A Quantum Annealing Computer Team Addresses Climate Change Predictability

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Overview

• Quad+ Milestone

• Quantum Annealing Computing (QAC) Objectives

• Current Accomplishments:
  - QAC algorithmic developments
  - OCO-2 Satellite data applications
  - Science Applications

• Budgets

• Current TRL Evaluations

• Activities – Next 6 months/12 months
Objective

- Develop quantum enabled annealing algorithms to extract CO2 fluxes from OCO-2 data to calculate annual Net Carbon Uptake for three ground truth sites
  - Satellite image registration for test sites & CO2.
  - Perform data assimilation (VarDA/K-F).
  - Calculate CO2 flux and Assimilate into LIS/Noah hydrological model
- Evaluate the potential for quantum annealing computing (QAC) to be a disruptive technology to advance Earth science.
- Improve NASA's understanding of the range of applications of quantum computing.

Approach:

- Generalize QAC Neural Nets for satellite data processing for high spatial and temporal locality
- Develop and test QAC algorithms for LIS 3D-Var/K-F
- Derive Atmospheric CO2 Transfer Matrices for 3 regions
- Enable time-step data transfer between QC and LIS*
- Implement OCO-2 observation function for LIS*
- Implement QAC Image Registration on Dwave
- Derive maps of vegetation and vegetation change
- Demonstrate Data Assimilation on LIS*
- Estimate and evaluate Net Carbon Uptake for 3 sites

Key Milestones

- Start 06/01
- Develop QAC Image Registration/neural nets 11/15
- Complete QAC Image Registration/CO2flux from OCO2 06/16
- Complete 3D VarDA/K-F QAC algorithm 06/16
- Time step Data Transfer between QAC and LIS 12/16
- QAC Image Registration on MODIS imagery 12/16
- Demo and evaluate QAC Data Assimilation Of OCO2 data for LIS (TRL 4) 05/17


TRL_{in} = 4
QAC Objectives

• Assess technology readiness of Quantum Annealing Computers (QAC) to evolve into a game changing technology for NASA science related missions.

• A by-product of assessment studies by UMBC/GSFC/Columbia Univ. team will determine potential of current or future D-Wave systems to improve Land Surface Model predictions of Net Ecosystem Exchange through the use of satellite surface observations.

• The initial focus of the UMBC/GSFC/CU team will employ the NASA Ames D-Wave system to infer surface CO2 flux from the Orbiting Carbon Observatory measurements of CO2 concentrations and assimilate into the GSFC Land Information Surface (LIS) model to predict net ecosystem exchange (NEE).

• The research approach draws on the D-Wave to solve 3 Neural Net optimization problems; (i) calculating CO2 Fluxes from CO2, (ii) Image registration of MODIS’ EVI products and (iii) 3-D VAR or K-F data assimilation of CO2 fluxes into LIS model.

• We address a fundamental Climate Change question based on NASA satellite missions and models, “Can future Quantum Annealing Computers infer correlations between satellite CO2 observations and in-situ CO2 flux measurements more accurately or faster than classical computers to determine whether land cover vegetation will continue to absorb 25% of the net annual anthropogenic CO2 emissions.
QAC Team Accomplishments To Date

• Developed and compared performance of an RBM algorithm on D-Wave2X with same algorithm on a classical IBM cloud for MNIST data set showing comparable accuracies.

• Developed 1st Deep Belief Learning Boltzman Machine (BM) on the Ames D-Wave2 as generic NN tool uploaded in Github. Still exploring performance. (J. Dorband UMBC)

• Downloaded and archived 20 months of OCO-2 CO2 L2 Lite data as well as Fluorescence data for period Sept. 6, 2014- present. Collected and co-located L2 lite data with 20 Fluxnet distributed globally. (M. Barr-Dallas, K. Brady, M. Halem UMBC)

• Acquired CO2 and CO2 flux measurements at ARM tower sites located at 2 sites, Barrows Alaska, Oklahoma City (A. Radov, M. Halem UMBC). Negotiating Ameriflux access in the Amazon (K34) (P. Gentine CU).

• Initiated CO2 flux calculations with co-located targeted OCO-2 satellite CO2 data with the RBM tool and obtained first comparative statistical results with classical Feed Forward algorithm.
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)

• Performance comparison of time continuous CO2flux assimilation with D-Wave and classical computer BM implementation. (G. Nearing, J. Dorband, N. Tilak, M. Halem)

• 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

• Developing HAAR wavelet algorithm for image registration implementation with full adder on D-Wave. (A. Shehab, S. Lomonaco, J. LeMoigne) Performed image registration of MODIS EVI data vegetation Indices for 3 sites initially using classical neural nets. (J. LeMoigne, D. Simpson)
Team Presentations


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

1. **A. Radov** – ARM Tower data, CO2, CO2 fluxes and colocation statistics.

