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Delivering science and technology
to protect our nation
and promote world stability

Unraveling Quantum Annealers with Machine Learning

Marc Vuffray, PIML 2018

Joint work with A. Lokhov, Y. Kharkov, C. Coffrin, M. Chertkov, S. Misra

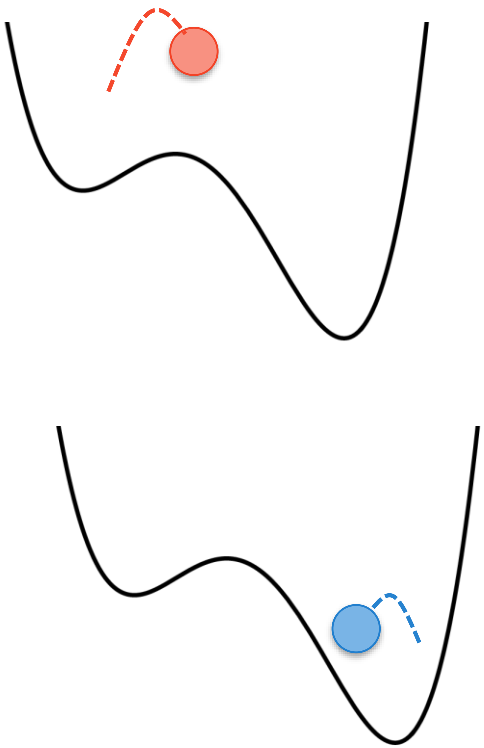
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

LA-UR-18-20555

Quantum Annealing

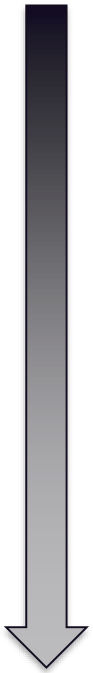
Quantum Annealing is a Global Optimization Heuristic

Classical Annealing:

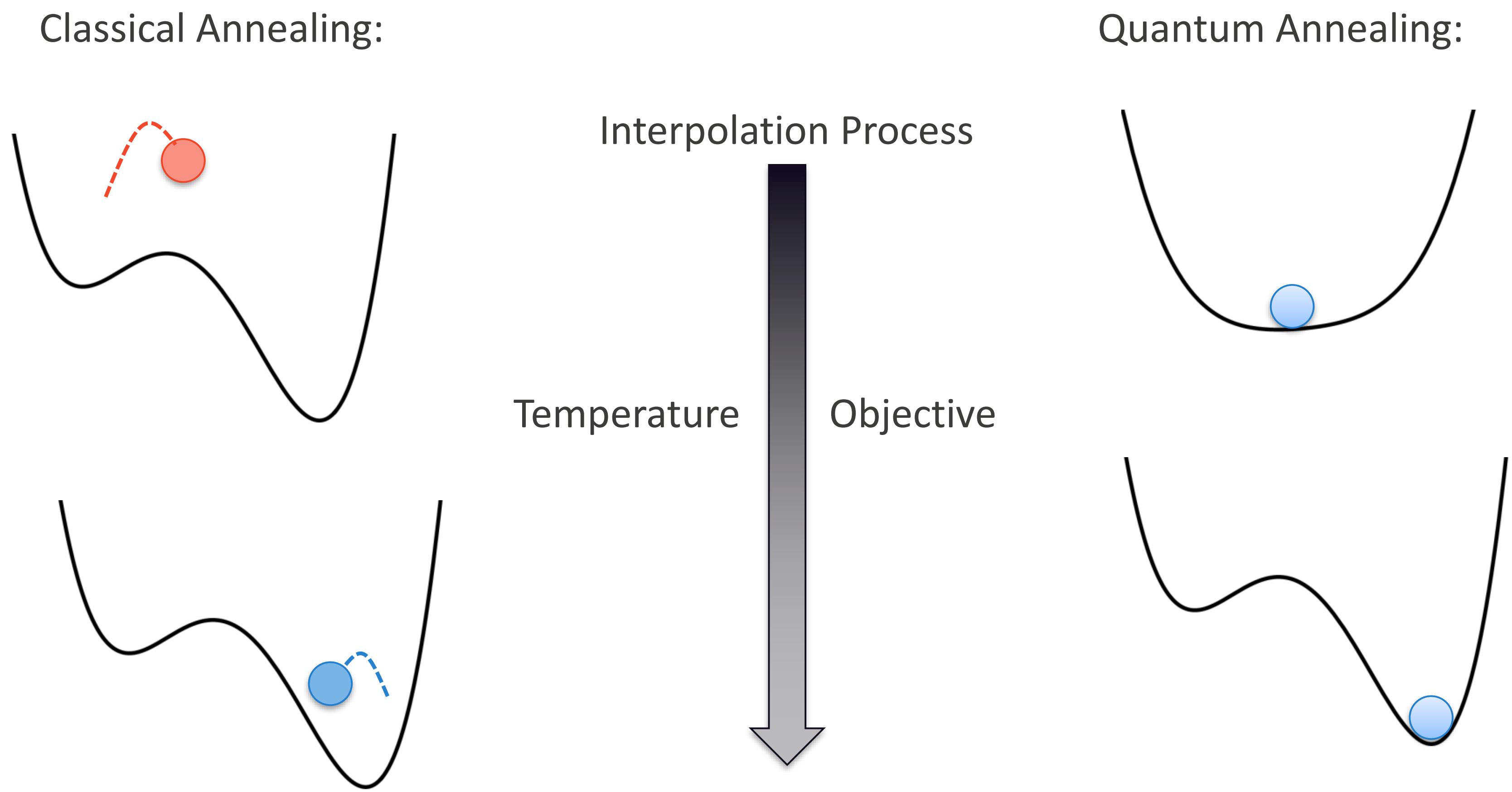


Interpolation Process

Temperature



Quantum Annealing is a Global Optimization Heuristic



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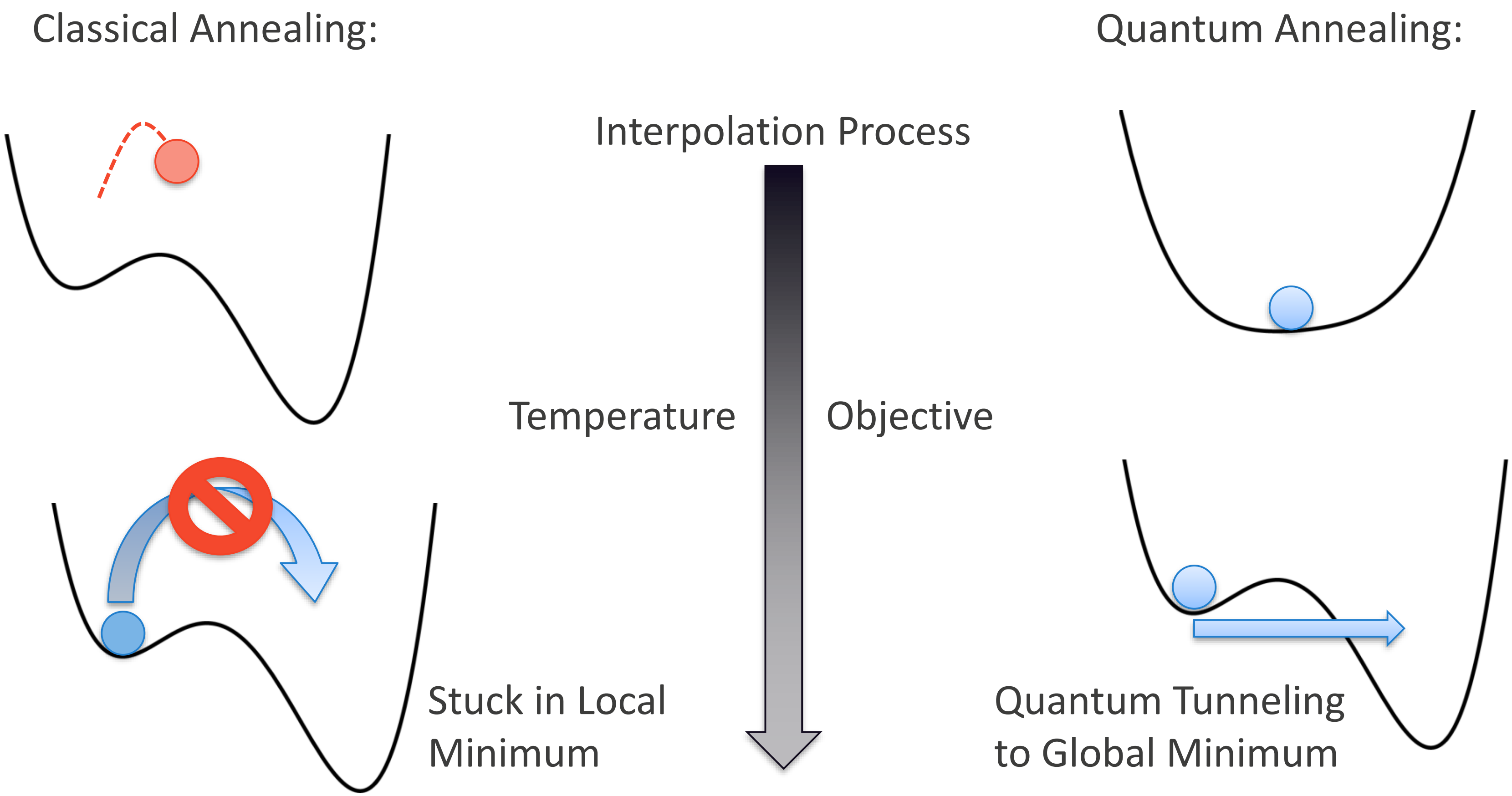

Quantum Annealing for Solving QUBO

Quadratic
Unconstrained
Binary
Optimization

Quantum Annealing for Solving QUBO

Quadratic
Unconstrained
Binary
Optimization

$$\arg\min_{\underline{x}} \sum_{i=1}^{N} b_i x_i + \sum_{i=1}^{N} \sum_{j=1}^{i} a_{ij} x_i x_j$$

$$\text{s.t.} \quad \forall i, x_i \in \{0,1\}$$

Input: $a_{ij}, b_i \in \mathbb{R}$

Output: $x_i \in \{0,1\}$

Quantum Annealing for Solving QUBO

Quadratic
Unconstrained
Binary
Optimization

$$\arg\min_{\underline{x}} \sum_{i=1}^{N} b_i\, x_i + \sum_{i=1}^{N} \sum_{j=1}^{i} a_{ij}\, x_i\, x_j$$

s.t. $\forall i, x_i \in \{0,1\}$

Input: $a_{ij}, b_i \in \mathbb{R}$

Output: $x_i \in \{0,1\}$

NP Hard

General class of combinatorial problems

$$E(\underline{x}) = b^T \underline{x} + \underline{x}^T A \underline{x}$$

QUBO = Finding Ground States of Ising Models

Quadratic
Unconstrained
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Ground States
of Ising Models

$$\arg\min_{\underline{\sigma}} \sum_{i=1}^{N} h_i\, \sigma_i + \sum_{i=1}^{N} \sum_{j=1}^{i} J_{ij}\, \sigma_i\, \sigma_j$$

$$\text{s.t.} \quad \forall i, \sigma_i \in \{-1,+1\}$$

Input: $J_{ij}, h_i \in \mathbb{R}$

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Input: $J_{ij}, h_i \in \mathbb{R}$

Output: $\sigma_i \in \{-1, +1\}$

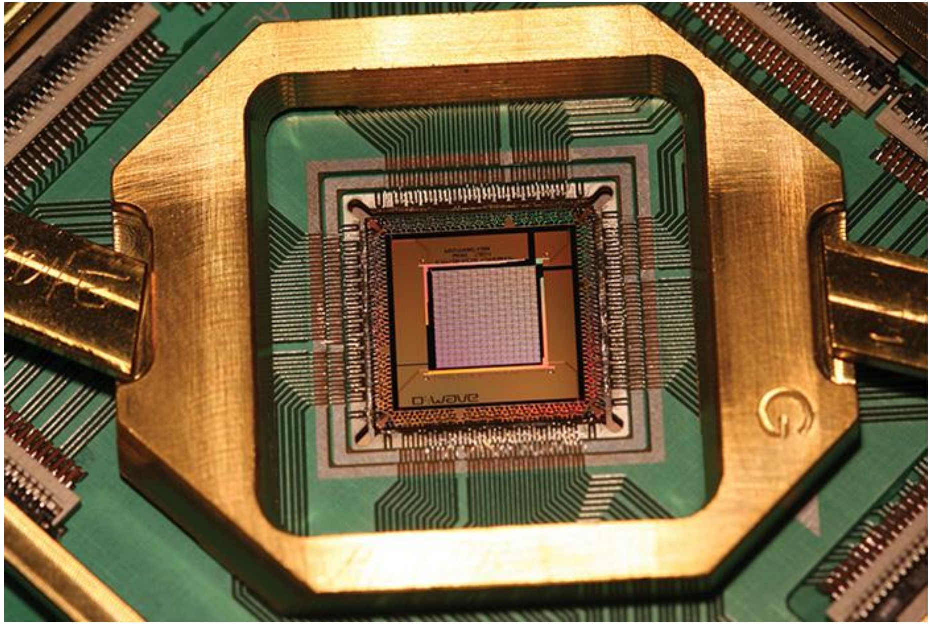
Magnetic field = h_i

Coupler = J_{ij}

Spin = σ_i

The D-Wave Implementation

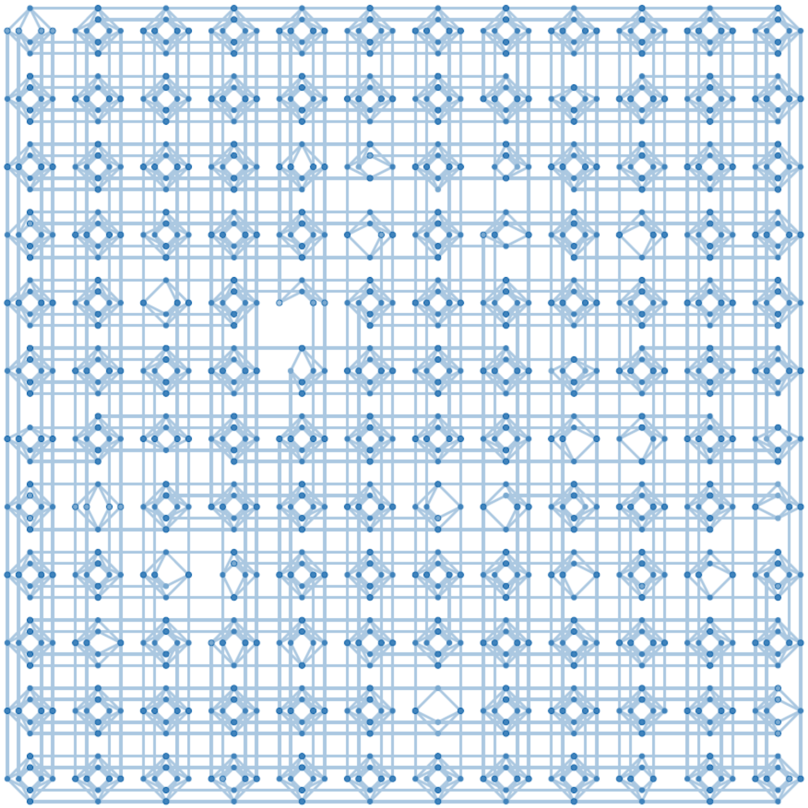
D-Wave: A Quantum Annealer for Solving QUBO



# of qubits	1,095 (95.1%)
# of couplers	3,061 (91.1%)
Temperature	10.45 mK

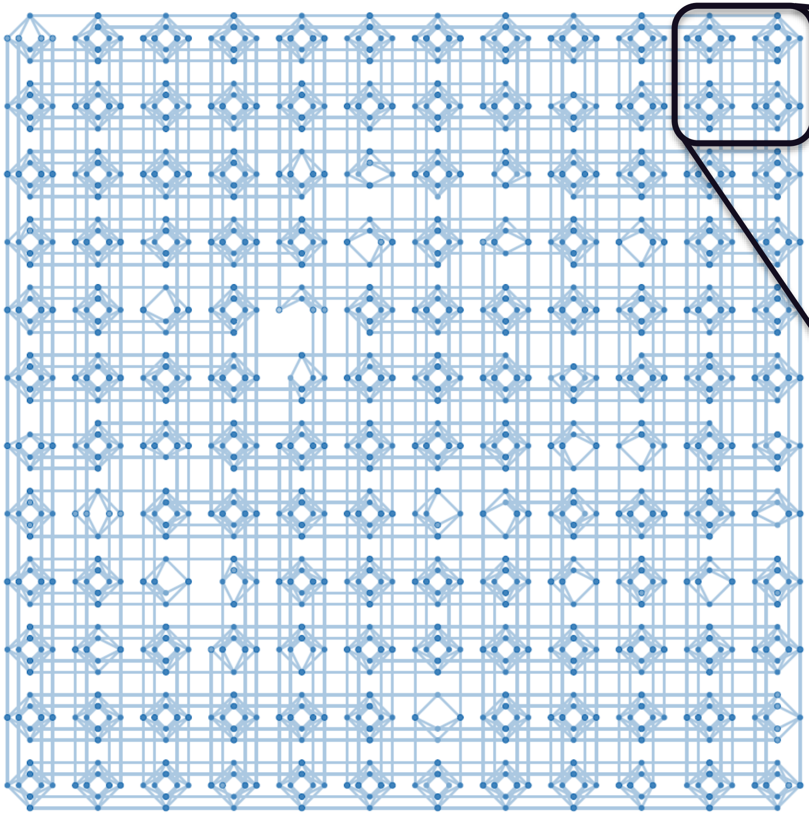
Annealing time	5–2000 μs
h range	[-2, +2]
J range	[-1, +1]

