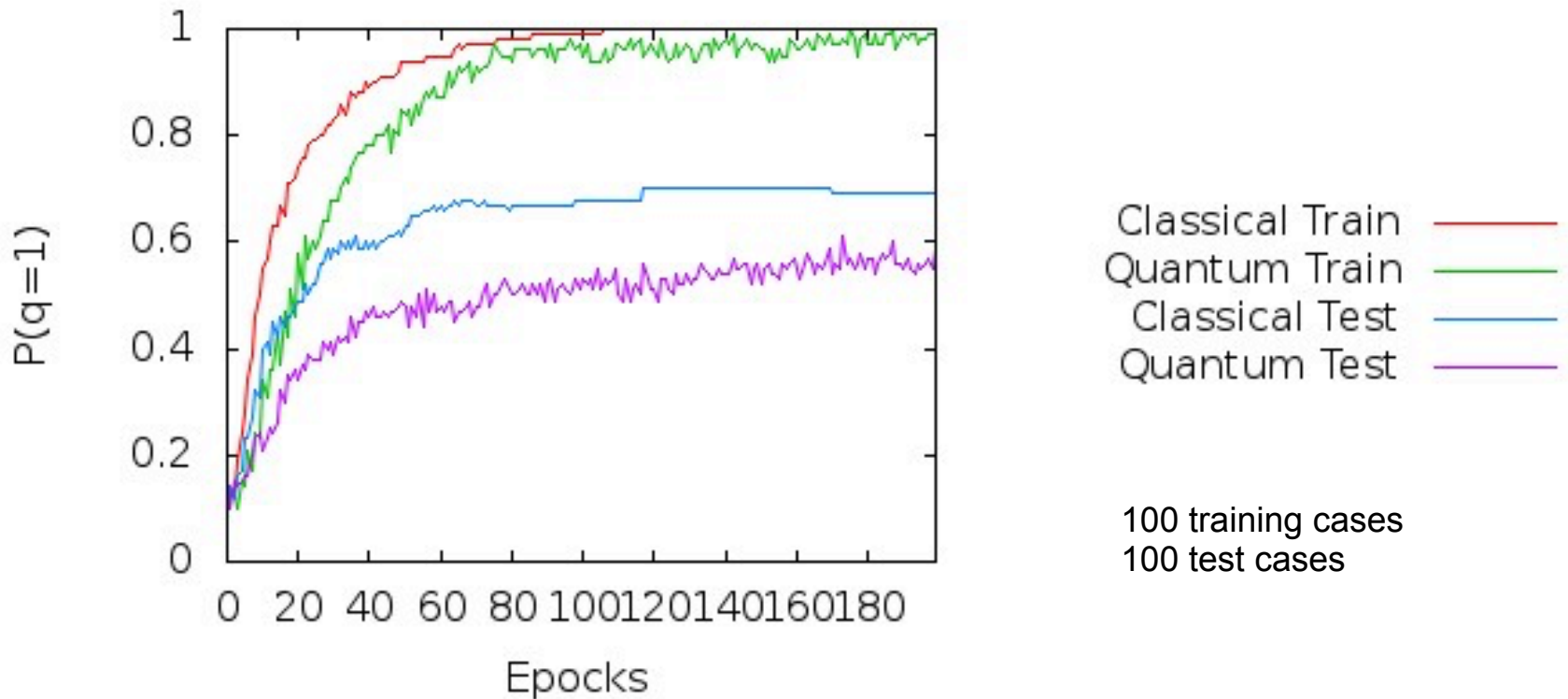
A Prototype RBM Evaluation using MNIST

- 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



Observation Regions



Barrow, Alaska



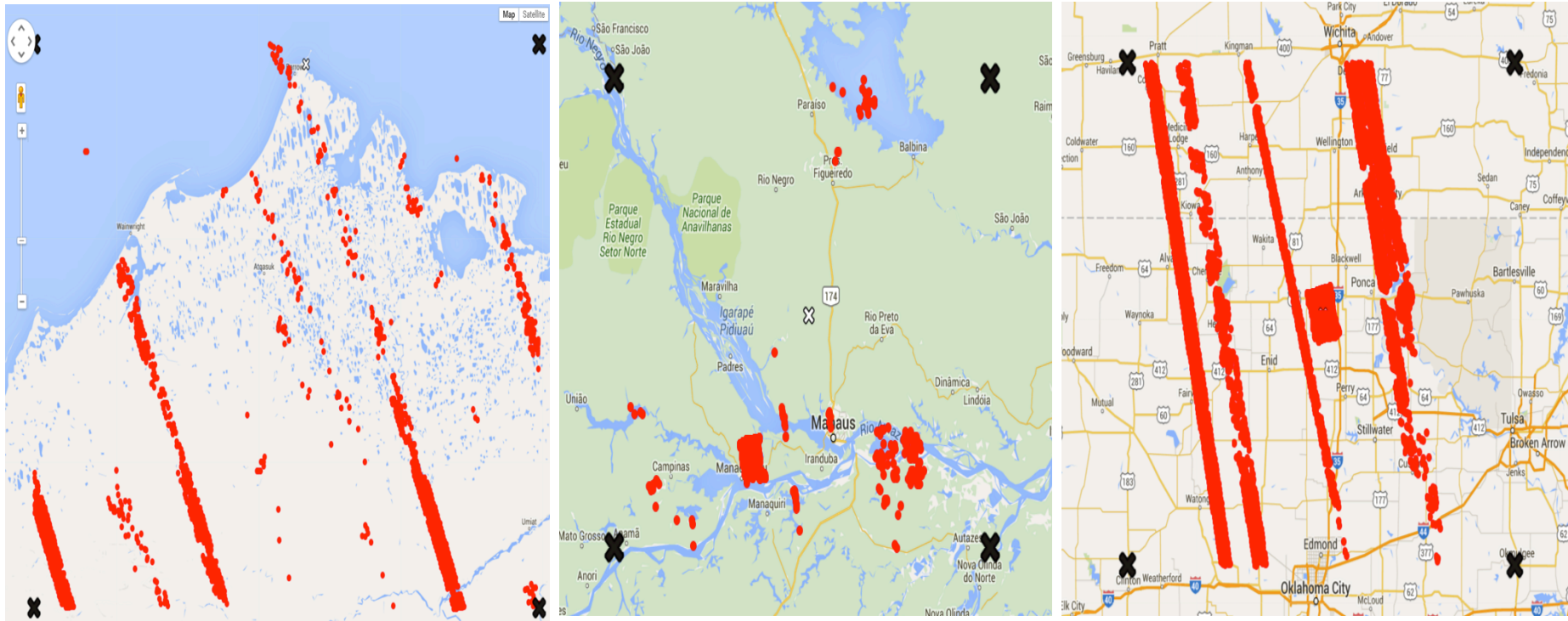
Oklahoma City, Oklahoma



K34, Brazil

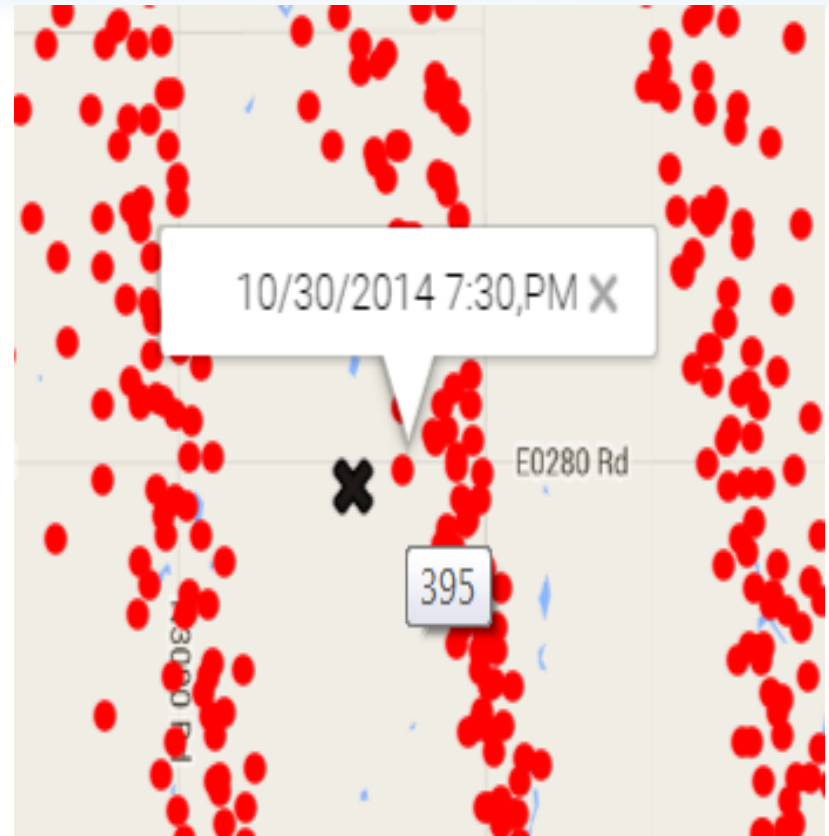
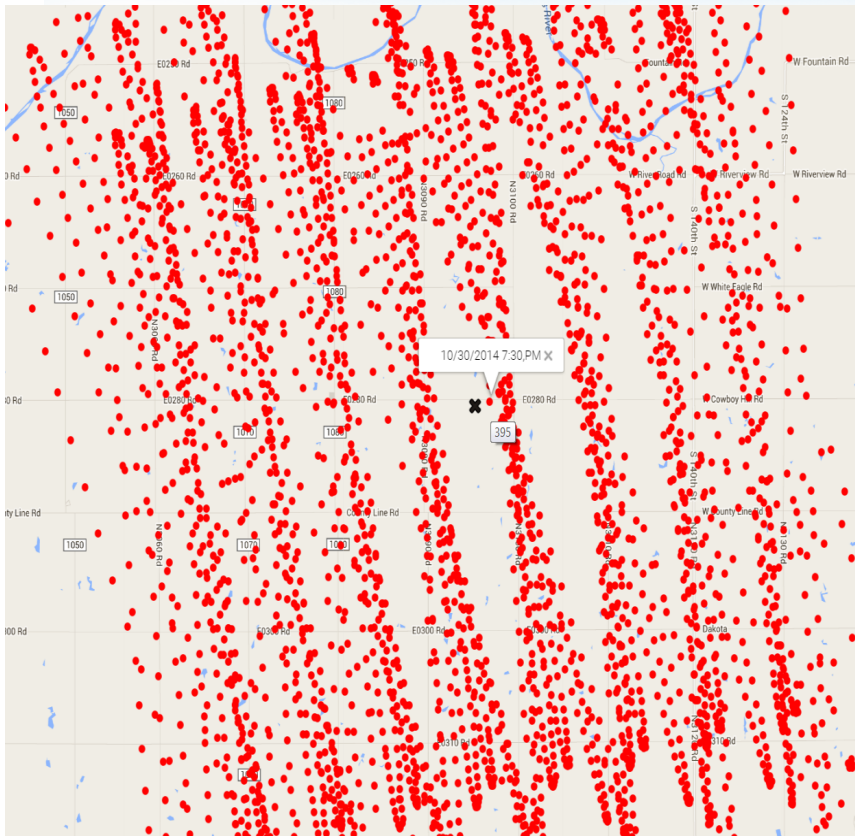
- 3 primary regions selected for observations:
- Barrow, (69.0,-162.0) (71.4,-152.0), Oklahoma City, (34.5,-99.5)(36.5, -96.5), K34, Brazil (-3.6, -61.5) (-1.6, -59.0)
- OCO2 – Orbiting Carbon Observatory 2 Launched July of 2014. Level 2 lite data has been collected and processed since September of 2014 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

OCO2 Tracks with CO2 values



- 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.