1. **N. Talik**- CO2 Flux Prediction Using Restricted Boltzmann Machines

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

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

1. **D. Simpson**- MODIS image registration using NN

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

1. **M. Halem**- Current and Future QAC TRLs and Next 6 Months Activities
Computing on the DWAVE

**Quadratic Unconstrained Binary Optimizations (QUBOs)**

**Numerical Task:**

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

\(\alpha_{ij}\) = 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”.

Hidden Stochastic Binary Neural Network

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

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

Energy/solutions

Solution Statistics

DWAVE is a physical realization of a RBM!
Hardware

DWAVE 2X™

- 1152 (8x12x12) qubit processor
- 1097 qubits in “Working Graph”
- Max operating temperature (13 mK nominal)
- Key feature: A small reduction in temperature provides a significant boost in performance
- 3.5% and 2% precision level for h and J (couplings)
- ~10xT (~4x improvement of adiabatic process)
- Graph connectivity: 6 per qubit (Chimera architecture)

IBM Quantum Experience

- Universal quantum computer with 5-qubits.
- Silicon based chip with superconducting qubits.
- Claims reliability.
- Claims scalable architecture.
- Open to the public through the cloud.

Lincoln Labs Quantum Computer

Current:
- 100 qubits operationally.
- Lower de-coherence time than DWAVE.
- 3rd and 4th order interactions.

Project roadmap:

Table 1. Select QEO program metrics (minimum requirements)

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<th>Design Space</th>
<th>Year</th>
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<th>3</th>
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<td>≥ 7</td>
<td>≥ 7</td>
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<td>≥ 8</td>
<td>≥ 10</td>
<td>≥ 16</td>
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<td>≥ 2</td>
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<td>≥ 4</td>
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<td>Speed-up projected</td>
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<td>10²</td>
<td>10¹0</td>
<td>10¹</td>
<td>10¹</td>
<td>10¹</td>
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<tr>
<td>Speed-up corroborated</td>
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<td>&gt; n¹³</td>
<td>n¹¹</td>
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<tr>
<td>Polynomial scaling improvement (all modeled at Application-Scale)</td>
<td>10¹</td>
<td>10²</td>
<td>10¹0</td>
<td>10¹</td>
<td>10¹</td>
<td>10¹</td>
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Computing using QUBOs on the Dwave 2X™

1. Map target problem into a QUBO.

2. Embed problem into Dwave 2X™ Hardware.

   - Bipartite graph (chimera graph)
   - Sparsely connected 6 connections / qubit.
   - $U_q \propto \sum_{i,j} \alpha_{ij} q_i q_j$

   Problem graph

   Hardware graph

3. Generate statistics and select the best answer.

   - Execute ~10,000 of anneals (4s including reset and readout) to collect statistics, and take the best answer.
   - Gauge symmetries, error checking, bias correction to eliminate systematic errors.
   - Pre/Post processing to improve results.
   - Optimization of constraints.

Image registration:

Data assimilation:

\[ O(q) = \sum_{i,j} \alpha_{ij} q_i q_j \]

$\alpha_{ij}$: define problem; user set

$\propto$ works well.

Requires more hardware qubits ($< N^2$)

Finding the best embedding is an NP-hard problem.

Need to chain qubits together. Long chains often (>10) break down due to limited hardware precision.

$U_q \propto q_i q_j$ after machine is cooled due to trapped magnetic flux, so graph is broken.
## Image Registration Steps

1. **Consider a reference image and target image for alignment.**
   - Reference image
   - Target image

2. **Filter image to reduce pixels and focus on important features.**
   - Reference image
   - Target image

3. **Transform target image by a combination of a rotation + translation ($\theta, ax, ay$).**
   - Reference image
   - Target image

4. **Compare pixel intensities.**
   $$\min \Delta(\theta, ax, ay)$$

## Formulating a QUBO

Real valued parameter represented with fixed precision:

$$x = x_{\text{min}} + \Delta x \sum_{i=1}^{N_b} 2^{i-1} q_i, \quad \Delta x = \frac{x_{\text{max}} - x_{\text{min}}}{2N_b}$$

Search all possible labeling (permutations):

$$\begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix}$$

Add constraints so all rows and columns sum to unity.

Rotation:

$$\begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \rightarrow \begin{pmatrix} c & s \\ -s & c \end{pmatrix}$$

Add constraint $c^2 + s^2 = 1$

Translation:

$$\begin{pmatrix} x \\ y \end{pmatrix} \rightarrow \begin{pmatrix} x + ax \\ y + ay \end{pmatrix}$$

No constraint needed!