The Set of Possible Couplings: A Bipartite Graph



Ensemble of Spins and Couplers

The Set of Possible Couplings: A Bipartite Graph



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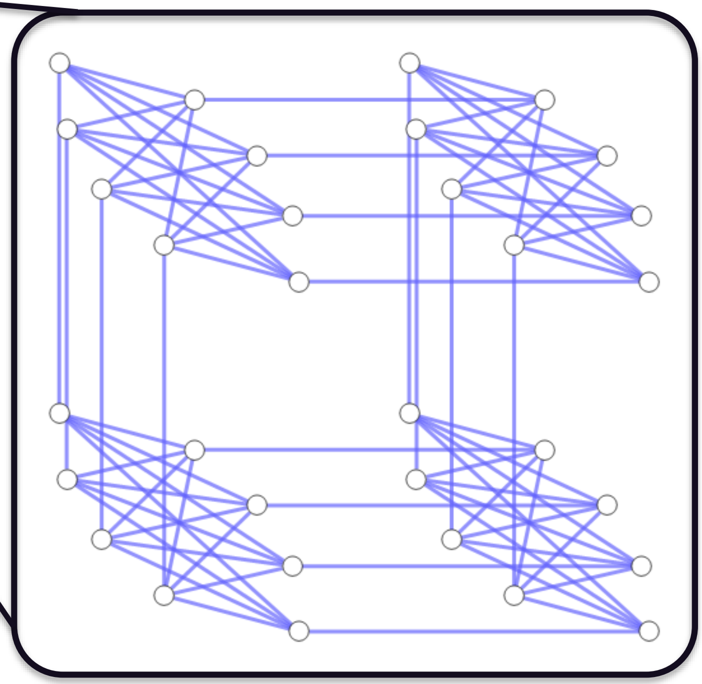

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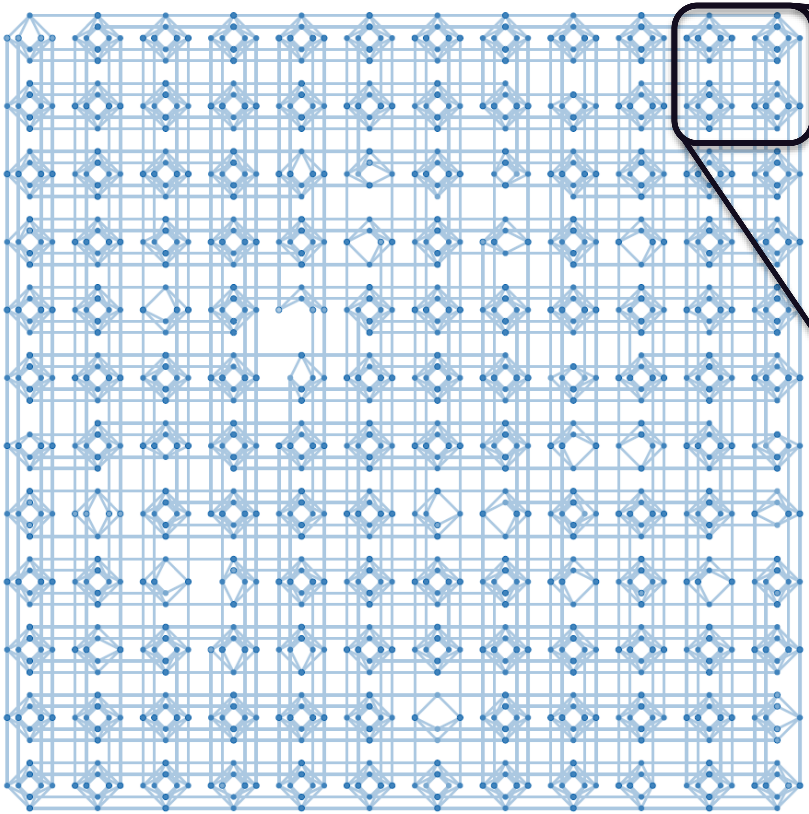

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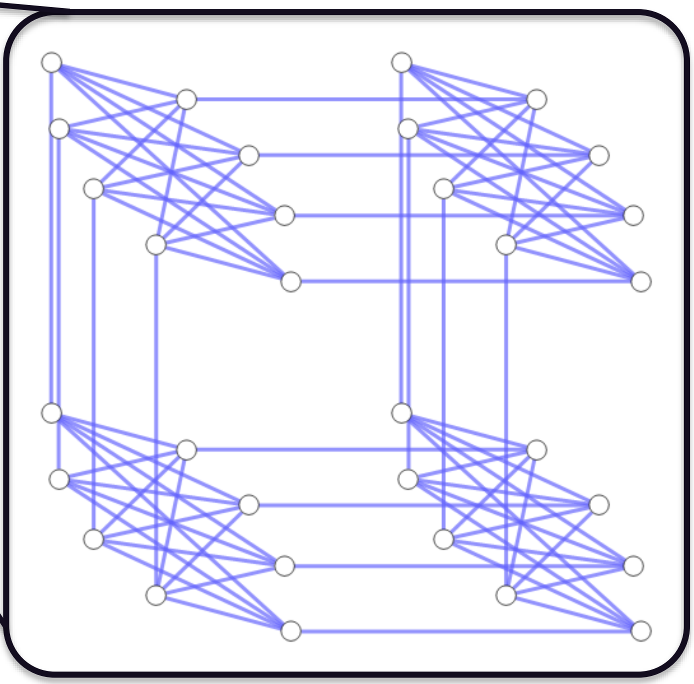
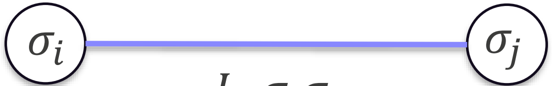




$J_{ij}\sigma_i\sigma_j$

Programming the D-Wave

Input

Couplings J_{ij}

Fields h_i

→

Annealing

D-Wave — The Quantum Computing Company™

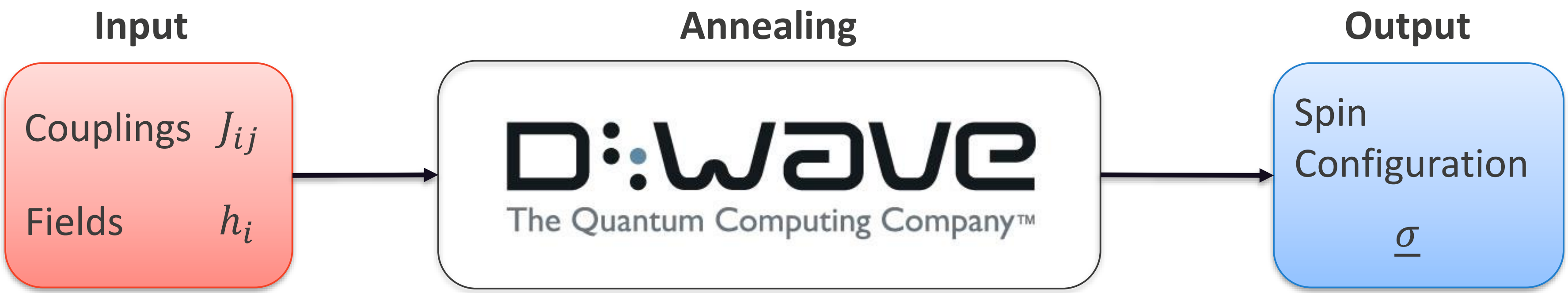
→

Output

Spin Configuration

$\underline{\sigma}$

Programming the D-Wave



Question 1: Can we characterize the probability distribution on $\underline{\sigma}$?

Programming the D-Wave

Input

Couplings J_{ij}

Fields h_i

Annealing

D:Wave The Quantum Computing Company™

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Spin Configuration

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Question 1: Can we characterize the probability distribution on $\underline{\sigma}$?

Question 2: What can we learn about the machine from the probability distribution?

Programming the D-Wave

Input

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Fields h_i

Annealing

The Quantum Computing Company™

Output

Spin Configuration $\underline{\sigma}$

Question 1: Can we characterize the probability distribution on $\underline{\sigma}$?

Inverse Problem

Question 2: What can we learn about the machine from the probability distribution?

Interaction Screening for Solving Inverse Problems

The Generalized Inverse Ising Problem

Random spin configurations: $\underline{\sigma} \in \{-1, +1\}^N$

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Inverse Ising = **Learning** $\boldsymbol{h}$ & $\boldsymbol{J}$ from **i.i.d. samples** $\underline{\sigma}^{(1)}, \underline{\sigma}^{(2)}, \ldots, \underline{\sigma}^{M}$

The Restricted Interaction Screening Estimator (RISE)

Estimated couplings are the results of a convex optimization:

$$\arg\min_{h,J} \mathbb{E}\left[\exp\left(-\sum_{i} h_i\sigma_i - \sum_{ij} J_{ij}\sigma_i\sigma_j - \sum_{ijk} J_{ijk}\sigma_i\sigma_j\sigma_k - \sum_{ijkl} J_{ijkl}\sigma_i\sigma_j\sigma_k\sigma_l - \cdots\right)\right]$$

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NIPS (2016)

Interaction Screening: Efficient and Sample-Optimal Learning of Ising Models

M. Vuffray, S. Misra, A. Lokhov, M. Chertkov

SciAdv AAAS (In press)

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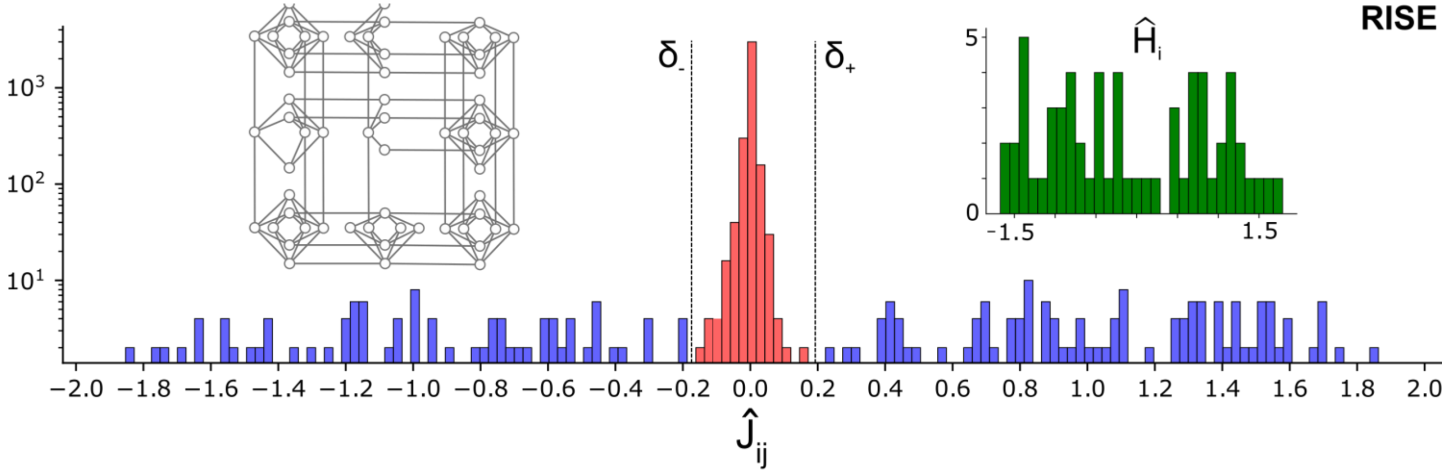
GitHub https://github.com/lanl-ansi/inverse_ising

Comparing RISE with Mean Field Methods



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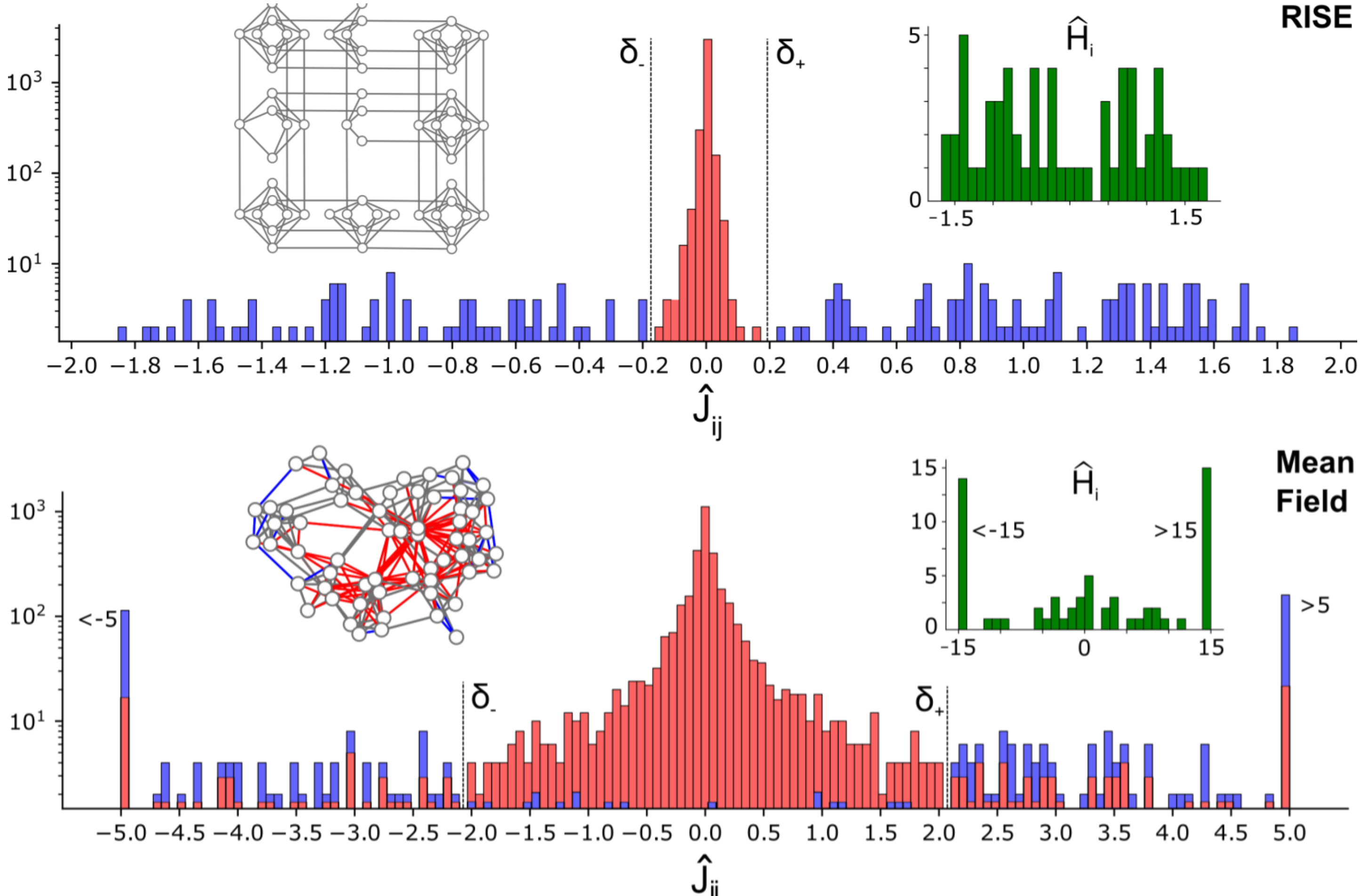

Going Back to Studying D-Wave

Input

Couplings J_{ij}

Fields h_i

Annealing

The Quantum Computing Company™

Output

Spin Configuration $\underline{\sigma}$

✓ **Question 1:** Can we characterize the probability distribution on $\underline{\sigma}$?

Inverse Problem

Question 2: What can we learn about the machine from the probability distribution?

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D-Wave The Quantum Computing Company™

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- **Multi-Body Interactions? (orders >2?)**

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D:WAVE
The Quantum Computing Company™

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- **Multi-Body Interactions? (orders >2?)**
- **Structure of Interactions?**
- **Couplings Input-Output Response?**

Type of Multi-Body Interactions

What are Multi-Body Interactions?

