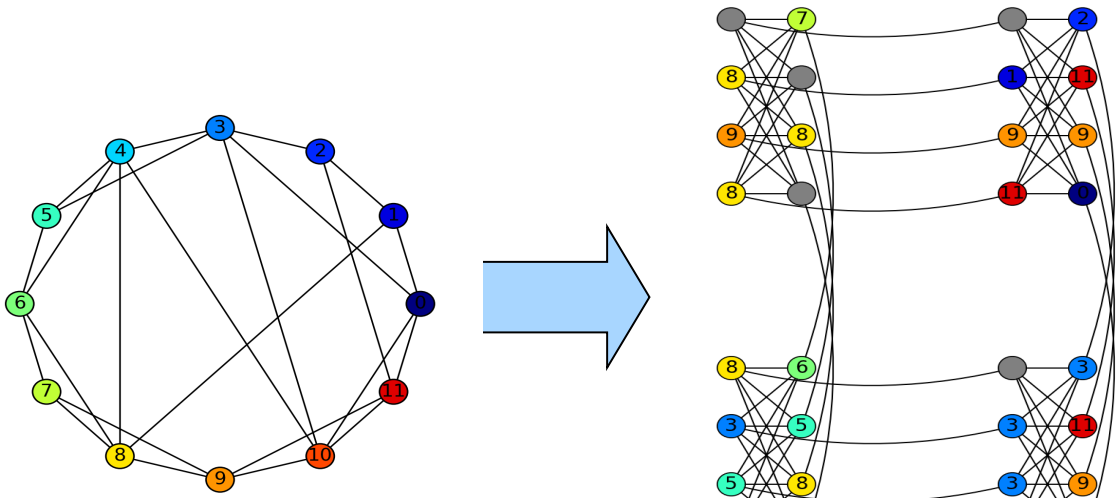
Solving Practical Problems with Quantum Computing Hardware

- Roles of software in CMOS-based computing environment
  - Provide the abstraction for users to expression their tasks
  - Correct hardware faults
  - …
  - Software makes hardware useable!
- Expected roles of software in quantum computing: more of the same
  - Can we do something useful with what we got so far?
- What can software guys do, while quantum computing hardware is emerging?
  - In the future: models of computation, hardware virtualization, programing tools, software development environment
  - What could be done now: (1) tools to make the hardware useful, (2) develop early applications

Practical Problem 1: Minor Embedding

- The hardware graph for a quantum computing device is likely to have many physical and engineering limitations, e.g., the graph is likely to be linear, planar, or having limited number of connections per qubit
- Real-word problems to be solved are unlikely to be subject to the same limitation
- **Challenge**: how to translate real-world problems onto a quantum emulation hardware? The problem is known as the minor embedding problem in literature. It is known to be a NP hard problem, therefore, brute-force solution is not going to work beyond a few qubits.
- **Approach**: develop a set of efficient software heuristics to solve the minor embedding problems.



