Integer Boltzmann Machines for Future Generation Digital Annealing Units

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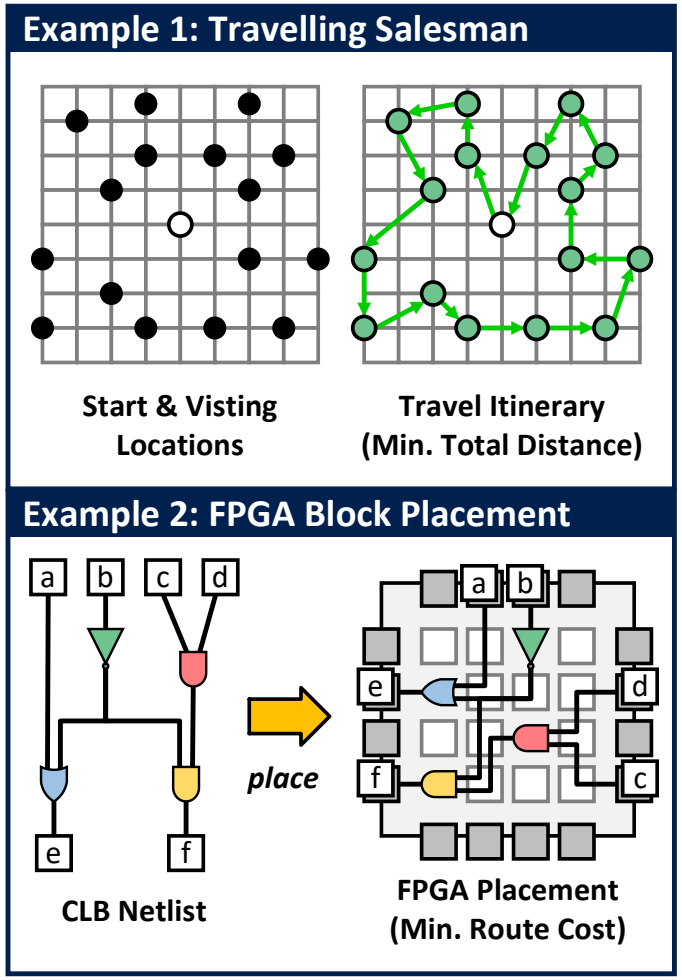
Outline

- **Motivation and Background**
  - Quadratic Assignment Problems
  - Local Search Algorithms
- Integer Boltzmann Machine
- Parallel Tempering Solver Design
  - Algorithm and SIMD
  - Load Balancing
- Benchmark Results
- Conclusion

Integer Assignment Problems

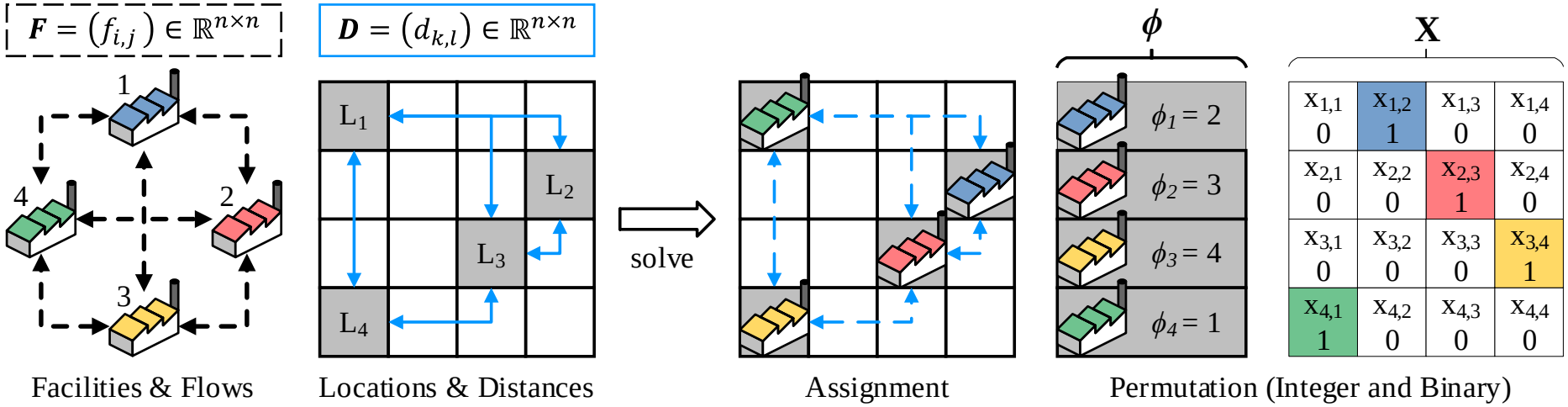


- Class of NP-hard combinatorial optimization problems with integer variables
  - Quadratic Assignment Problem (QAP) [1]
- Simple formulation but difficult to solve even with modern CPU and GPU hardware