Random spin configurations: $\underline{\sigma} \in \{-1, +1\}^N$

with probability distribution:

$$\mu(\underline{\sigma}) \propto \exp\left(\underbrace{\sum_i h_i \sigma_i}_{1^{st}\ \text{Order}} + \underbrace{\sum_{ij} J_{ij} \sigma_i \sigma_j}_{2^{nd}\ \text{Order}} + \underbrace{\sum_{ijk} J_{ijk} \sigma_i \sigma_j \sigma_k}_{3^{rd}\ \text{Order}} + \underbrace{\sum_{ijkl} J_{ijkl} \sigma_i \sigma_j \sigma_k \sigma_l}_{4^{th}\ \text{Order}} + \cdots \right)$$

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Single Spin Term

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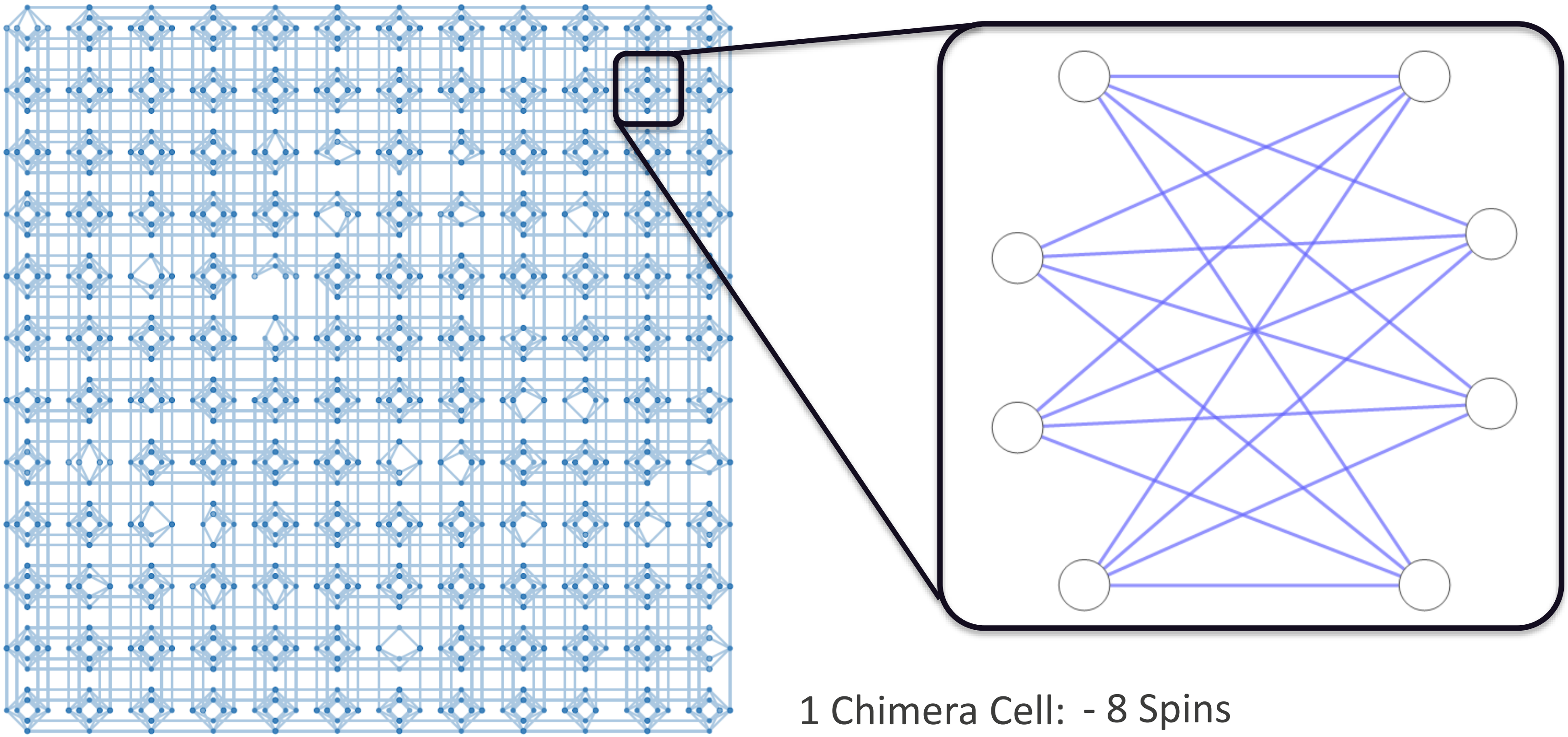
Single Spin Term

Multi-Body Interactions

Bias or Prior

Conditional Dependences

Multi-Body Interactions: Results on Chimera Cell



1 Chimera Cell: - 8 Spins

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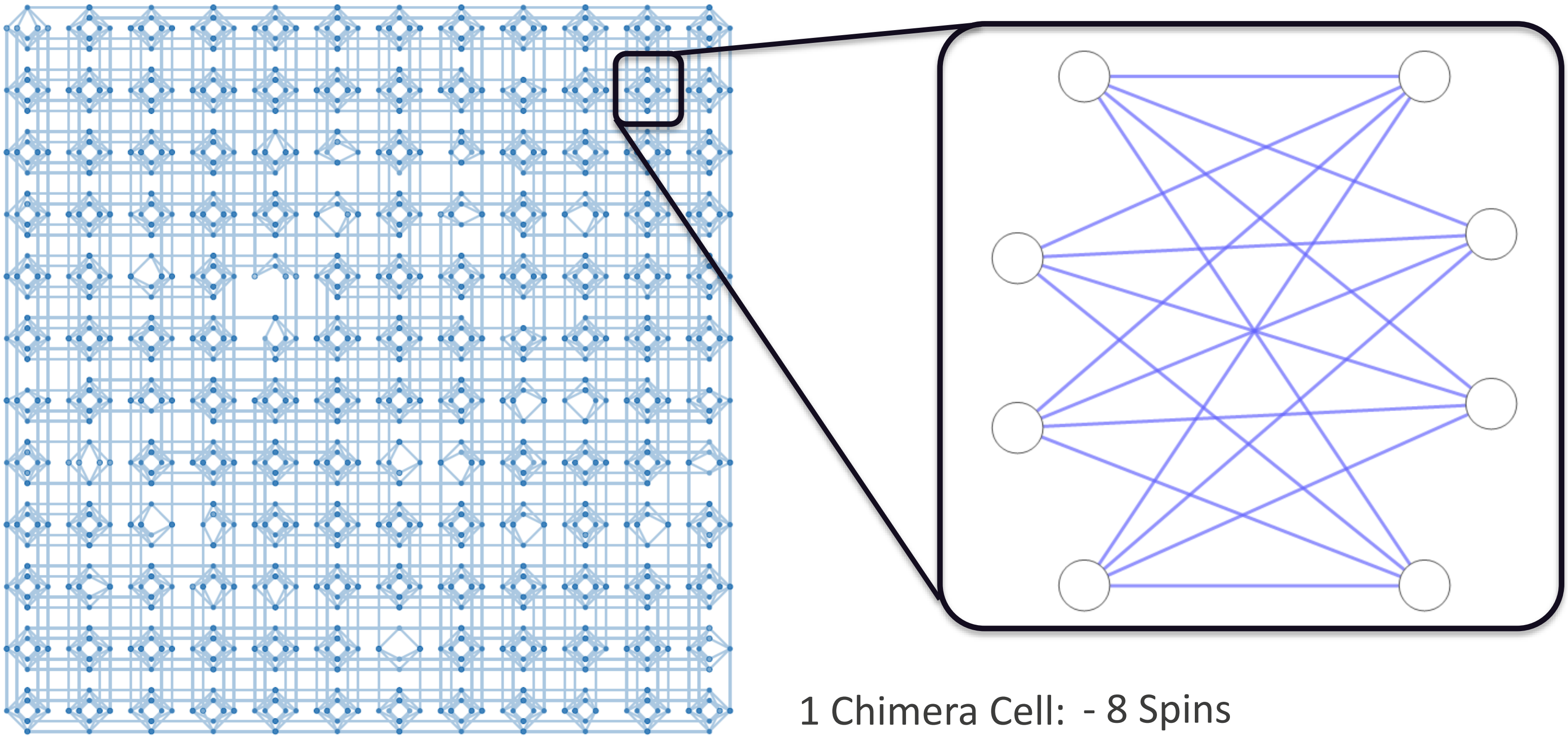
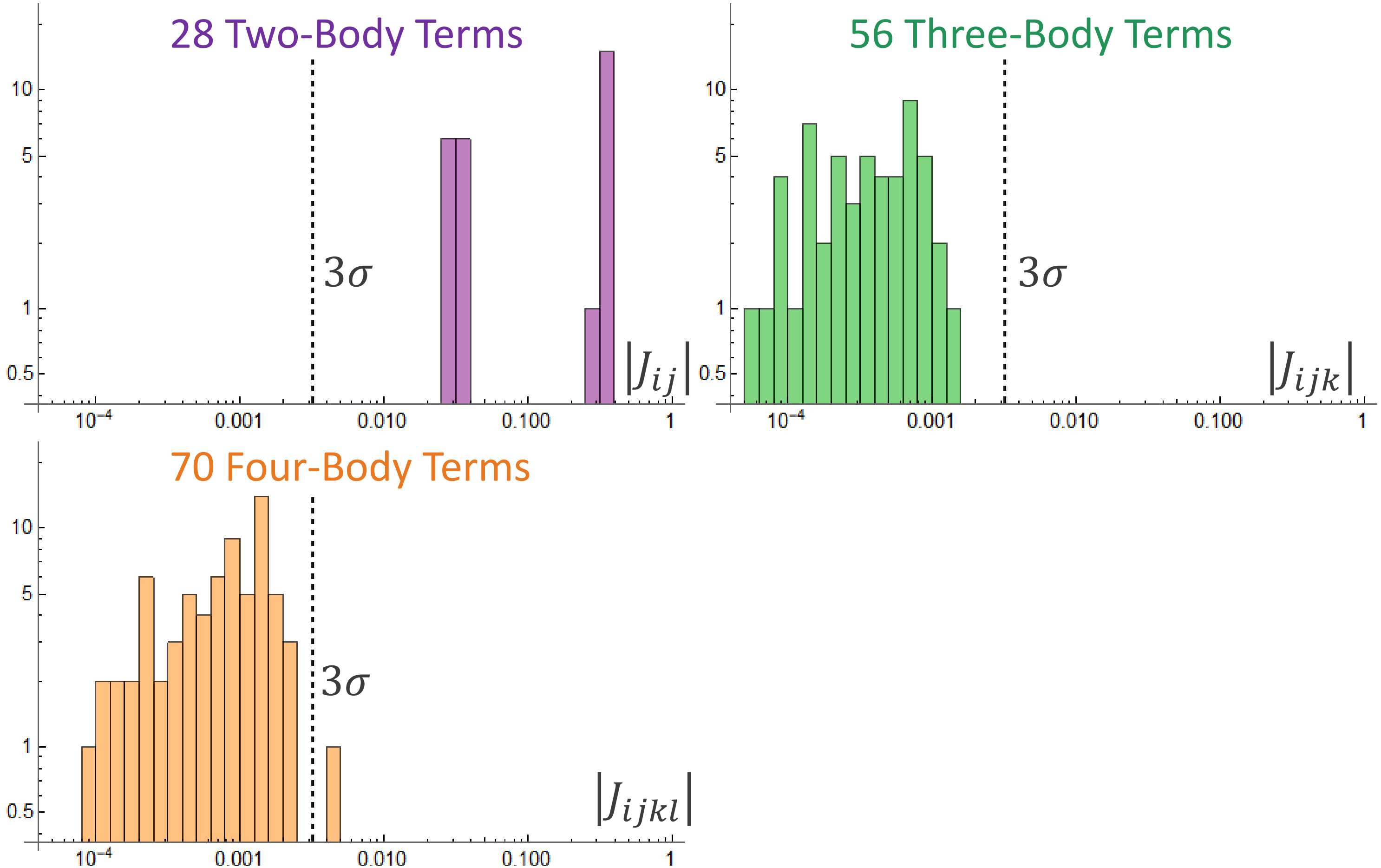


1 Chimera Cell:
- 8 Spins
- 16 **Input** Couplers set to 0.025
- 0 **Input** Magnetic Fields

Log-Histogram of Reconstructed Multi-Interactions



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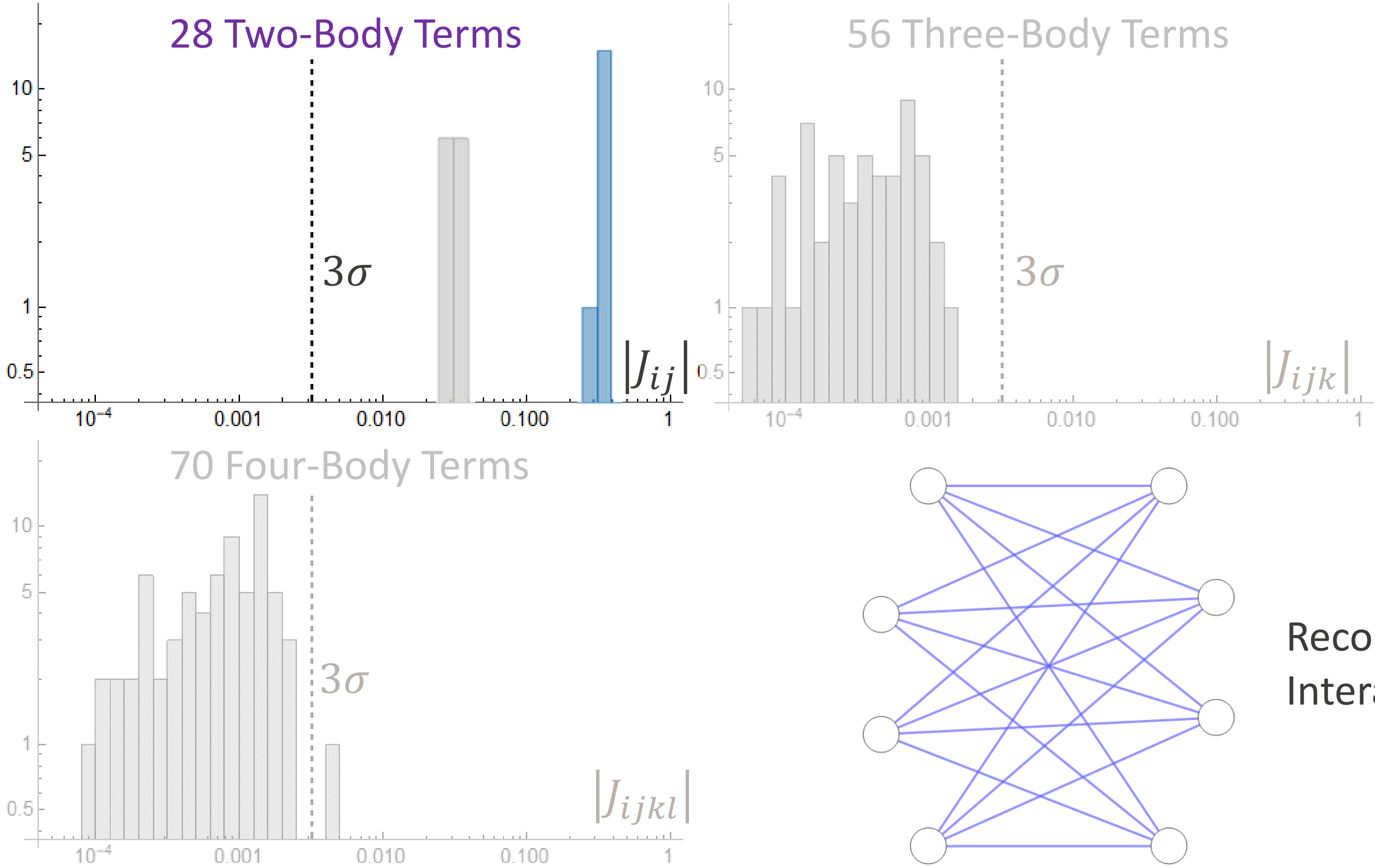

Reconstructed Interactions

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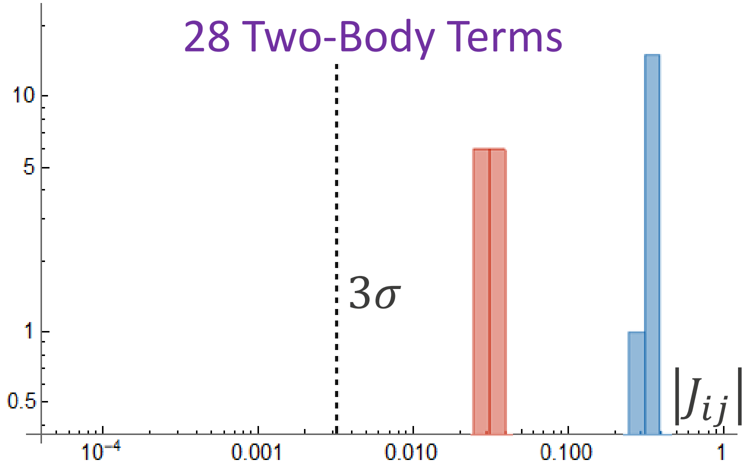