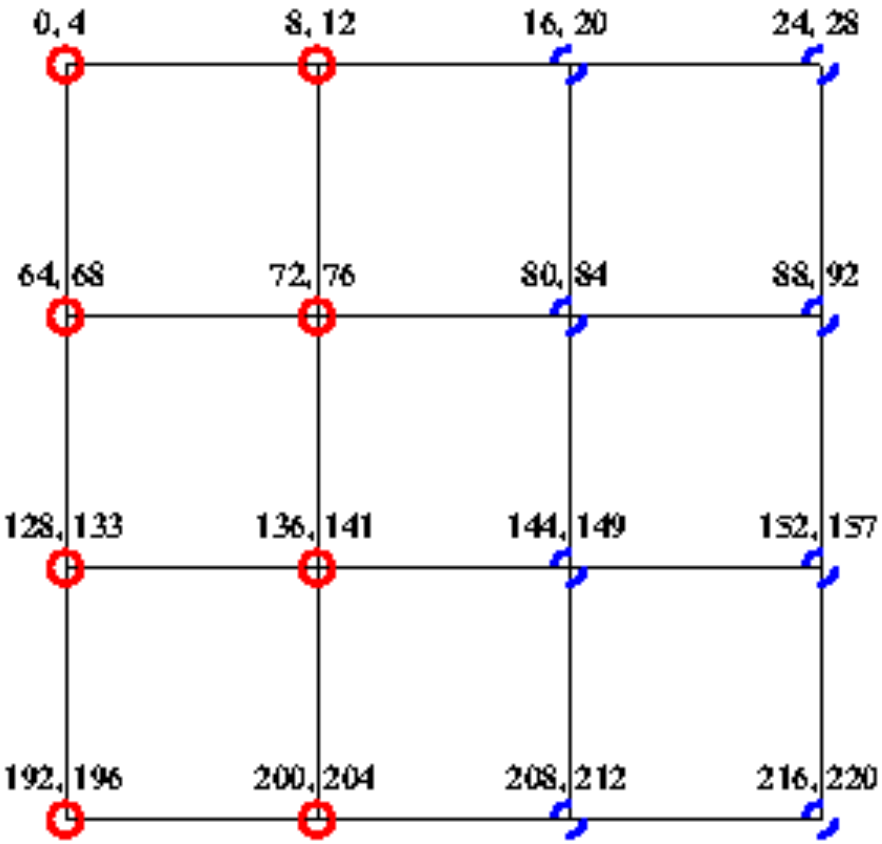
User problem: an example

Embedded into D-Wave

Practical Problem 2.1: Graph Partitioning

- Graph partitioning as a test problem of the clustering problem
- Turn graph partition problem into a Ising model
- Solved with D-Wave

- Figure on the right shows a mapping of the 4x4 mesh to the Vesuvius chip
- The colored circles illustrate an observed solution

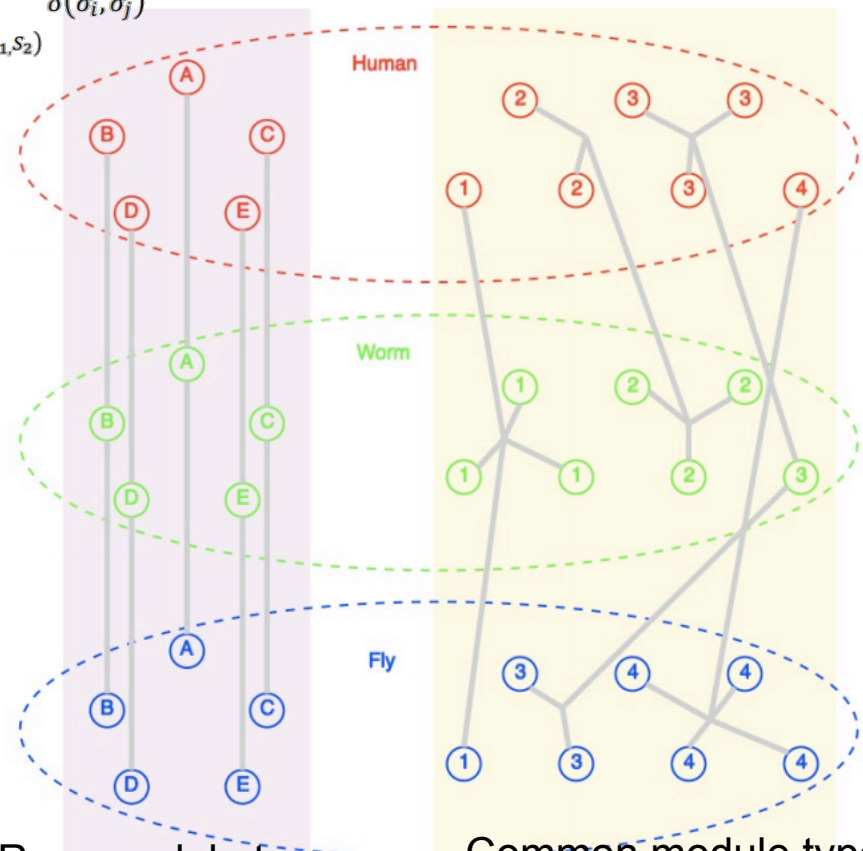


$$H = A \underbrace{\left(\sum_{i \in V} \sigma_i\right)^2}_{\text{penalize config. that doesn't bisect}} + B \sum_{ij \in E} \underbrace{\frac{1 - \sigma_i \sigma_j}{2}}_{\text{penalty } B \text{ for each edge btwn two subsets}}$$