OCO-2 Data Validation



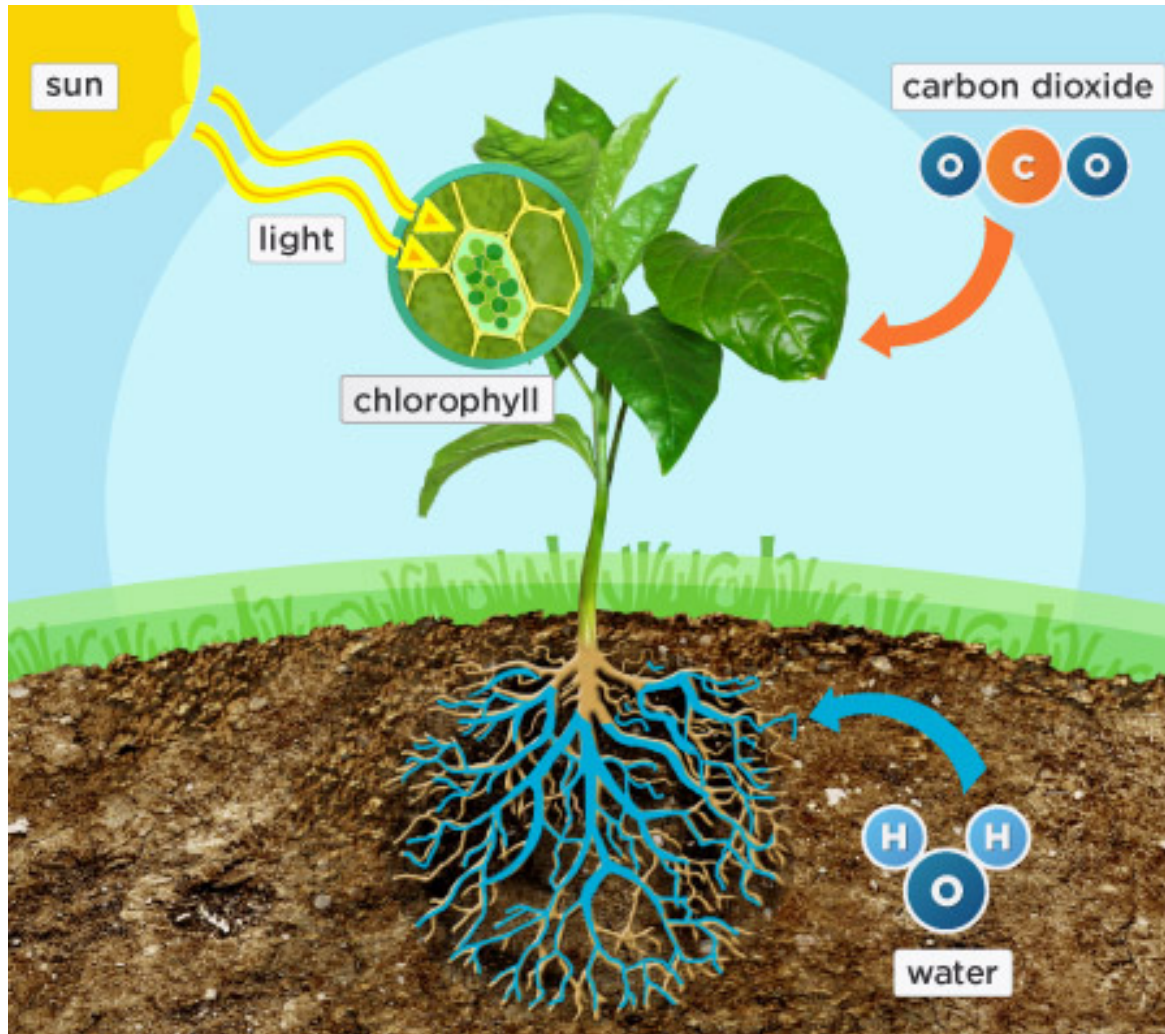
Oklahoma City

- 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



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

Value	CO2 Flux($\mu\text{mol m}^{-2} \text{s}^{-1}$)	CO2(mol m^{-3})	H2O(mol m^{-3})	Temperature($^\circ\text{C}$)	Pressure (kPa)	Wind Speed(m s^{-1})	horizontal wind direction	rotation to zero w(theta)	rotation to zero v(phi)
Min	-140.5	0.0792	0	-17.31	0.38	0.158	0.0087	0	0
Max	69.271	139.33	2108.7	40.55	100.95	15.314	359.99	61.592	180.00
Average	-0.626	16.092	688.89	21.8193	97.7852	4.6211	173.368	1.416	73.327
Standard Deviation	4.4978	1.7935	384.35	9.57815	1.6441	2.5330	94.668	1.1683	60.240

10 years of $\frac{1}{2}$ 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

Mean Error	0.065
Error standard deviation	3.936
Root Mean Squared Error	3.939

2. Error for test data after removing outliers

Mean Error	1.133
Error standard deviation	4.43
Root Mean Squared Error	4.58

Prediction Accuracy of RBM

1. Error for complete test data

Mean Error	12.67
Error standard deviation	4.30
Root Mean Squared Error	13.38

2. Error for test data after removing outliers

Mean Error	6.60
Error standard deviation	2.62
Root Mean Squared Error	7.10

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.