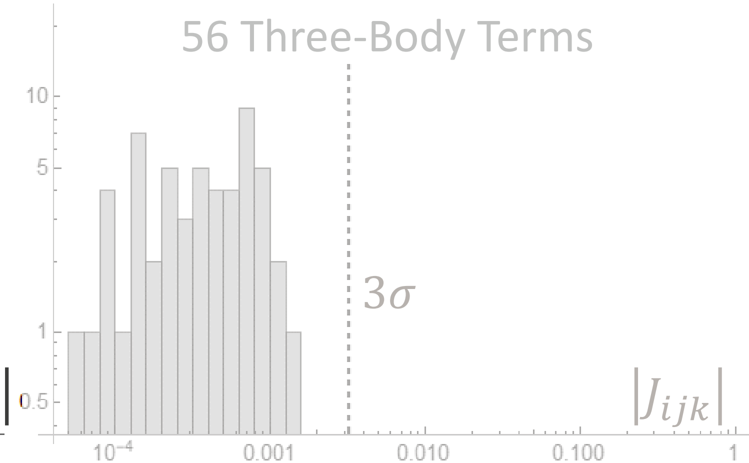

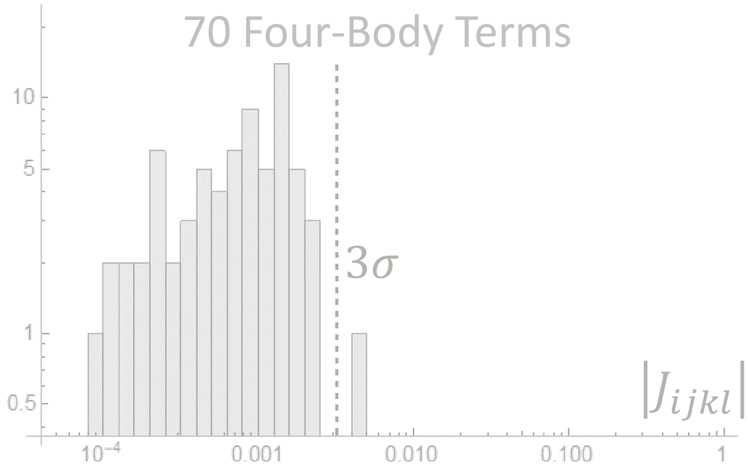

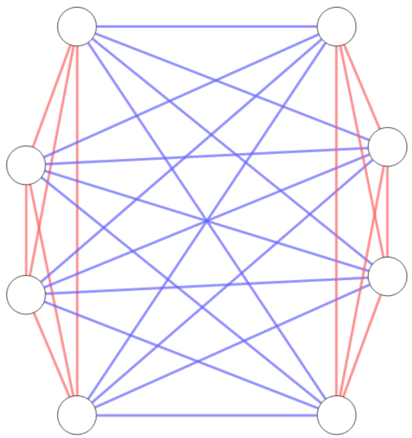

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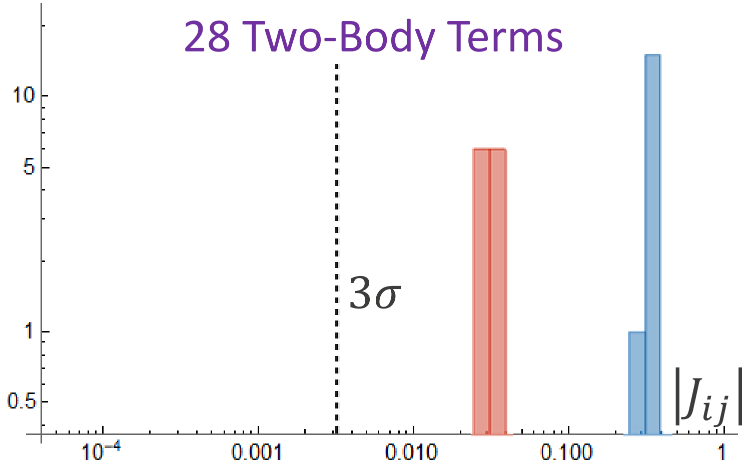

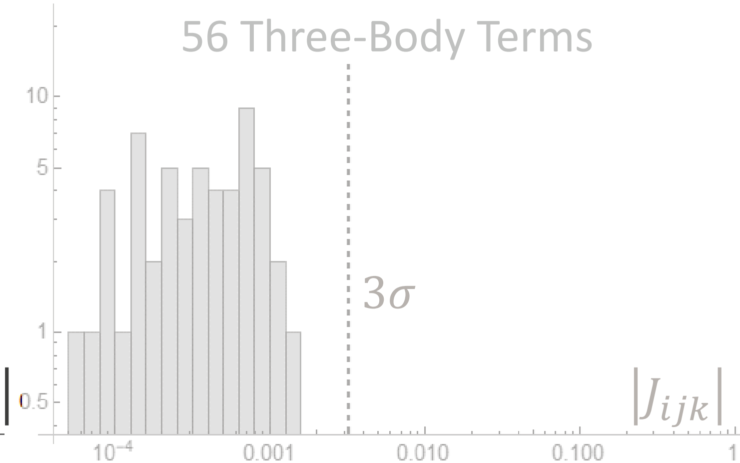

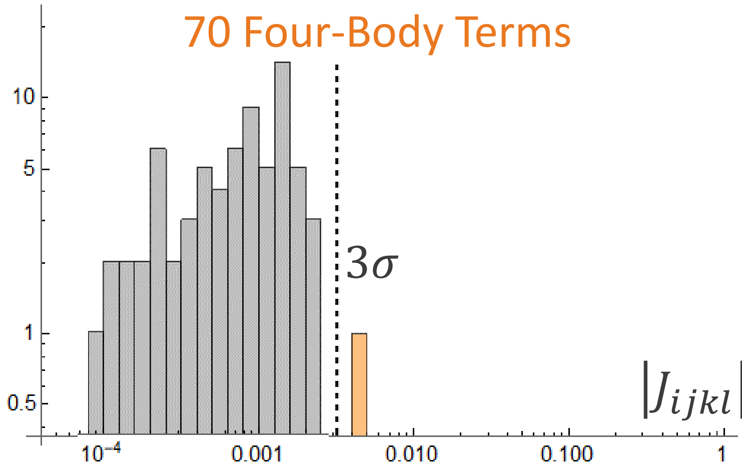

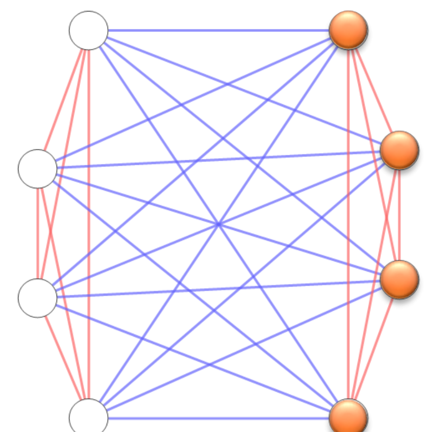

Reconstructed Interactions

Conclusion: Pair Interactions are Dominant

D-Wave Random Configurations: $\underline{\sigma} \in \{-1, +1\}^N$

have probability distribution:

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Single Spin Term

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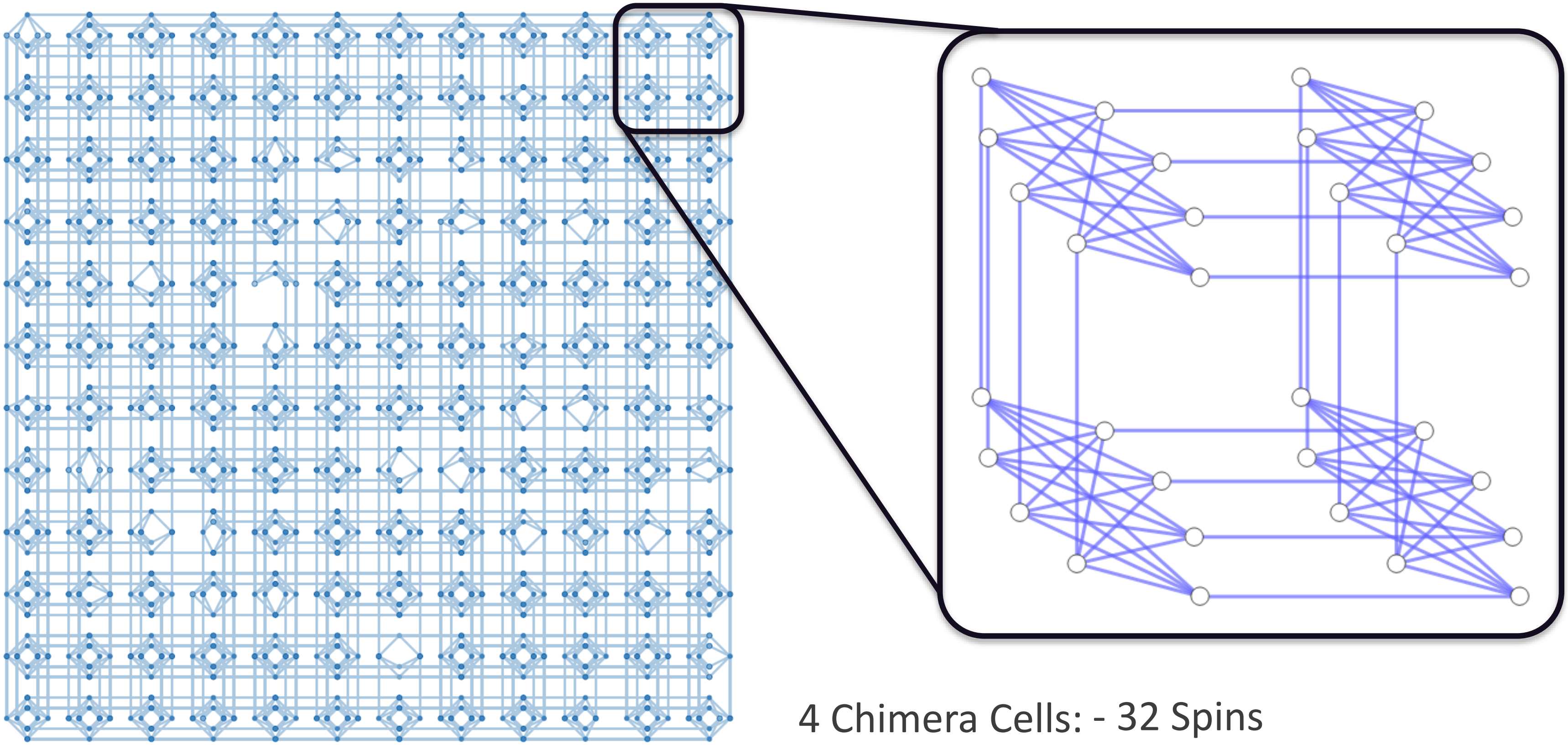
Single Spin Term

Pair Interactions

Question: What is the structure spanned by pair interactions?

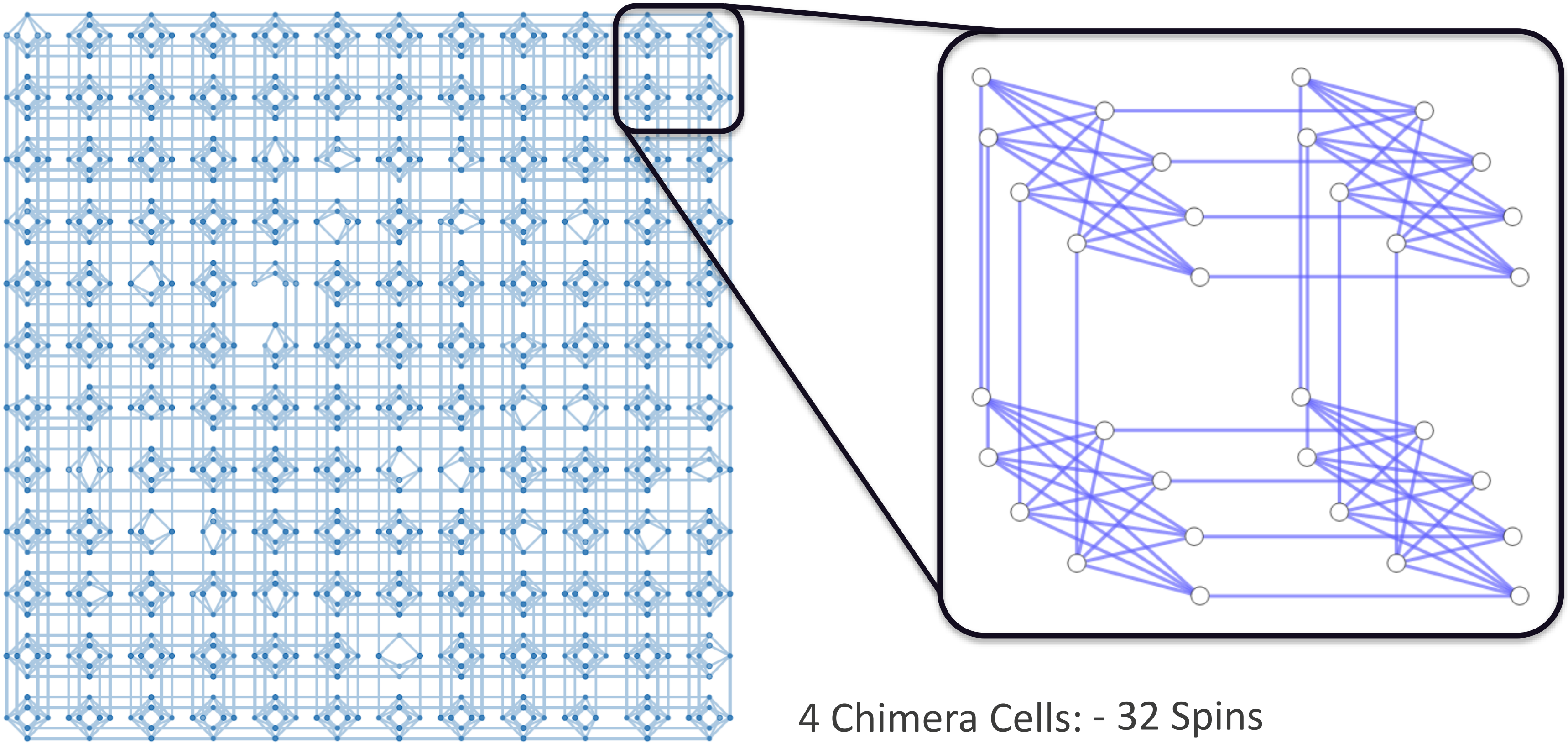
The Structure of the Two-Body Interactions

Pair Interactions: Results on 4 Chimera Cells



4 Chimera Cells: - 32 Spins

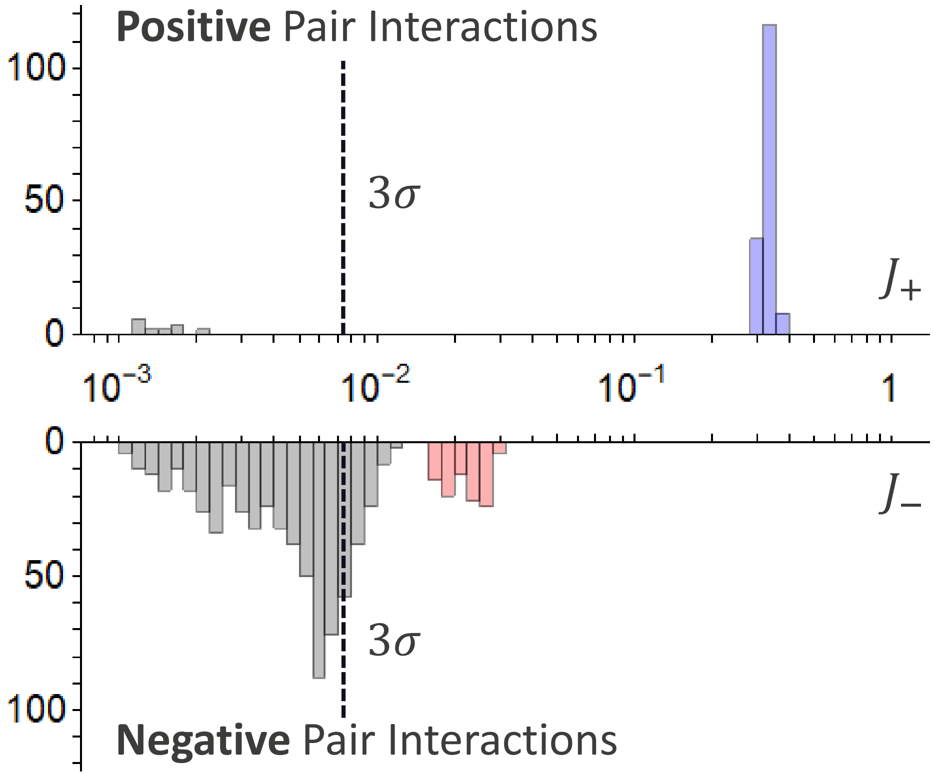
Pair Interactions: Results on 4 Chimera Cells