Goal

- Create an integer Boltzmann Machine variant to accelerate search for QAP
- Presentation covers formulation for symmetric, bias-less QAPs but concepts are directly transferrable to asymmetric + biased problems

QAP Formulation



- Given n facilities and n locations
- Find a permutation $\boldsymbol{\phi} = (\phi_i) \in \boldsymbol{\Phi}$, where $\boldsymbol{\Phi}$ is set of all possible permutations
  - $\boldsymbol{\phi}$ assigns each facility i, to a unique location ϕ_i such that the total cost of the assignment (1) is minimized:

$$C(\boldsymbol{\phi}) = \sum_{i=1}^{n}\sum_{j=1}^{n} f_{i,j} d_{\phi_i,\phi_j} \quad (1)$$

$$x_{i,j} = \begin{cases} 1, & if\ \phi_i = 1 \\ 0, & otherwise \end{cases}, \mathbf{X} = (\mathrm{x_{i,j}}) \in \{0,1\}^{n \times n} \quad (2)$$

Local Search

1. Propose new states as perturbations of the current state
   - Exchange locations of 2 facilities

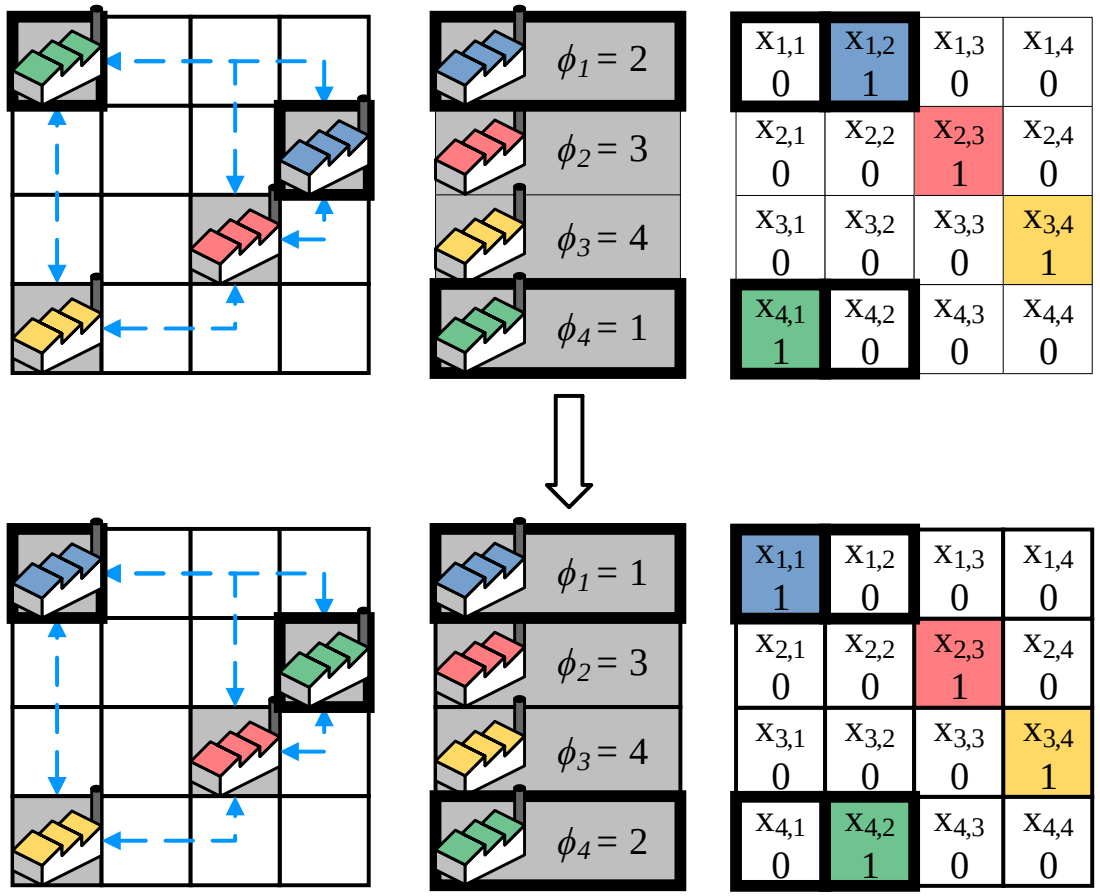
2. Calculate difference in cost function (ΔC) between previous and proposed state