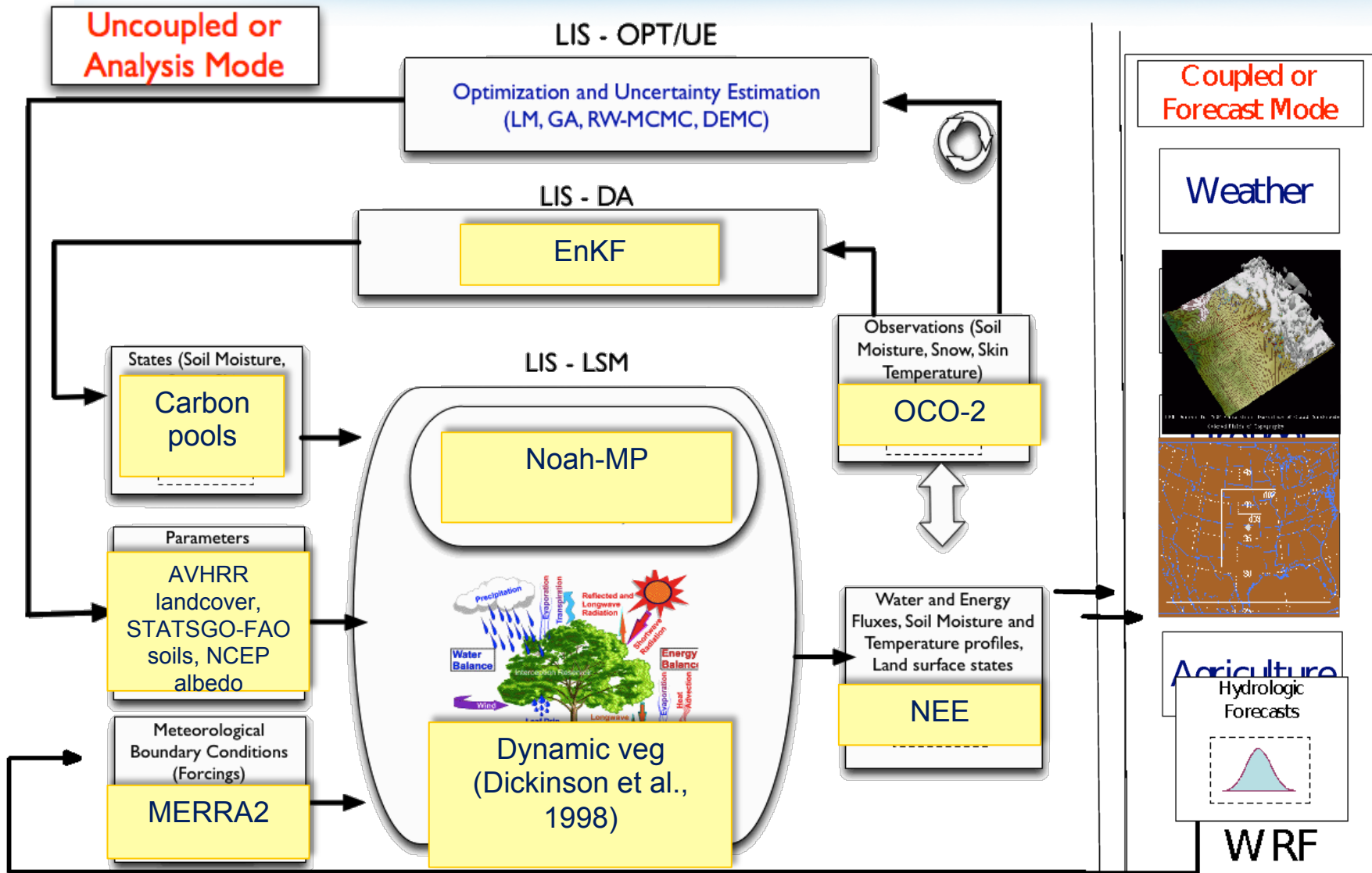
Main role of LIS in QAC project

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

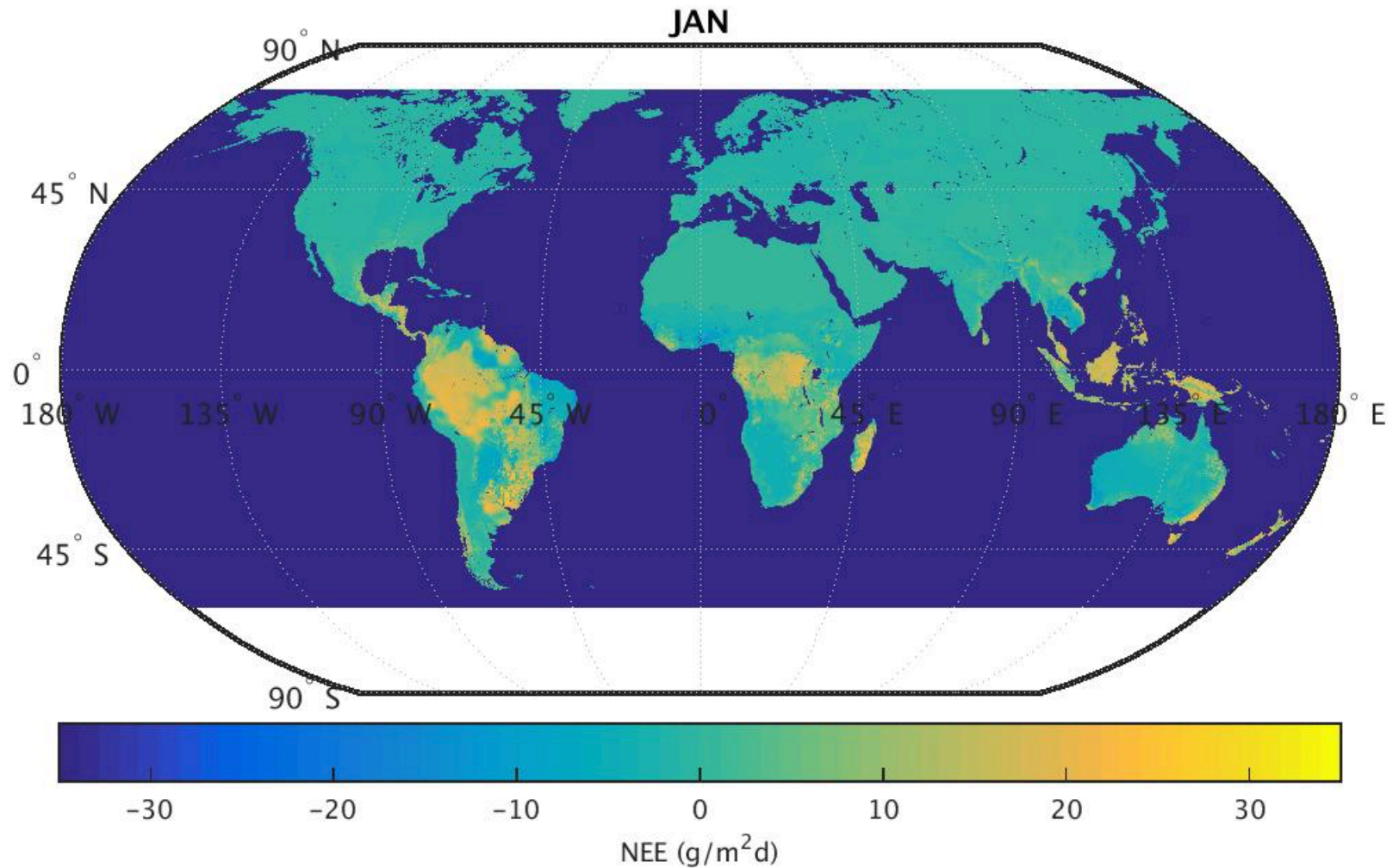
We have completed a 10-year CONUS run and a 5-year global run.

1. Noah-MP is NCEP's newest version of the WRF with lower boundary condition. It is 1st 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)