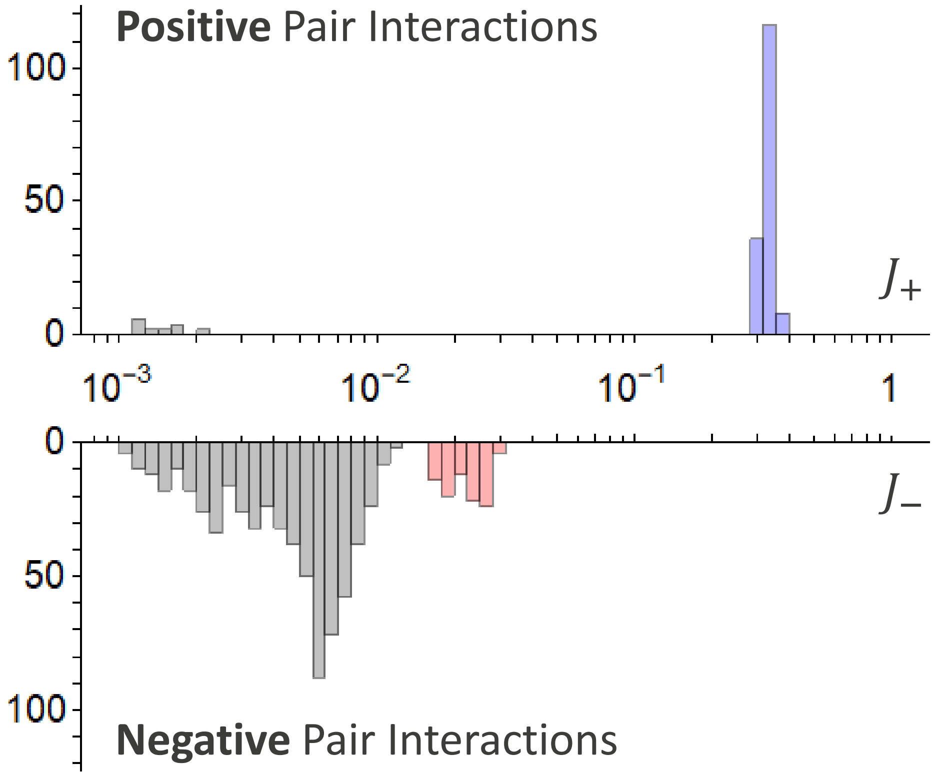
4 Chimera Cells: - 32 Spins

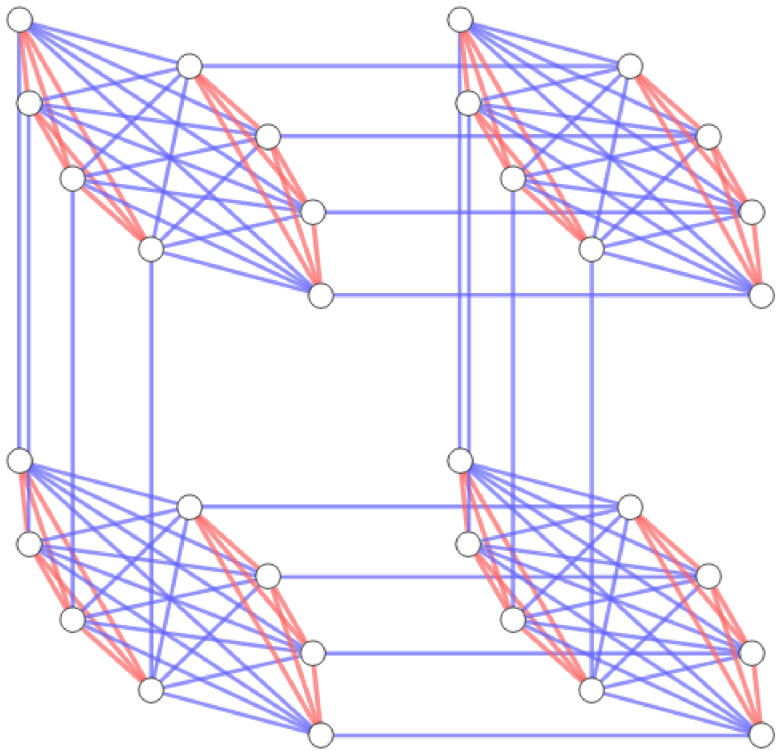
- 80 **Input** Couplers set to 0.025
- 0 **Input** Magnetic Fields

The Structure of Pair-Interactions



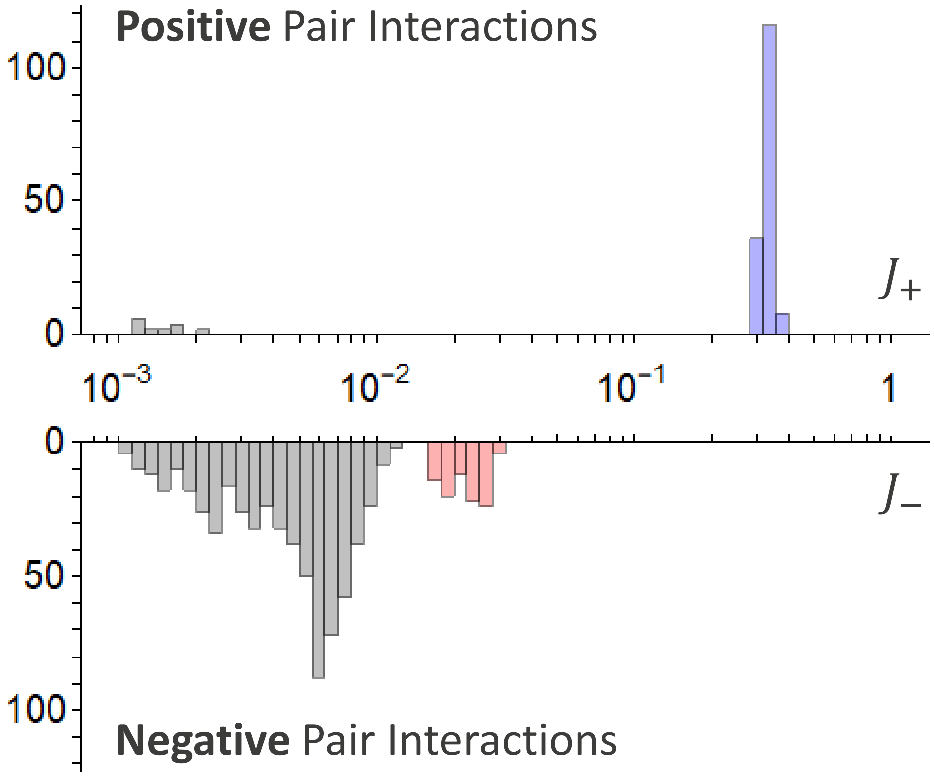
The Structure of Pair-Interactions

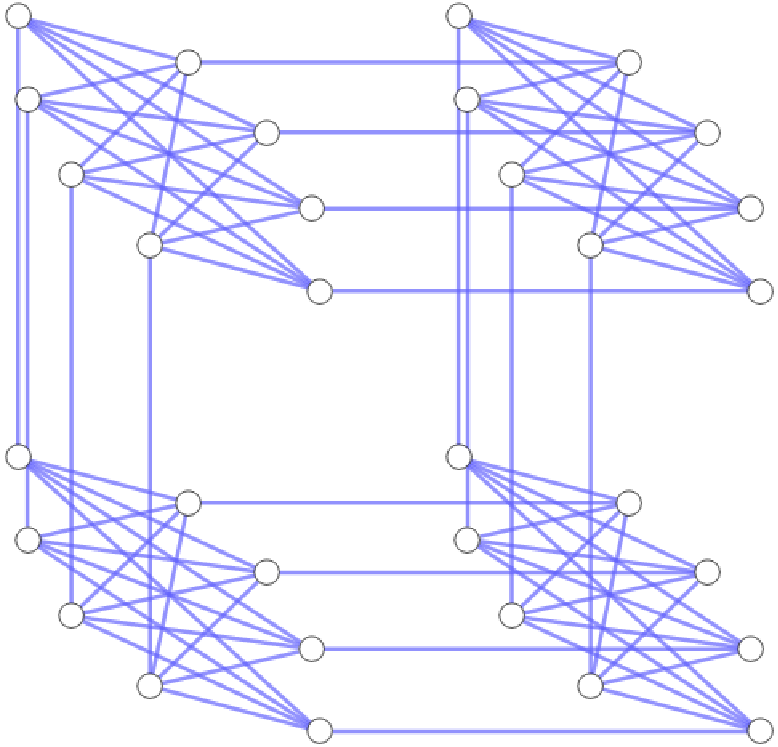




Reconstructed **Structure**

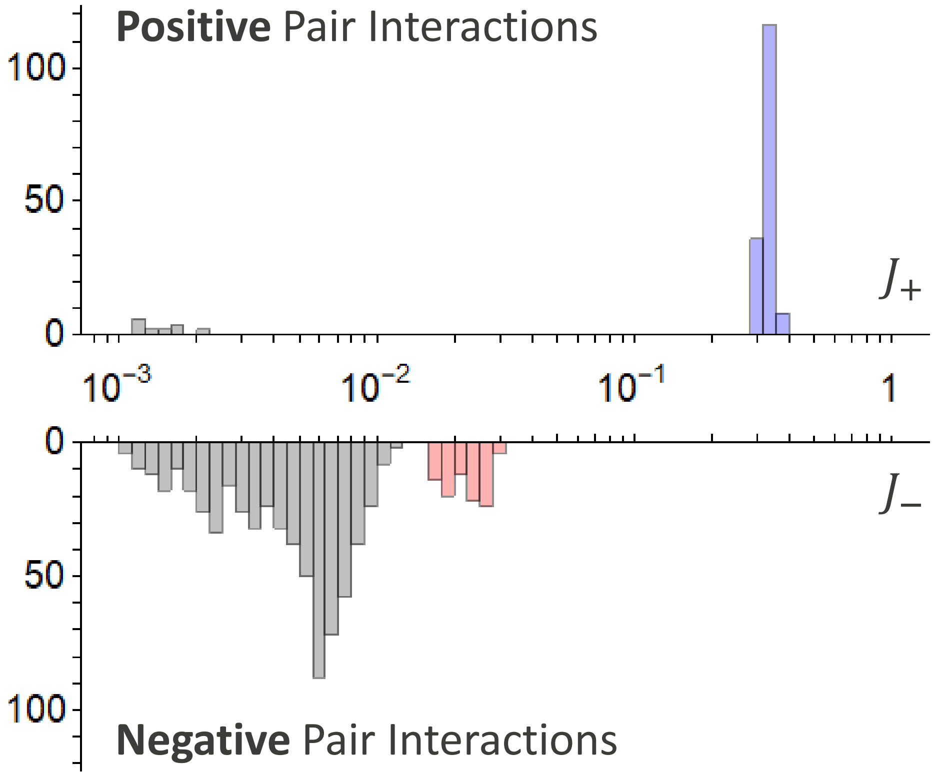
The Structure of Pair-Interactions

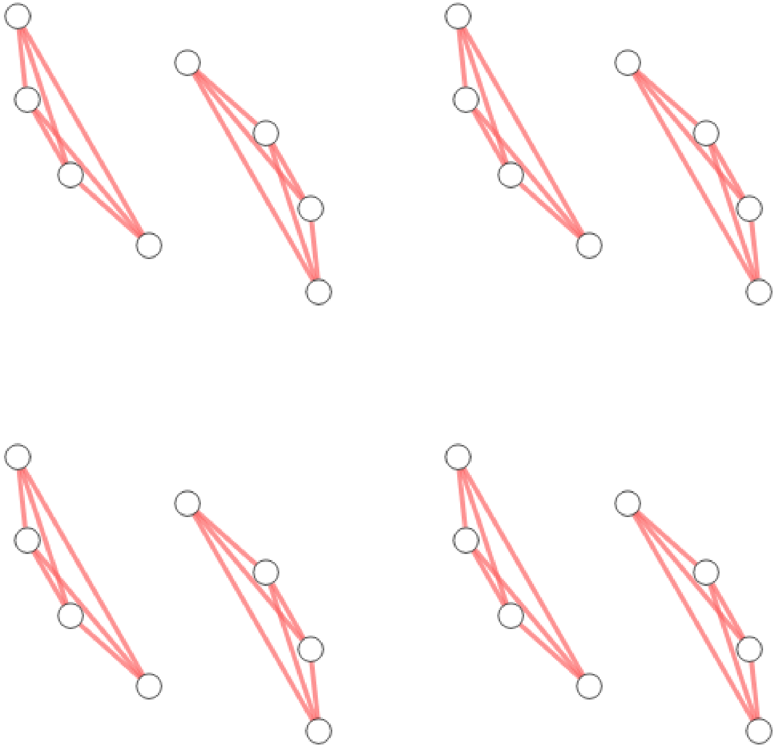




Most **Significant** Interactions ≡ D-Wave **Couplers**

The Structure of Pair-Interactions

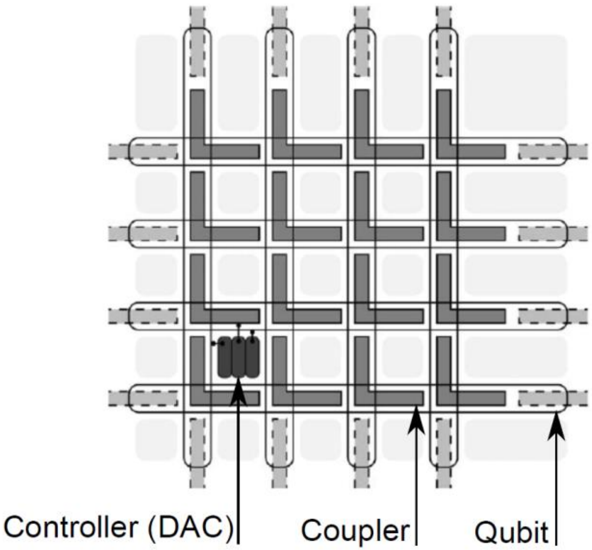




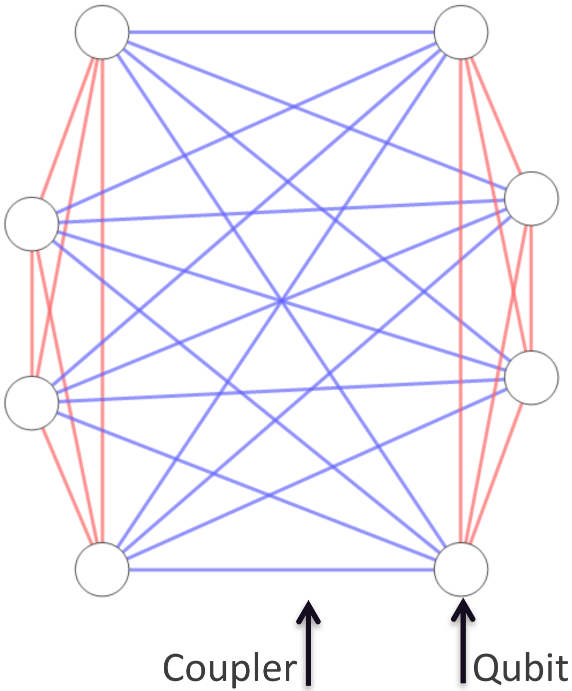
Weak **Spurious** Interactions between Spins

Spurious Interactions & Echo of the Chip Architecture

Chimera Cell Controller



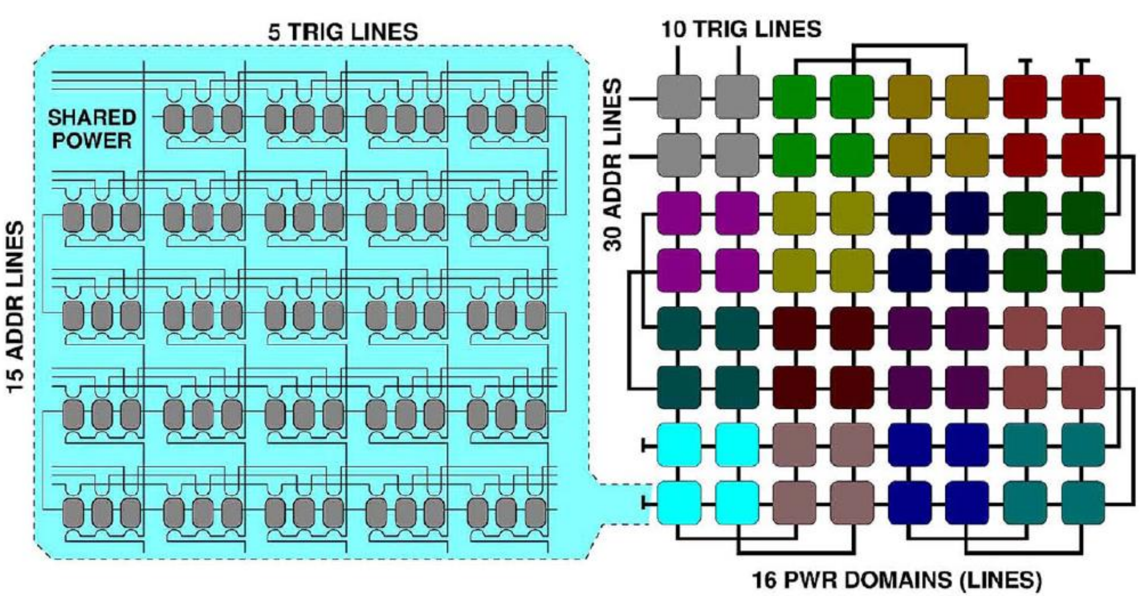
Reconstructed Cell



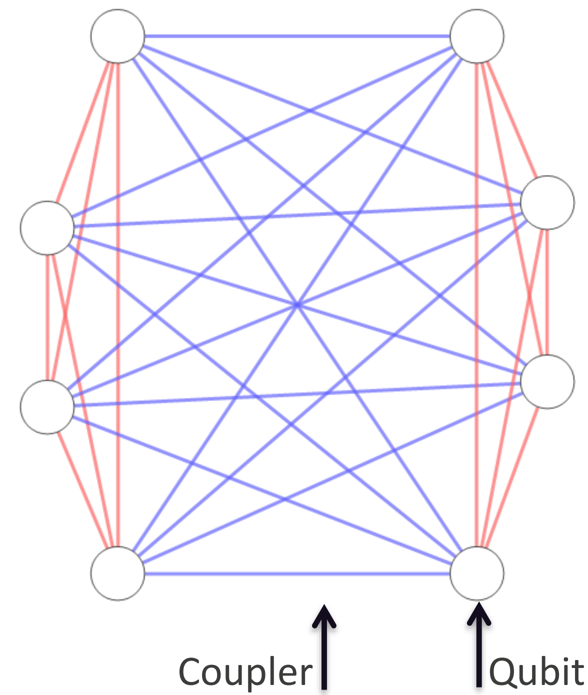
Reference & figure credit: [Bunyk et al., *IEEE Trans. Appl. Supercond.* (2014)]