- Results in 4\textsuperscript{th} order binary objective function. Can be reduced with ancillary variables.
- Small angle approximation leads to a QUBO.
**Data assimilation as a QUBO**

**Data Assimilation**

Real valued parameter represented with fixed precision:

\[ x = x_{\text{min}} + \Delta x \sum_{i=1}^{N_b} 2^{i-1} q_i , \quad \Delta x = \frac{x_{\text{max}} - x_{\text{min}}}{2N_b} \]

Approximate as a polynomial (Taylor series):

\[ J(x, x_0) = \sum_{k=0}^{\infty} \frac{1}{k!} \left[ \sum_{i=1}^{d_{x}} (x_i - x_{0,i}) \frac{\partial}{\partial x_i} \right]^k J \approx \sum_{c_{i_1,\ldots,i_n}} \prod_{n=1}^{N} x_{i_n} \]

Reduce higher order terms with ancillary variables:

\[ q_1q_2q_3 \rightarrow q_1z + s(q_2, q_3, z) \]

\[ s(q_2, q_3, z) = 3z + q_2q_3 - 2z(q_2 + q_3) \]

**Bayesian approach --- maximize posterior (minimize log posterior probability).**

**Observation function**

\[ J(x_i) = \frac{[H(x_i, U_i) - y_i]^2}{R_i} + [x_{i-1} - M(x_{i-1}, U_i)]^T Q^{-1} [x_{i-1} - M(x_{i-1}, U_i)] \]

**Surface respiration model**

- Real valued non-linear optimization problem.
- Find optimal model (land respiration) parameters ~3 - 10

**Formulating a QUBO**

- Repeated application can reduce any order to quadratic.
- DWAVE SAPI APIs available to do this for you.
- Higher order terms require substantially more binary variables.
QUBO Results and outlook

Data Assimilation

Quadratic equation (simplest example):

\[ J(x) = ax^2 + bx \]

\[ x = x_{\text{min}} + \Delta x \sum_{i=1}^{N_{b}} 2^{i-1} q_i, \quad \Delta x = \frac{x_{\text{max}} - x_{\text{min}}}{2N_b} \]

\[ J(q) = \sum_{i,j} \alpha_{ij} q_i q_j \]

Likelihood of correct solution with increased precision

Issues:
- Requires entire machine to register 6 points.
- Embedding almost always broken down (400/10000).
- Possible to improve accuracy with error correction and careful adjustment of constraint parameters.
- Image registration algorithms perform the same task in polynomial time ~N^2.

Image Registration

Solution Statistics

Energy/solutions

Issues:
- Higher order terms require substantially more qubits and decrease reliability of the result.
- Quadratic already difficult.
- Polynomial simplification can be carried out efficiently on traditional computers.

Outlook

- Problems (approximation to) can be solved in polynomial time on a traditional computer.
- Sparse connectivity restricts size and results become more unreliable. Better connectivity in the future?
- Limited precision, thermal fluctuations, and errors make it impossible to achieve high precision if required.
- Restricted Boltzmann machines looking more promising, but RBMs are not suited for all problems.
- Probably better to investigate computationally hard problems on classical computers to get potential gains in the near future.
LIS Noah-MP Open Loop runs

Ken Harrison
LIS’s role in QAC project

• Facilitate the conduct of an OSSE to evaluate land surface model prediction improvements from OCO-2 data assimilation
• First step: Run the land surface model without the OCO-2 data (“Open Loop” run)
• This is the main focus of Yr. 1
NASA Land Information System (LIS)

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

LIS - DA
EnKF

LIS - LSM
Noah-MP
Dynamic veg (Dickinson et al., 1998)

Weather

Coupled or Forecast Mode

WRF

Carbon pools

Coupled or Forecast Mode

Meteorological Boundary Conditions (Forcings)
MERRA2

AVHRR landcover, STATSGO-FAO soils, NCEP albedo

States (Soil Moisture)

Observations (Soil Moisture, Snow, Skin Temperature)

CO2

Floods

Agriculture

First year LIS task is completed

• Open Loop runs completed
  – Globally, with daily 10km output
  – At the three study sites, with hourly 10km output
Noah MP: Global run: NEE seasonal cycle
Noah MP: Site runs

Showing daily min and max as there are large fluctuations within and across days.
Issues/Other

• Noah MP is new—our team has contributed several bug fixes back to the model developers
• The open loop data is being distributed to team members, each with their own specific requirements
• Next year’s task: OCO-2 Data Assimilation (addressed next by Grey Nearing)
LIS Noah-MP Open Loop

**LIS Noah-MP open loop runs are necessary for two reasons:**

1. To use as the baseline for measuring the added value of data assimilation
2. 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.
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.
Preliminary DA Results: Sensitivity Analysis

Sensitivity of $Q_{in}$ to Plant Mass Perturbations

Sensitivity of $Q_{in}$ to Soil Moisture Perturbations

Compare Sensitivity of $Q_{in}$ to SM and PM Perturbations

Compare Sensitivity of $Q_{in}$ to SM and PM Perturbations
Preliminary DA Results

Assimilating NEE directly

Italy - Grassland

Netherlands Evergreen Needleleaf

U.S. Evergreen Needleleaf
Information from LAI vs. SM
Our Ability to Extract Information

Info About NEE - After Cal/DA

- LPRM (AMSR-E) Soil Moisture | Noah
- MODIS MOD13 LAI | Noah
- LPRM (AMSR-E) Alone
- MODIS MOD13 Alone
- Noah Modeled (LPRM Cal/DA)
- Noah Modeled (MODIS Cal/DA)

Info About ET - After Cal/DA
What is happening inside the model?