Noah MP: Global run: NEE seasonal cycle

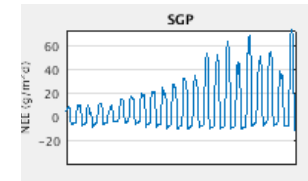
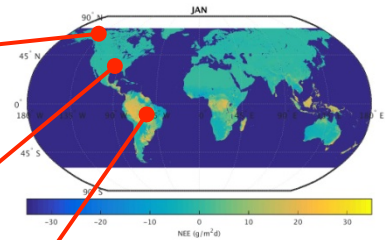
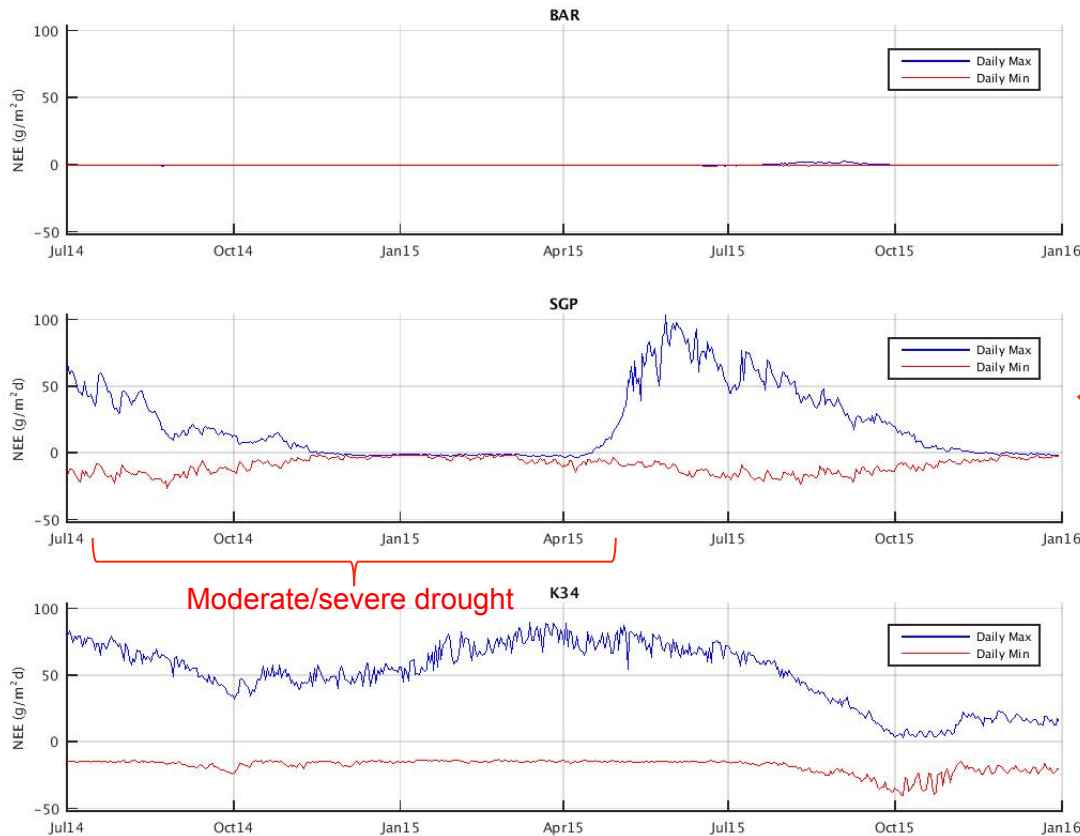


Noah-MP Data Assimilation

Basic Testing of a Kalman-Type Data Assimilation Algorithm for Surface Carbon Flux

- 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*.