Spurious Interactions & Echo of the Chip Architecture

Power Lines for Controllers



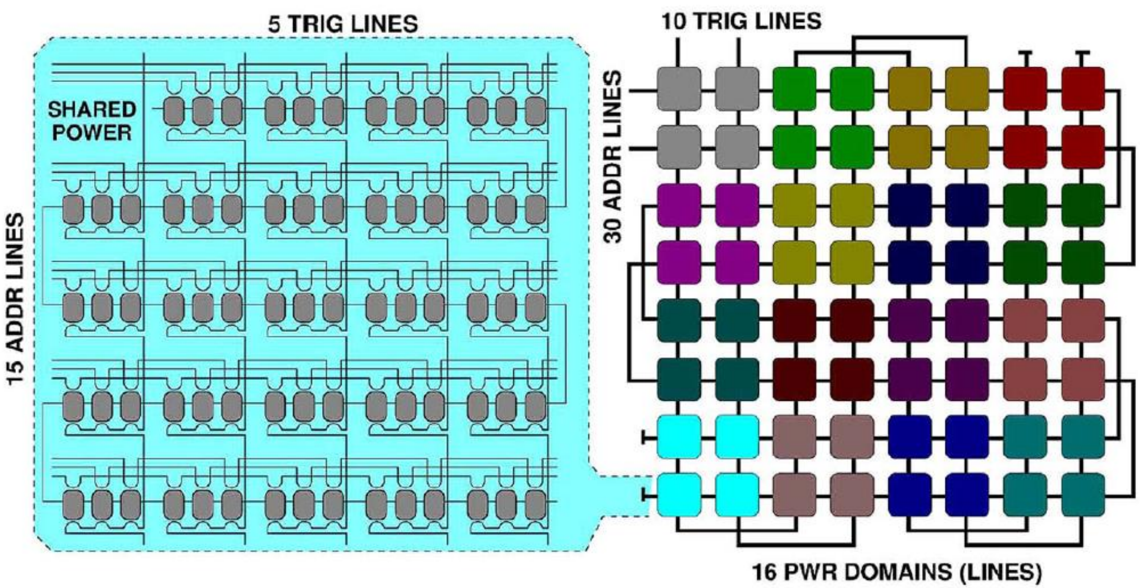
Reconstructed Cell



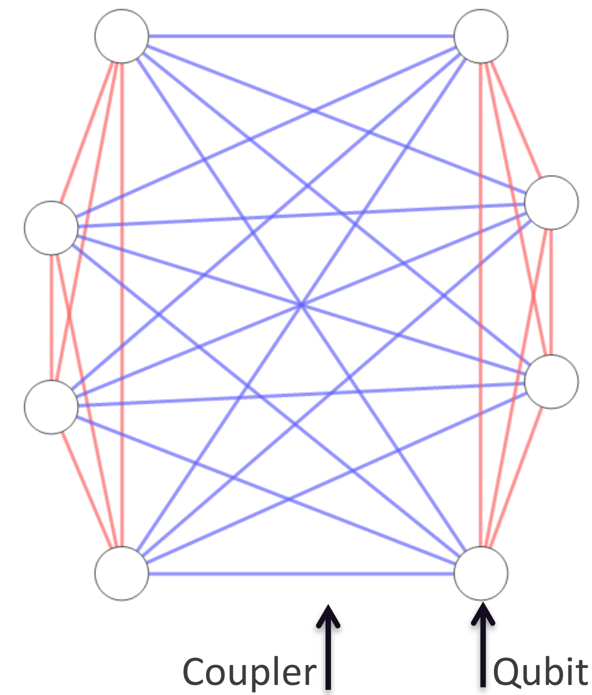
Reference & figure credit: [Bunyk et al., *IEEE Trans. Appl. Supercond.* (2014)]

Spurious Interactions & Echo of the Chip Architecture

Hypothesis: **Spurious** Interactions Reflects **Shared Control** Lines



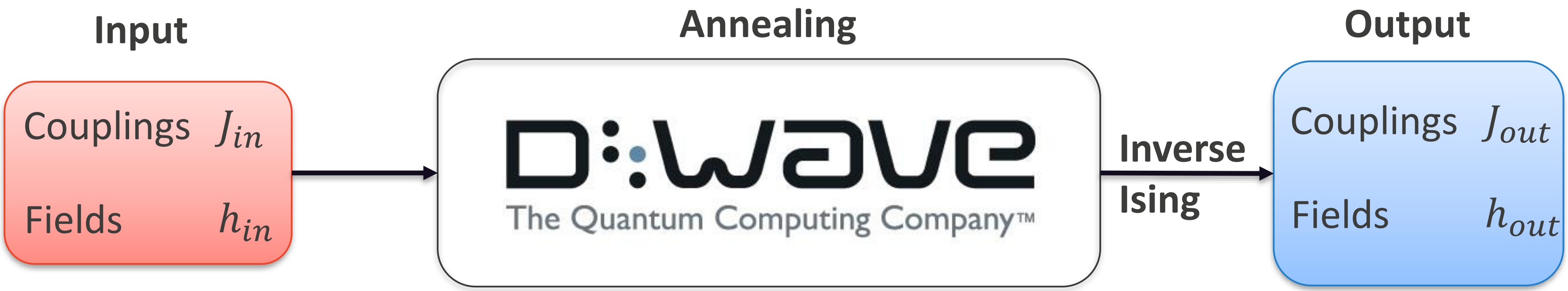
Reconstructed Cell



Reference & figure credit: [Bunyk et al., *IEEE Trans. Appl. Supercond.* (2014)]

Coupling Input-Output Response

What is the Input-Output Response?



What is the Input-Output Response?

Single Scaling (temperature) response:

$$h_{out} = \beta_{eff} h_{in}$$

$$J_{out} = \beta_{eff} J_{in}$$

Benedetti et al. *Phys. Rev. A,* (2016)
Raymond et al. *Front. In ICT,* (2017)
Marshall et al. *arXiv,* (2017)

What is the Input-Output Response?

Input

Couplings J_{in}

Fields h_{in}

Annealing

D:Wave The Quantum Computing Company™

Inverse Ising

Output

Couplings J_{out}

Fields h_{out}

Single Scaling (temperature) response:

$$h_{out} = \beta_{eff} h_{in}$$

$$J_{out} = \beta_{eff} J_{in}$$

Benedetti et al. *Phys. Rev. A,* (2016)

Raymond et al. *Front. In ICT,* (2017)

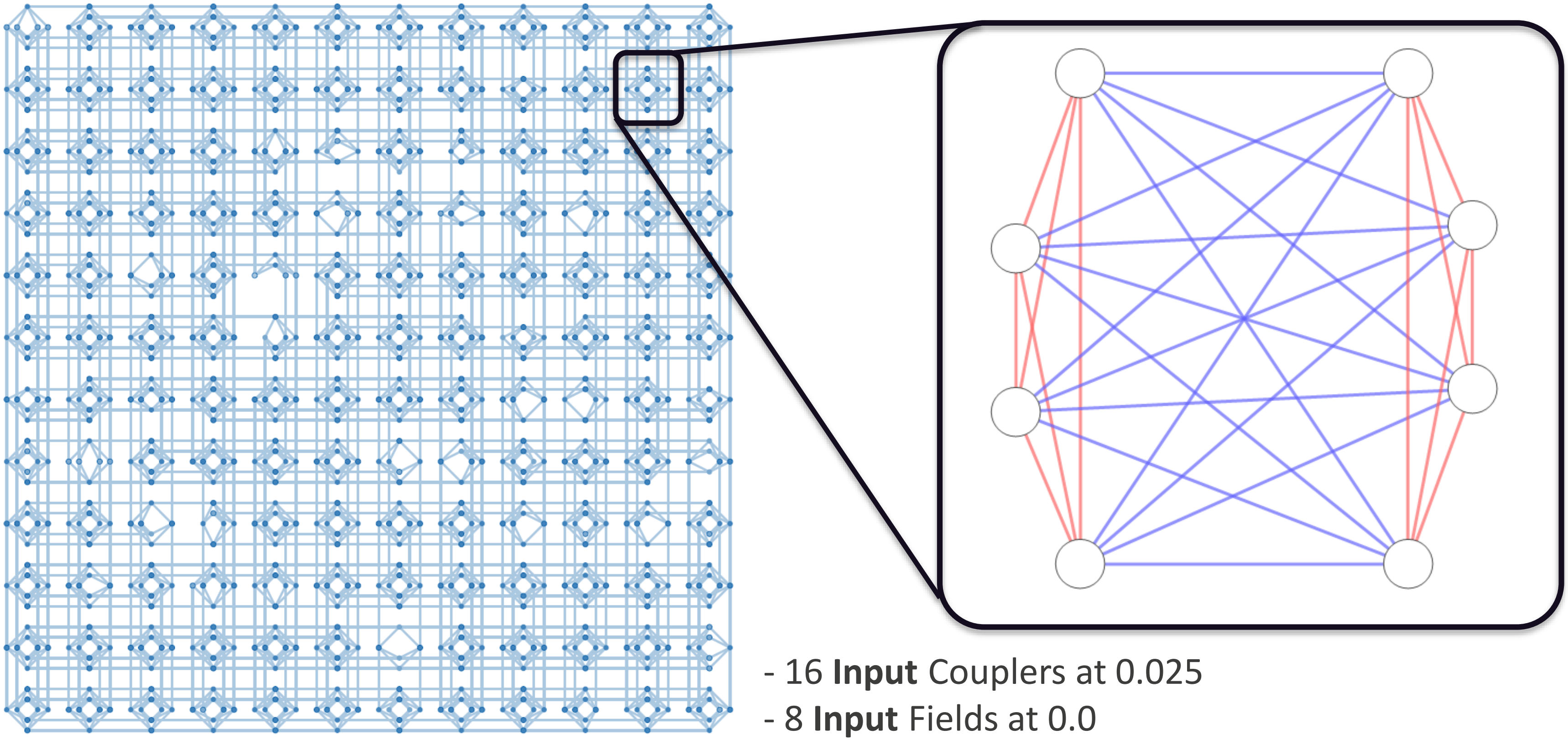
Marshall et al. *arXiv,* (2017)

General Linear response:

$$\begin{bmatrix} h_{out} \\ J_{out} \end{bmatrix} = \begin{bmatrix} \beta_{hh} & \beta_{hJ} \\ \beta_{Jh} & \beta_{JJ} \end{bmatrix} \begin{bmatrix} h_{in} \\ J_{in} \end{bmatrix} + \begin{bmatrix} c_h \\ c_J \end{bmatrix}$$

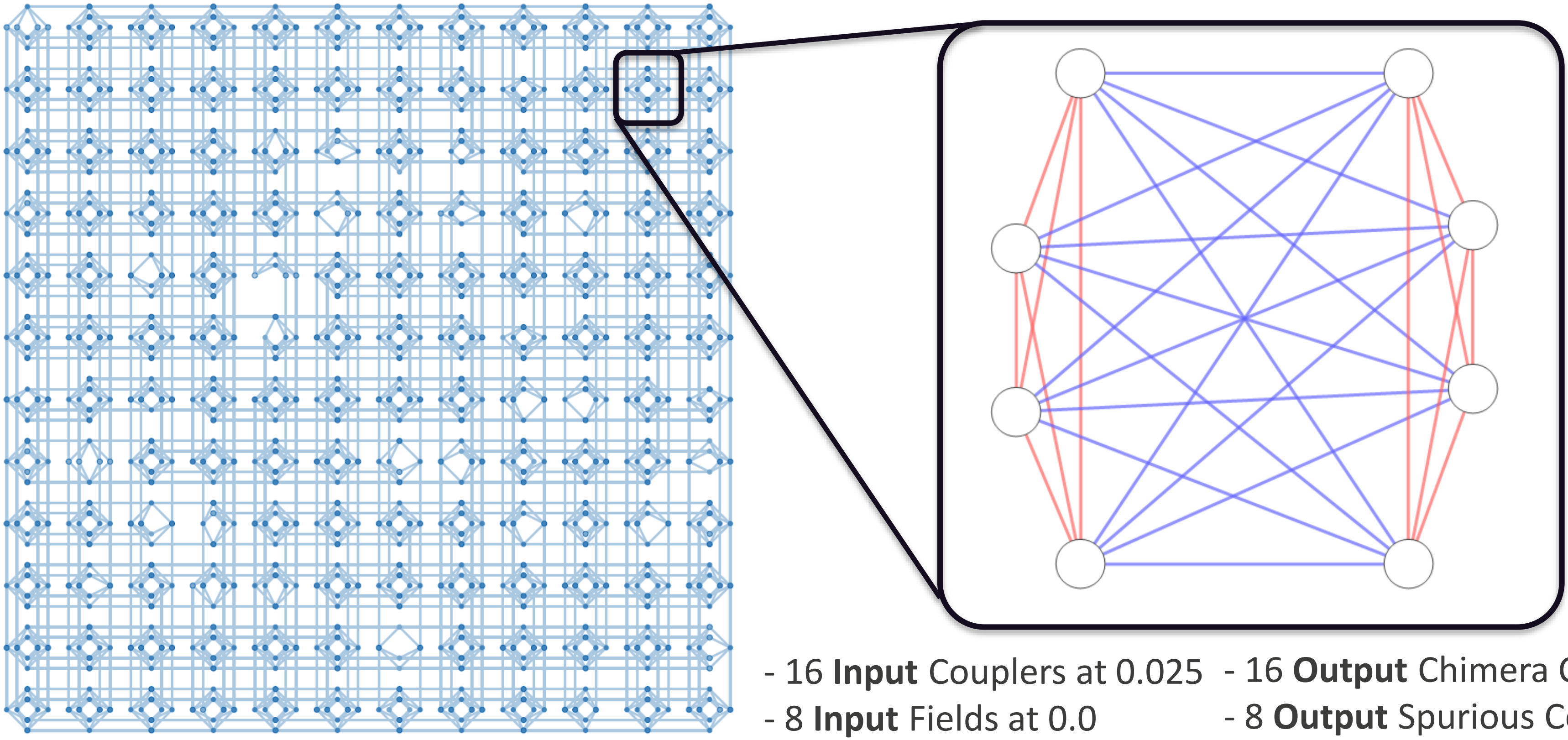
Testing effective temperature hypothesis

Input-Output Response: Results on 1 Chimera Cells



- 16 **Input** Couplers at 0.025
- 8 **Input** Fields at 0.0

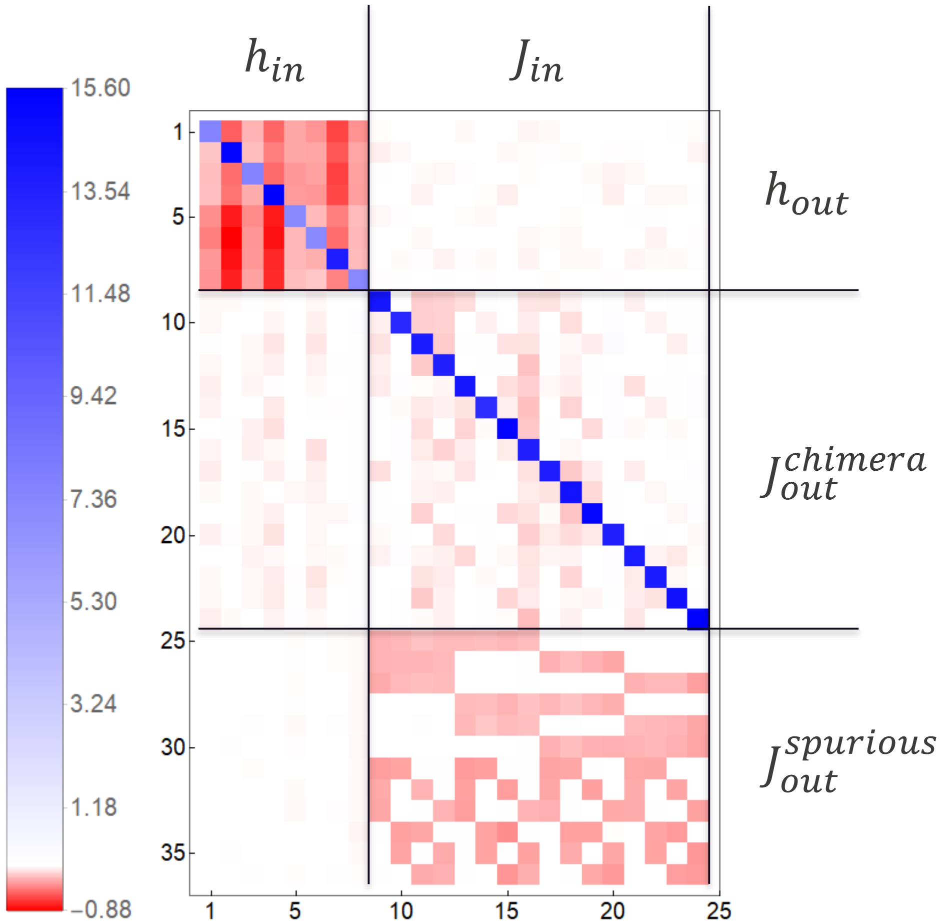
Input-Output Response: Results on 1 Chimera Cells