MODIS Calibration & Data Assimilation

LPRM Calibration & Data Assimilation
Port LIS/Noah Model to UMBC/Bluewave

• Provides a quantitative assessment of the potential impacts of proposed observing systems (OS) on climate modeling, data assimilation (DA), and NN processing of remote sensing data

• Will be used to evaluate BM sensitivity of new quantum annealing architectures of CO2/SIF

• OSSE analytics consist of following steps:

  - Generate reference system (‘nature run’) by running high-res predictive model
  - Simulate observations from output results
  - Observations are assimilated into low-res identical model and simulated forecasts are made
  - Forecasts from reference system are compared to simulated forecasts.

1: Kumar, S.V. et al. 2005
Summary of Port to UMBC

• Downloaded/ported LIS to UMBC/CHMPR BlueWave system

• The model is being implemented and tested for reproducibility with runs at NCCS. LIS on BlueWave is still experiencing compatibility errors

• Working with Nearing and Harrison at GSFC to correct issues

• Expected to debug system and complete a high-resolution full physics run by the end of June

• Will also run a coarse resolution run for three proposed regions

• Expected to generate simulated data with the aim of conducting an Identical Twin OSSE by the end of the 5th quarter
Image Registration on the D-Wave Quantum Computer

David Simpson
Craig Pelissier
Jacqueline Le Moigne
Overview

• 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:

1. Ohio River (ground-based radar with artificial translations)
2. Landsat images (with real translations and rotations)

RBM “votes” on what translations it thinks it sees in a test image
Restricted Boltzmann Machine (2)

• 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.
Test Image – Ohio River (Ground-Based Radar)
Test Image – Pacific NW (Landsat5-TM)
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.
As a first test of this approach, we have trained a feed-forward network on both Ohio River radar image and Landsat images at various translations and rotations. Initial results look promising – the feed-forward network seems to be able to correctly identify the image translations and rotations.

Initial results appear to be better with a feed-forward network than for the RBM – image registration estimates appear to be of better accuracy.
Plans for Future Image Registration Work

• Since feed-forward network appears to produce the best results so far, we plan to focus our efforts in that direction

• Continue testing feed-forward network on real images

• The next major task will be to implement an algorithm on the D-Wave to compute the feed-forward network weights
Separable Haar Wavelet Transform using Quantum Annealing

Omar Shehab
Milton Halem
Samuel Lomonaco
Jacqueline LeMoigne
John Dorband
Motivation

• Aims
  – Develop a quantum annealing algorithm which performs separable Haar wavelet transform

• Motivation
  – The goal is to compress the image keeping the features intact
  – Registration is an important image processing problem
  – Capability of quantum annealing computers needs to be studied in solving earth science problems
  – Quantum algorithms need to be benchmarked against classical algorithms

• Related work
Quantum Annealing Approach

• Develop a multi qubit full adder
  – We have developed a programmable half adder
  – Currently studying the error rate of a single qubit full adder

• Generalize it for floating point subtraction
  – We take the complement of the subtrahend and add

• Use the full adder for Haar transform
  – We adopt a divide and conquer approach and use the full adder in a repetitive manner

• Evaluate performance
  – We compute the cost in terms of ancilla qubits and study the error rate
Result

Haar (single iteration)

Separable Haar

Quantum Separable Haar
Challenges

• A single bit full adder has been used repetitively
• Expanding a half adder into full adder redistributes the success probability over a larger space
• Expanding single bit full adder to multibit may worsen the success probability even more
• The network roundtrip time for single bit a multibit is prohibiting
• Larger full adder will take the input magnetic field strengths below the stable threshold
Future Directions

• A dedicated quantum accelerator with on board classical processing unit will save the round trip network time
• A fifth order interaction quantum annealing device will reduce the number of ancilla qubits significantly
• A higher precision needs to be allowed for input field strengths
Quantum Annealing Approach

• Develop a multi qubit full adder
  – We have developed a programmable half adder
  – Currently studying the error rate of a single qubit full adder

• Generalize it for floating point subtraction
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  – We compute the cost in terms of ancilla qubits and study the error rate
Thank You