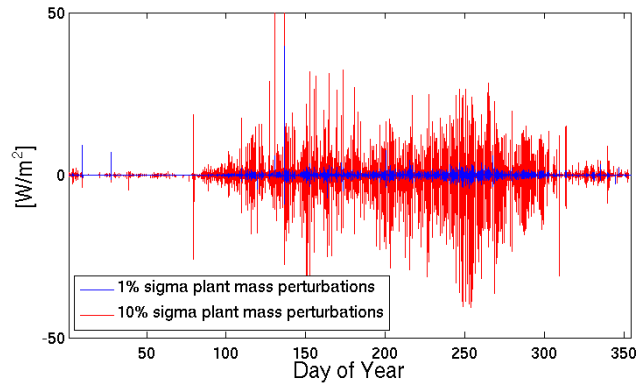
Noah MP: Site runs



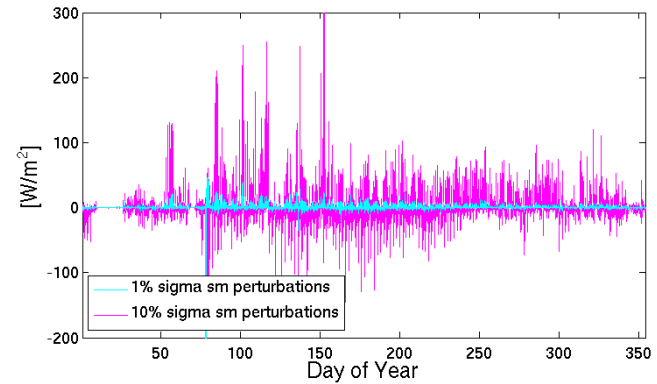
Showing daily min and max as there are large fluctuations within and across days

Preliminary DA Results: Sensitivity Analysis

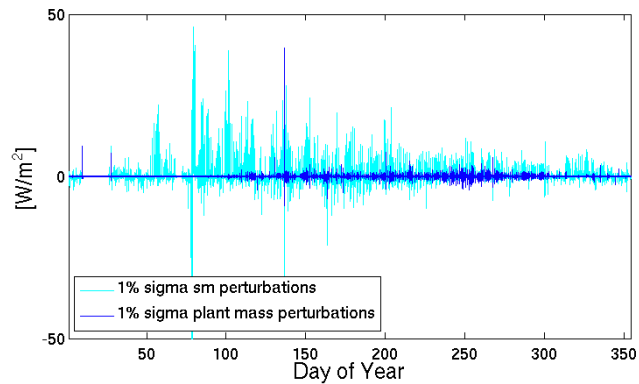
Sensitivity of Q_{ie} to Plant Mass Perturbations



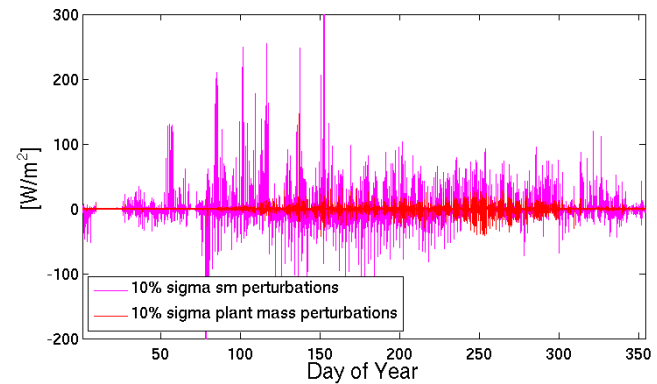
Sensitivity of Q_{ie} to Soil Moisture perturbations