Practical Problem 2.2: Gene co-expression in Potts Model

$$-\left\{\sum_{i,j\in S_k}\left(A_{ij}^{S_k+}-p_{ij}^{S_k+}\right)\delta(\sigma_i,\sigma_j)+\sum_{i,j\in S_k}\left(A_{ij}^{S_k-}-p_{ij}^{S_k-}\right)\delta(\sigma_i,\sigma_j)+\kappa\sum_{(i,j')\in O(S_1,S_2)}\delta(\sigma_i,\sigma_j)\right.$$
$$\left.+\kappa\sum_{(i,j')\in O(S_1,S_3)}\delta(\sigma_i,\sigma_{j'})+\kappa\sum_{(i,j')\in O(S_2,S_3)}\delta(\sigma_i,\sigma_{j'})\right\}$$

- Pairwise relationships between genes and species can be expressed as a Potts model
- The co-expressions are usually very complex and good solutions to the Potts models are hard to find
- **New computing technology such as D-Wave or Quantum Emulation devices promise to solve Potts models quickly**



Rare module type
Ultra-conserved
Enzymatic complexes

Common module type
Differing gene counts
Regulatory sub-network

Gerstein, *et al.* 2014. Nature.

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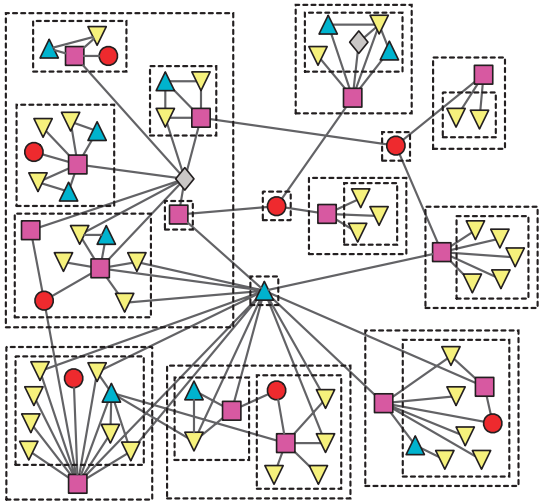
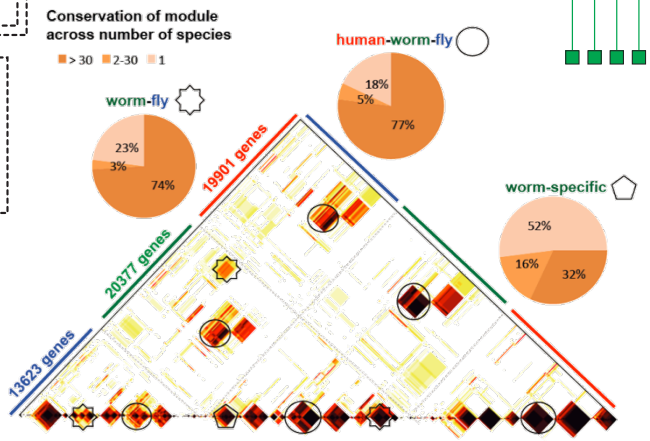
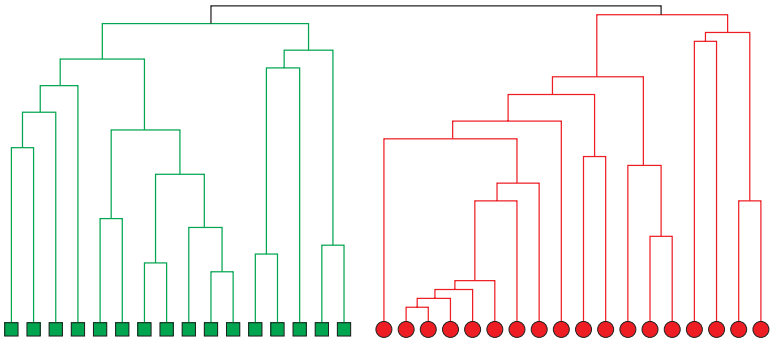
Practical Problems 2.3: Potts Model for Large-Scale Structure in Complex Networks

- Samples of graph problems solved with Potts models (left to right)
  - Grassland food web
  - Co-expression of genes from different animal models for toxicity study
  - Relatedness of species in a microbial community







Found a Killer App in Science?

- Potts models could express many NP-hard problems in large-scale graph structures from bioinformatics, chemoinformatics, among other applications
- We believe that the Potts model could be a practical demonstration of the usefulness of quantum annealing and quantum simulation
- Its application in determining the toxicology profile of new medicine could reduce the cost of pharmaceutical research and development and have imminent economic impact