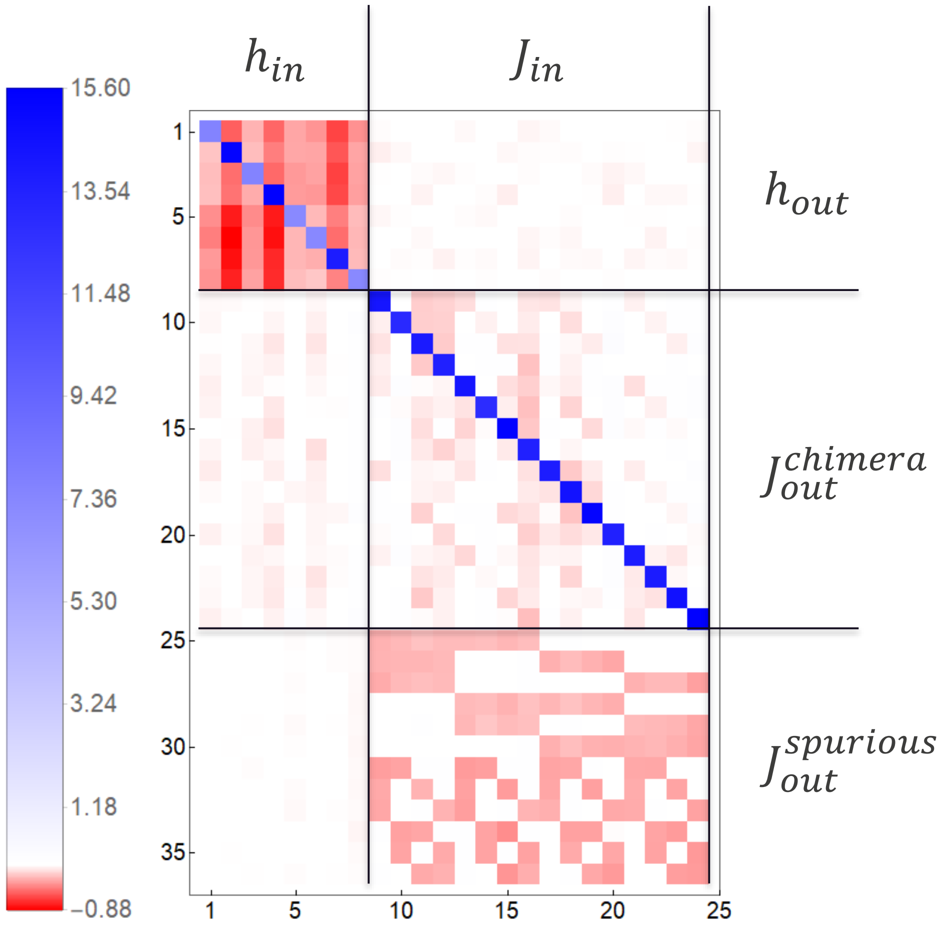
- 16 **Input** Couplers at 0.025
- 8 **Input** Fields at 0.0

- 16 **Output** Chimera Couplings
- 8 **Output** Spurious Couplings
- 8 **Output** Fields