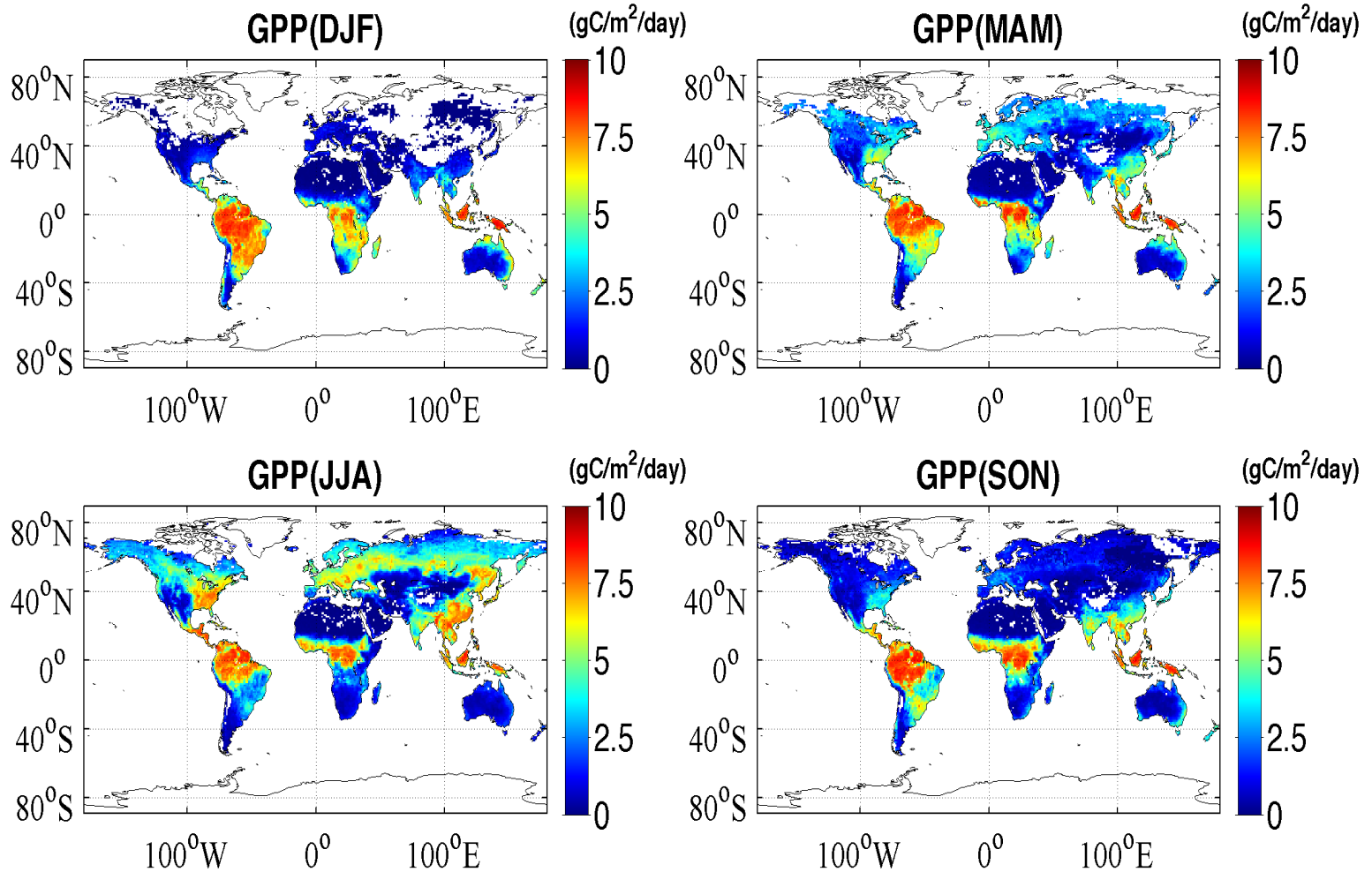
Compare Sensitivity of Q_{ie} to SM and PM Perturbations



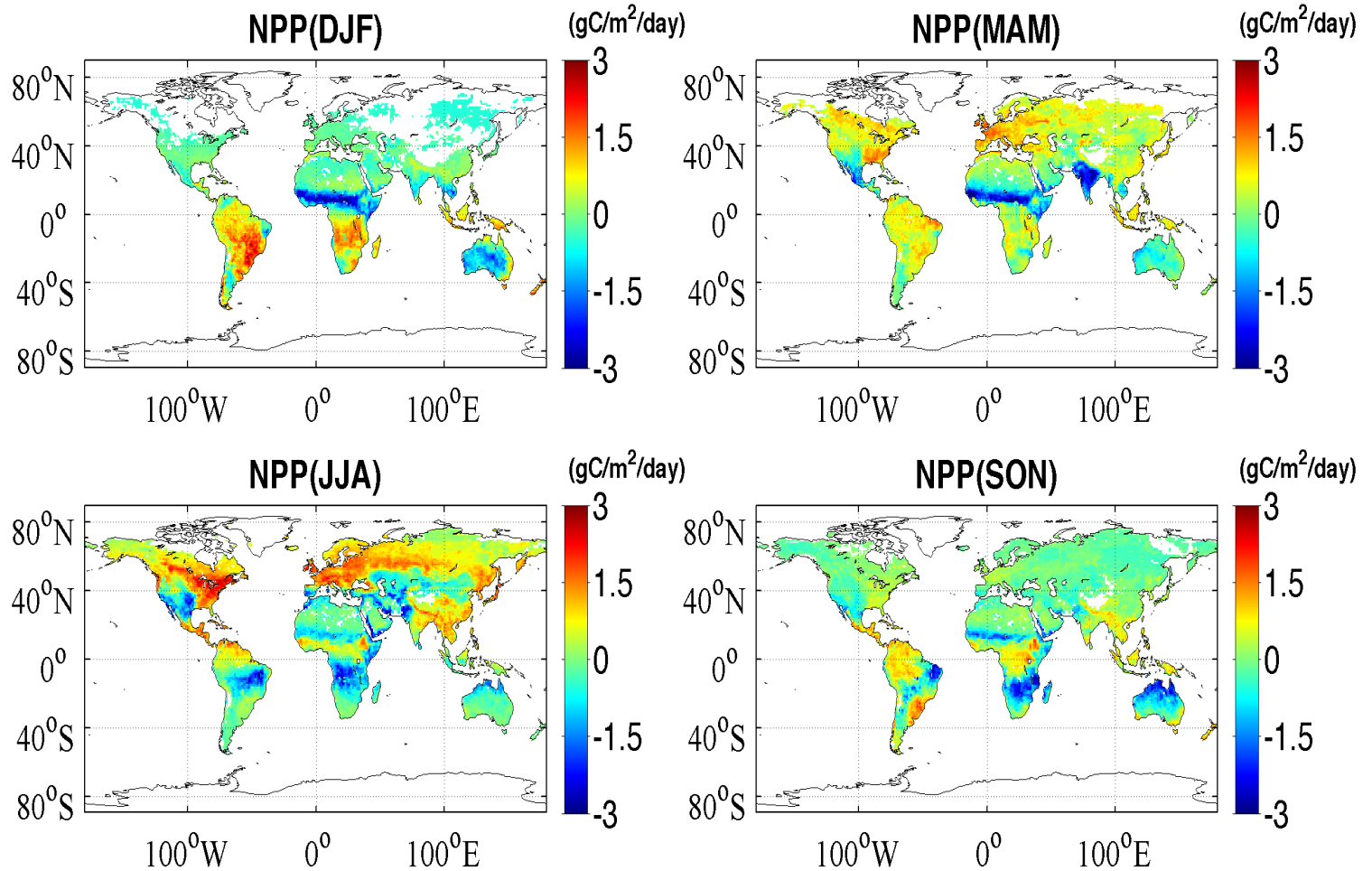
Compare Sensitivity of Q_{ie} to SM and PM Perturbations



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.

Restricted Boltzmann Machine

- 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.

Status of Quantum Annealing Machines

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



Quantum Gate comparisons with Quantum Annealing

	Gate model	Quantum annealing
Target	Universal computation	Combinatorial optimization
Strengths	A few algorithms are proven to be exponentially faster than their classical counterparts.	Many problems of practical importance, such as machine learning, can be represented as combinatorial optimization. Resilient against noise.
Weaknesses	Very susceptible to decoherence, i.e. easily destroyed by noise. Faster than conventional machines only for a few tasks.	Problems are yet to be found that can be solved exponentially more efficiently than by classical methods and are of practical significance.
Current Status of Implementation	About 10 qubits (ions, photons, quantum dots, superconductors,..)	More than 1,000 qubits (superconducting circuits)
Prospects	Needs extremely many qubits, millions or more, if one implements error corrections. Will take decades to realize.	Will need tens of thousands of qubits. May be realized within a decade.

Links to Data

- <http://www.nasa.gov/press-release/as-earth-warms-nasa-targets-other-half-of-carbon-climate-equation>
- <http://www.arm.gov/sites>
- <http://www.archive.arm.gov/discovery/#v/results/s/fcat::carbon>
- <http://www.archive.arm.gov/discovery/#v/home/s/>

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- 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
- M. Halem et. al., "A Quantum Annealing Computer Team Addresses Climate Change Predictability." Earth Science Technology Forum: Annapolis, MD. June 14-16.
- K. W. Harrison, Y. Tian, C. D. Peters-Lidard, S. Ringerud and S. V. Kumar, "Calibration to Improve Forward Model Simulation of Microwave Emissivity at GPM Frequencies Over the U.S. Southern Great Plains," in IEEE Transactions on Geoscience and Remote Sensing, vol. 54, no. 2, pp.1103-1117, Feb. 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.

References (Cont.)

- G. Nearing, “Data Assimilation on a Quantum Annealing Computer – Feasibility and Scalability”; American Geophysical Union Fall Meeting; San Francisco, CA, December, 2014.
- C. Pelissier, “Quantum Annealing in Earth Science : image registration and data assimilation in predicting annual net anthropogenic CO₂ uptake in land vegetation" Presented at Supercomputing '15 , Austin, TX
- A.M. O. Shehab, “Feasibility of Performing Arithmetic on a Quantum Annealing Computer”, (Poster) Adiabatic Quantum Computing Conference, 2016, LA, California.
- 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

References

- [1] MIT Lincoln Laboratory - annual report 2014. Technical report, MIT Lincoln Laboratory, 2014.
- [2] Broad agency announcement: Quantum enhanced optimization (qeo) - iarpa-baa-15-13. Technical report, Intelligence Advanced Research Projects Activity, February 2016.
- [3] MHS Amin, CJS Truncik, and DV Averin. Role of single-qubit decoherence time in adiabatic quantum computation. *Physical Review A*, 80(2):022303, 2009.
- [4] Neil G Dickson, MW Johnson, MH Amin, R Harris, F Altomare, AJ Berkley, P Bunyk, J Cai, EM Chapple, P Chavez, et al. Thermally assisted quantum annealing of a 16-qubit problem. *Nature communications*, 4:1903, 2013.
- [5] Richard Harris, MW Johnson, T Lanting, AJ Berkley, J Johansson, P Bunyk, E Tolkacheva, E Ladizinsky, N Ladizinsky, T Oh, et al. Experimental investigation of an eight-qubit unit cell in a superconducting optimization processor. *Physical Review B*, 82(2):024511, 2010.
- [6] MW Johnson, MHS Amin, S Gildert, T Lanting, F Hamze, N Dickson, R Harris, AJ Berkley, J Johansson, P Bunyk, et al. Quantum annealing with manufactured spins. *Nature*, 473(7346):194–198, 2011.
- [7] J Kelly, R Barends, AG Fowler, A Megrant, E Jeffrey, TC White, D Sank, JY Mutus, B Campbell, Yu Chen, et al. State preservation by repetitive error detection in a superconducting quantum circuit. *Nature*, 519(7541):66–69, 2015.
- [8] Stephen Nellis. Google, microsoft vie for ucsb top minds with quantum initiatives, September 2014. [Online; posted 12-September-2014].

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
- Mukherjee, S. and Chakrabarti, B.K. (2015) Multivariable optimization: Quantum annealing and computation. Eur. Phys. J. Special Topics 224, 17–24.

Team Presentations

1. C. Pelissier- Computing on the Dwave- QUBO, RBM,H/W Overviews.
2. J. Dorband - Deep Learning Boltzman Machine, Characterization of Qubit Chain on D-Wave;
3. A. Radov – ARM Tower data, CO₂, CO₂ fluxes and colocation statistics.
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