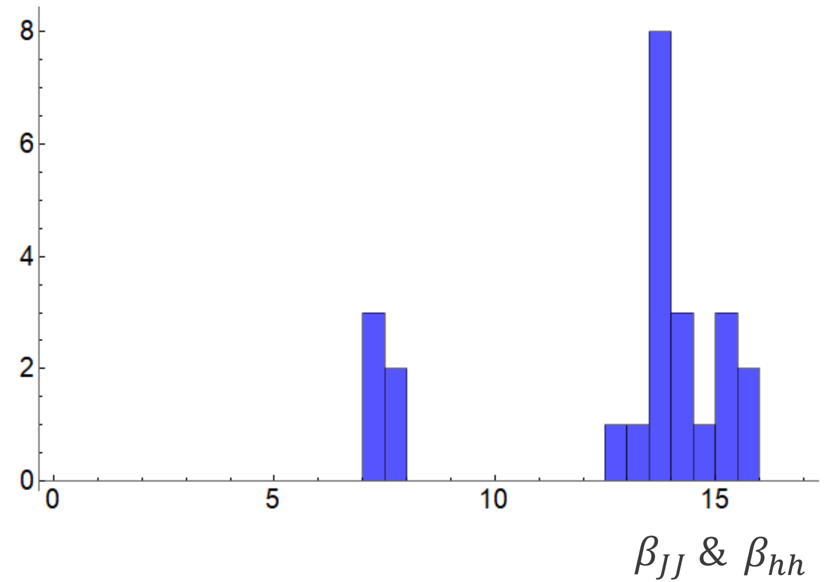
Input-Output Response Matrix



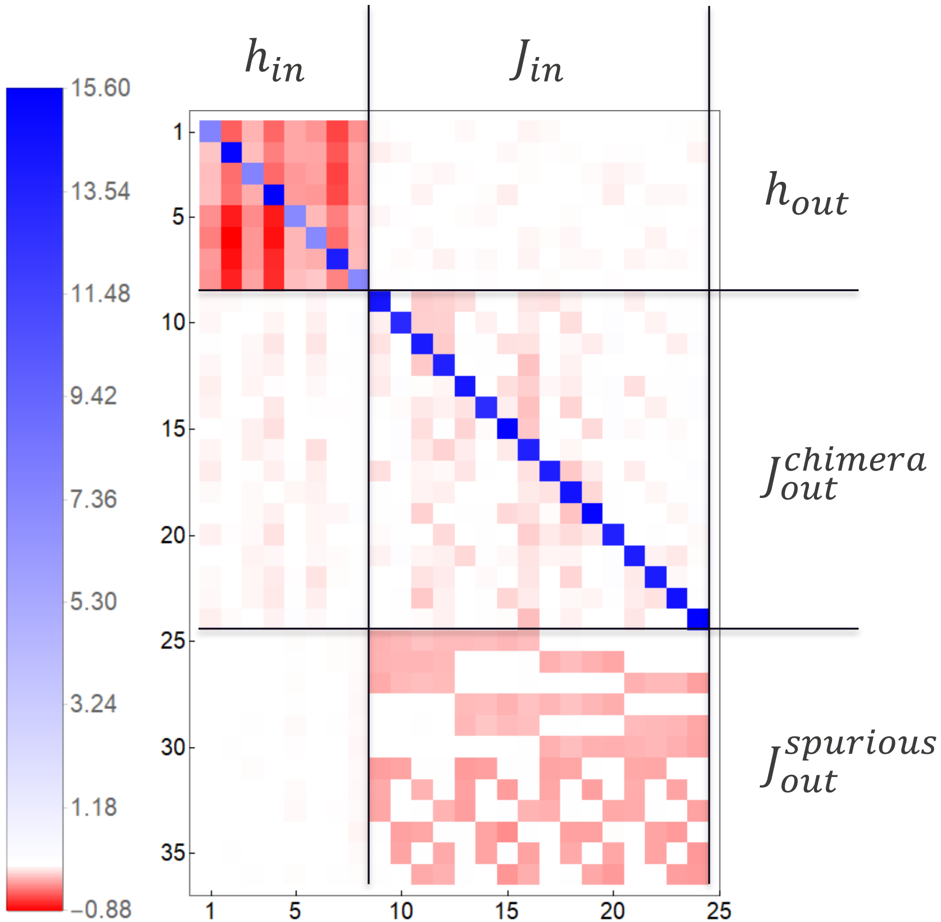
Input-Output Response Matrix



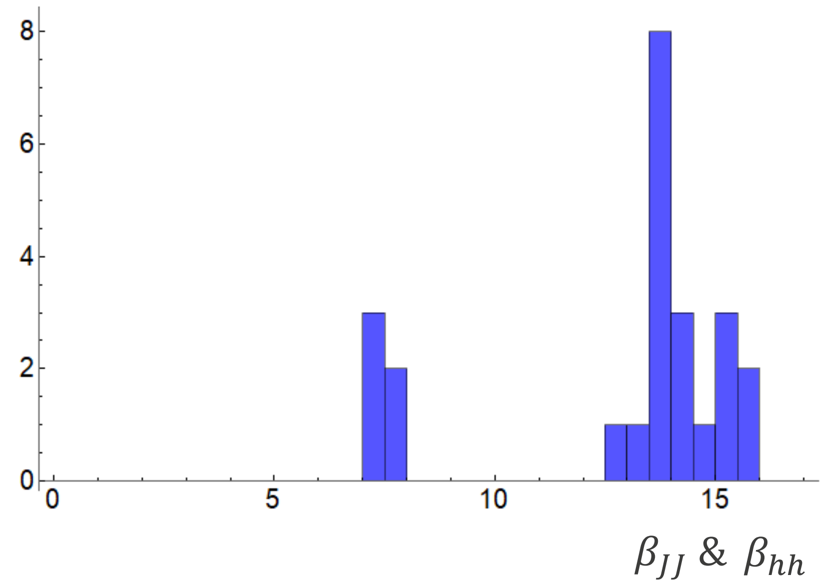
Diagonal Input-Output Response



Input-Output Response Matrix



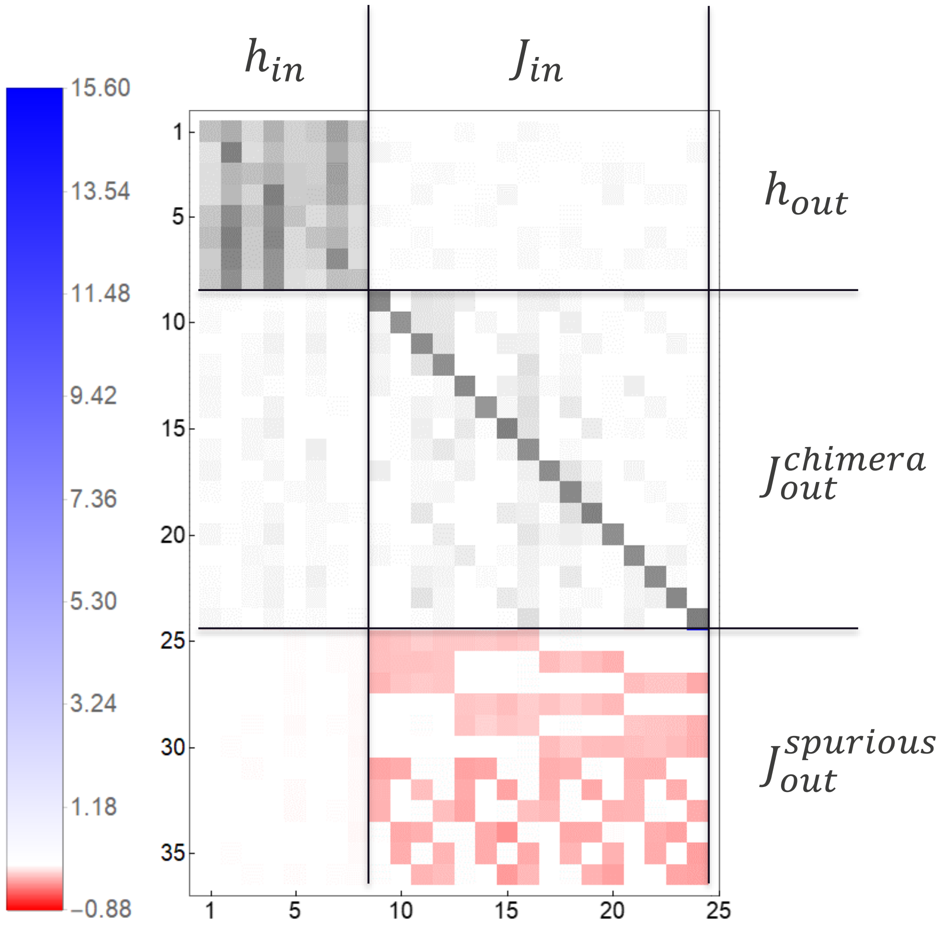
Diagonal Input-Output Response

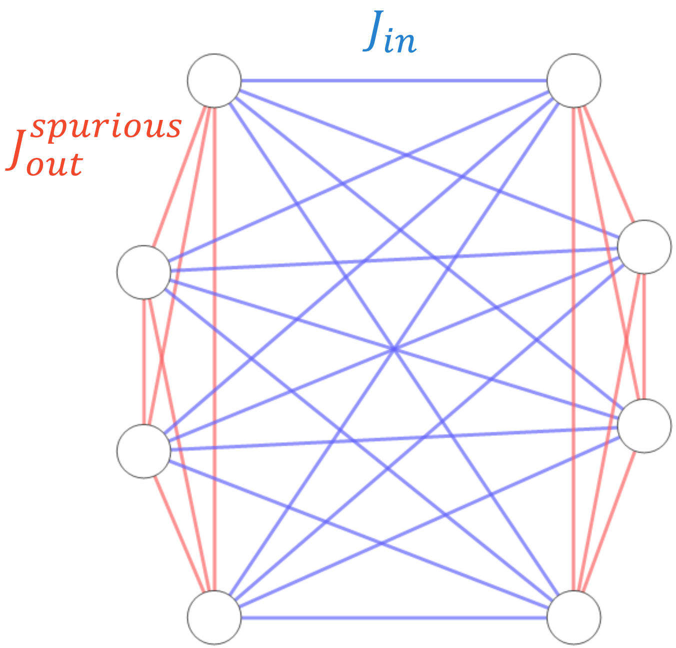


Different Scaling

No single effective **temperature**

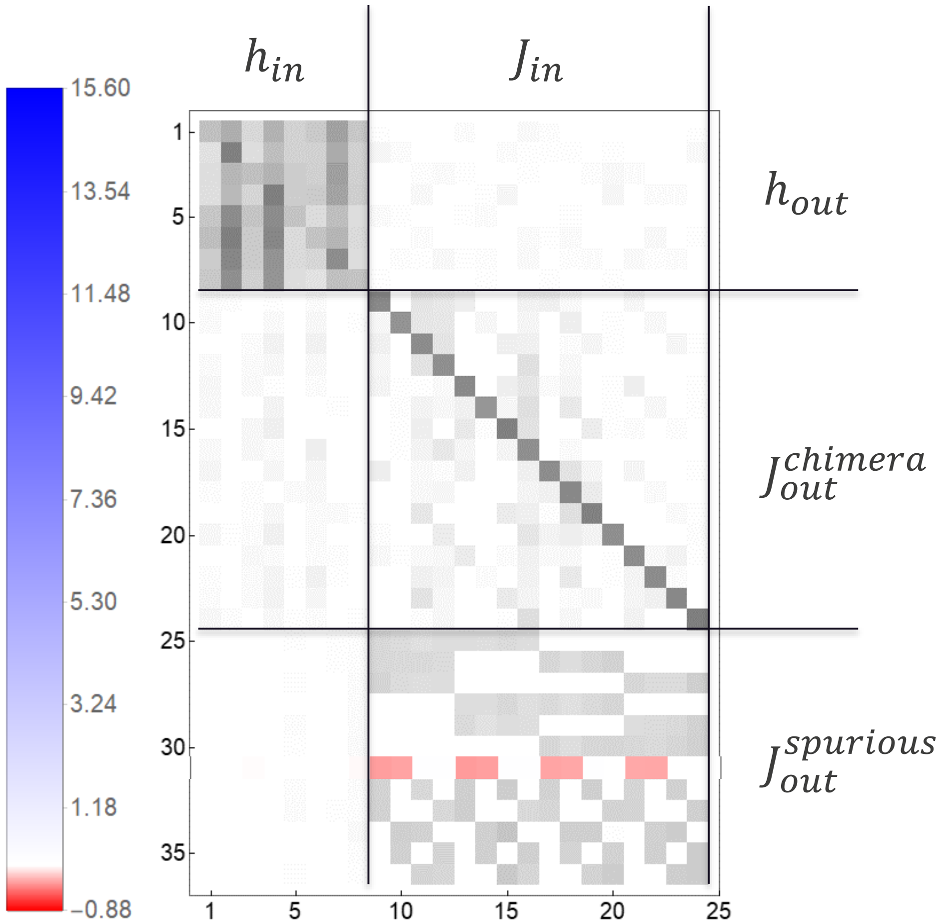
Input-Output Response Matrix

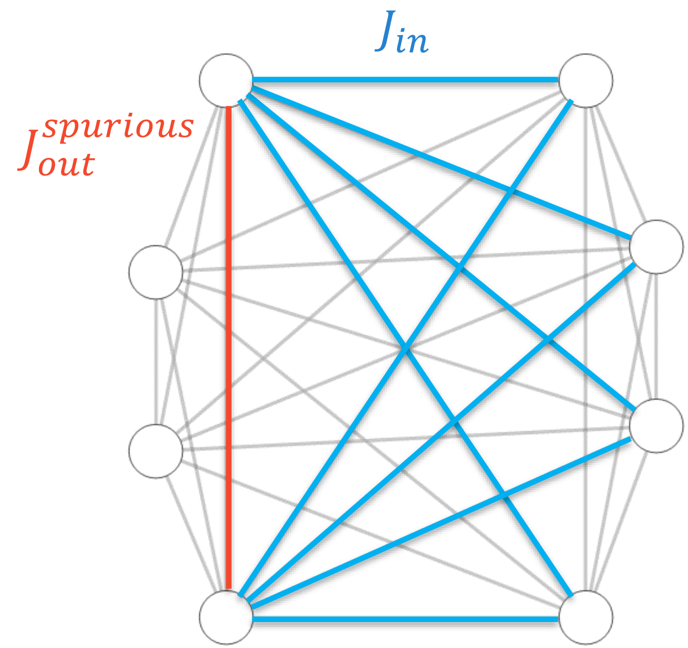




Spurious couplings response from **input** couplers

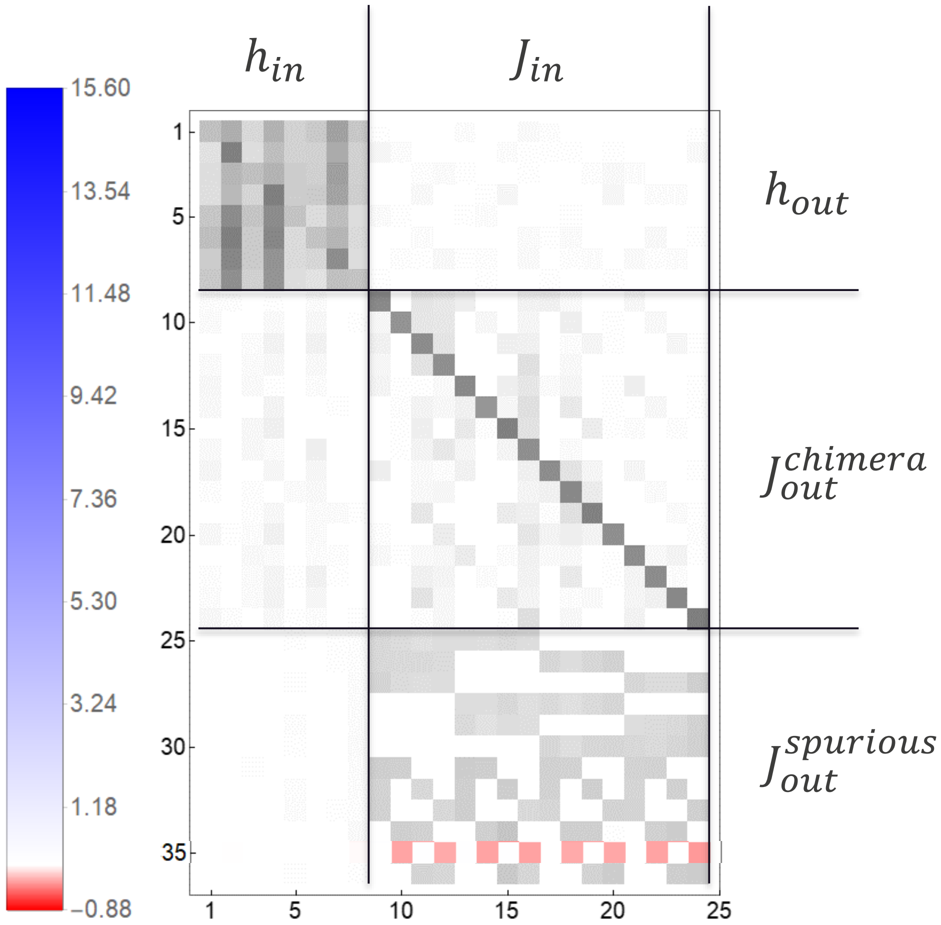
Input-Output Response Matrix

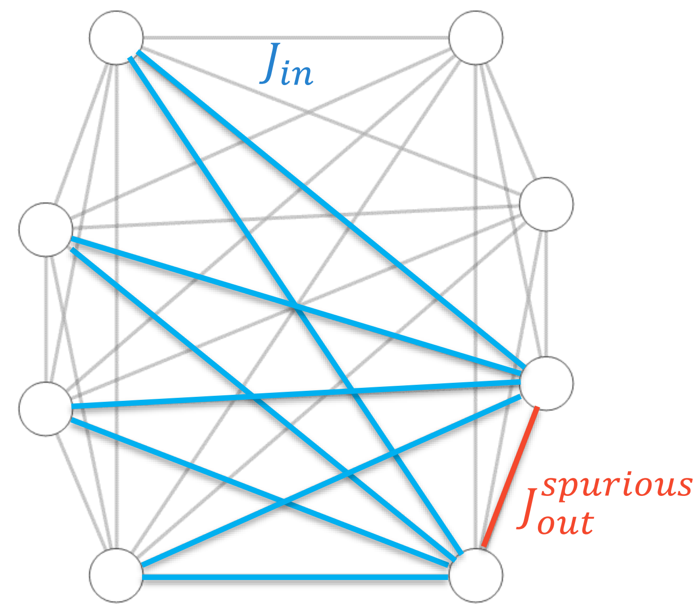




Spurious couplings only respond to **neighboring input** couplers

Input-Output Response Matrix





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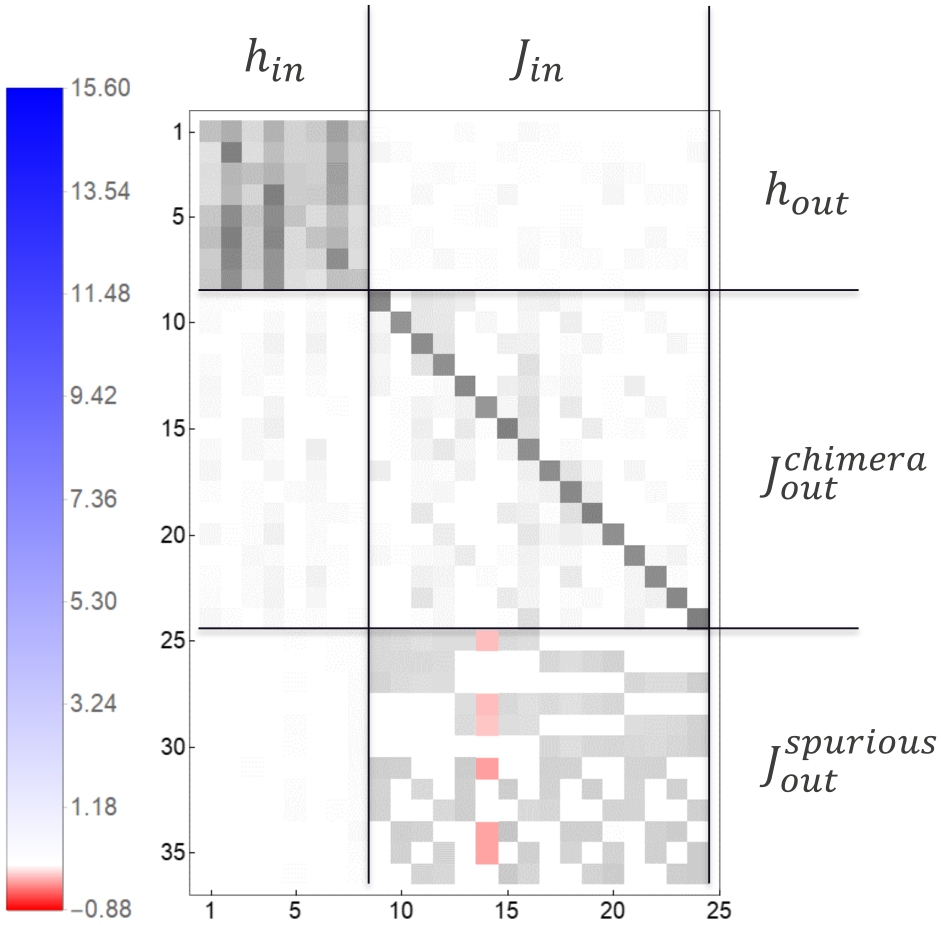
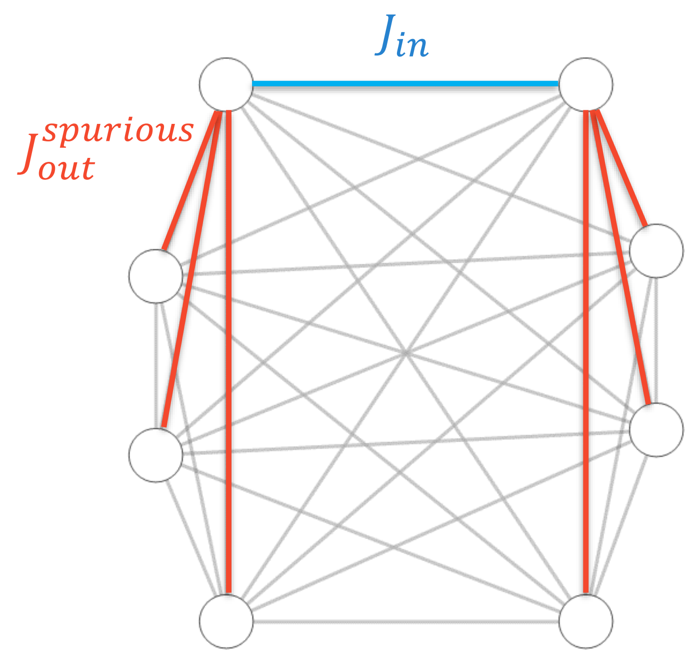
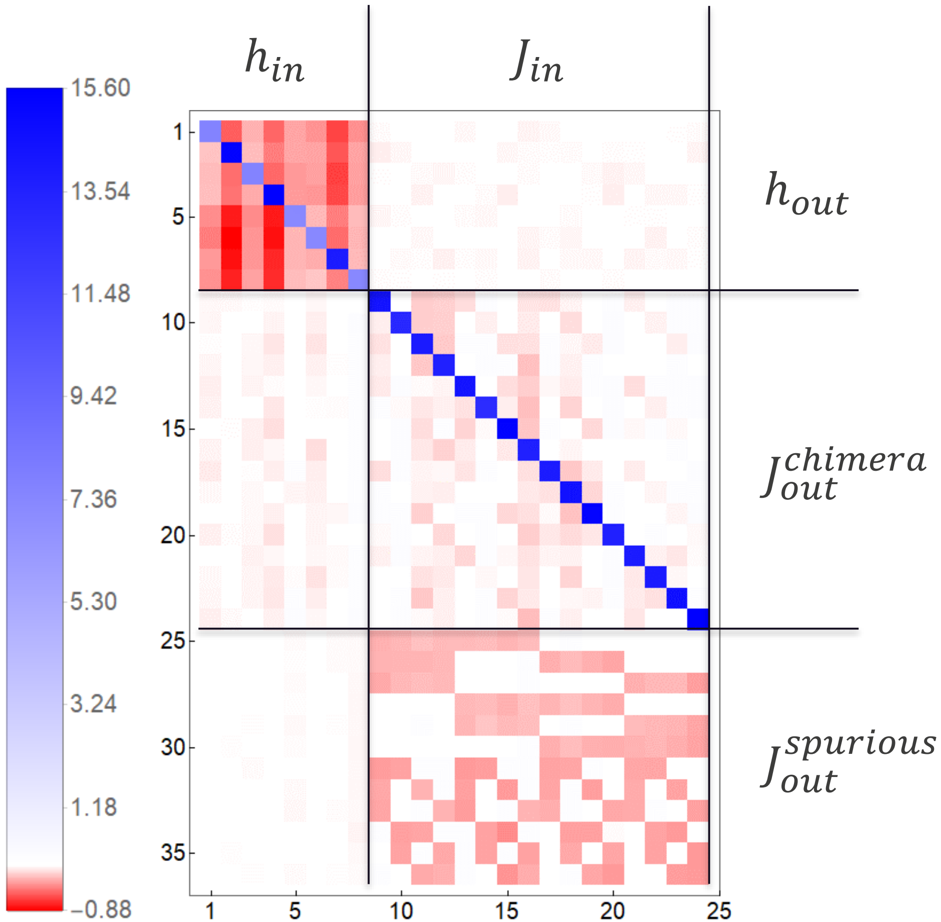
Input-Output Response Matrix

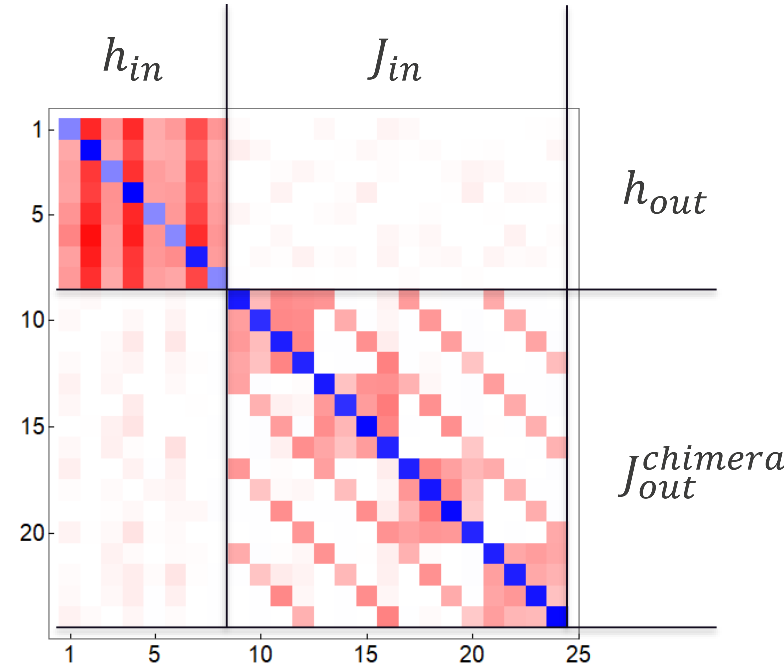




Input couplers induces response on **neighboring spurious** links

Input-Output Response Matrix





Best response matrix **ignoring spurious** links

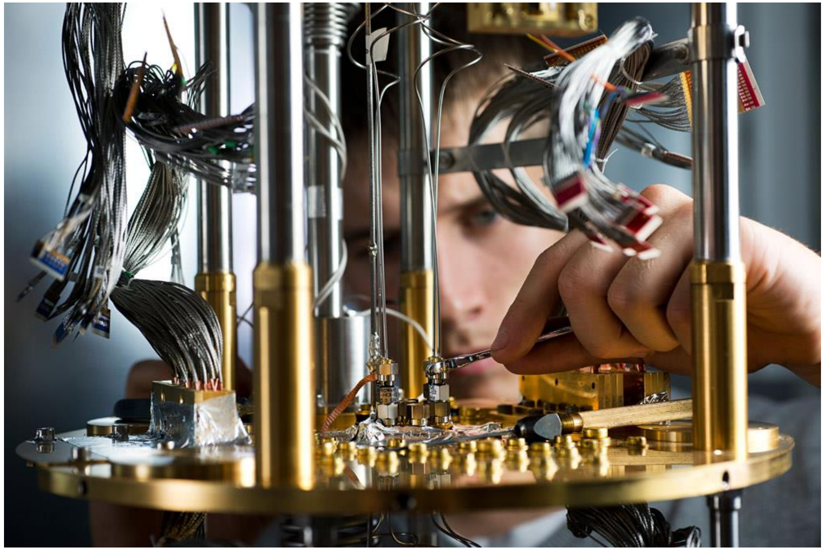
Conclusions

Summary

- ✓ D-Wave **samples** are well described by **pairwise Ising Models**
- ✓ **Multi-body** interactions **exists** but are **small**
- ✓ **Pairwise** structure is **approximately chimera** but with **spurious interactions**
- ✓ **Output-Input** response is mainly **diagonal**
- ✓ **No Single** effective **temperature**

Path forward

- Deeper study of **deviations** from **pairwise** Ising models → Enhance chip **architecture**
- Use **Input-Output** response for **calibration** → Enhance **optimization**/sampling



Acknowledgements

Center for Nonlinear Studies

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advanced network science initiative (ansi)