3. Decide whether to accept proposed state based on some criterion
   - Stochastic Approach (e.g. Simulated Annealing):

     Use a varying temperature variable (T) that is used to inject randomness into acceptance of moves via Metropolis Hastings acceptance probability generated using (3)
     - Proposal Acceptance Rate (PAR)
     - $T \to \infty, PAR \to 100\%$, all proposals are accepted regardless of ΔC value
     - $T \to 0, PAR \to 0\%$, search turns greedy

$$P_{acc} = \min\{1, \exp\left(-\frac{\Delta C}{T}\right)\} \qquad (3)$$

Local Search: QAP Exchange



- Exchange locations of two facilities a, b
- Change in cost calculated via (4)
- Implemented in software via simple loop(s) in $\mathcal{O}(n)$ time

$$\Delta C_{ex} = \sum_{i=1, i \neq a,b}^{n} 2(f_{b,i} - f_{a,i})(d_{\phi_a,\phi_i} - d_{\phi_b,\phi_i}) \quad (4)$$

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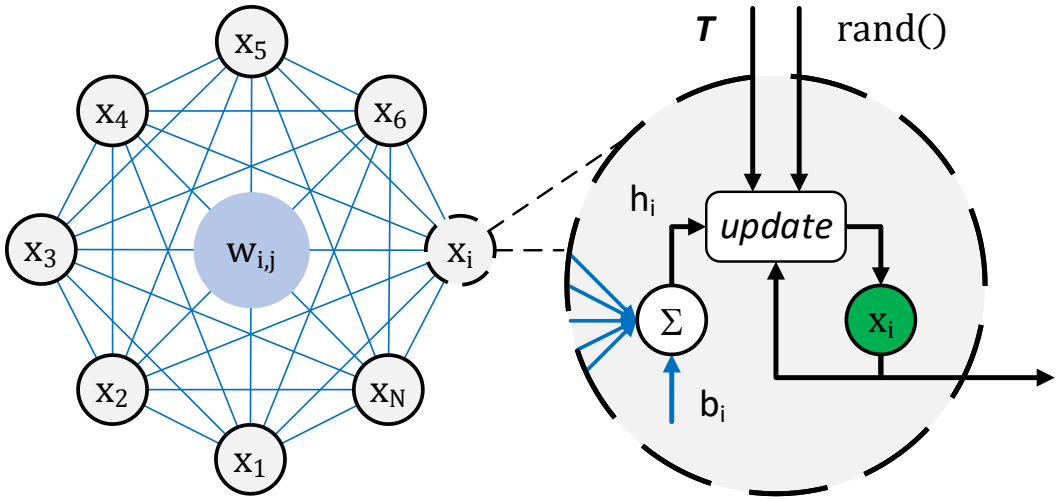
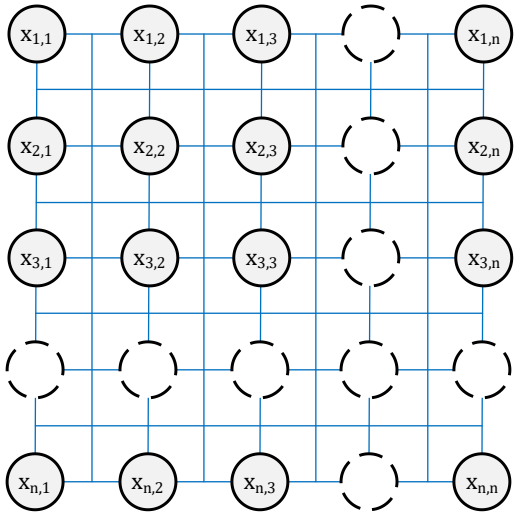
Boltzmann Machines

1D – N neurons

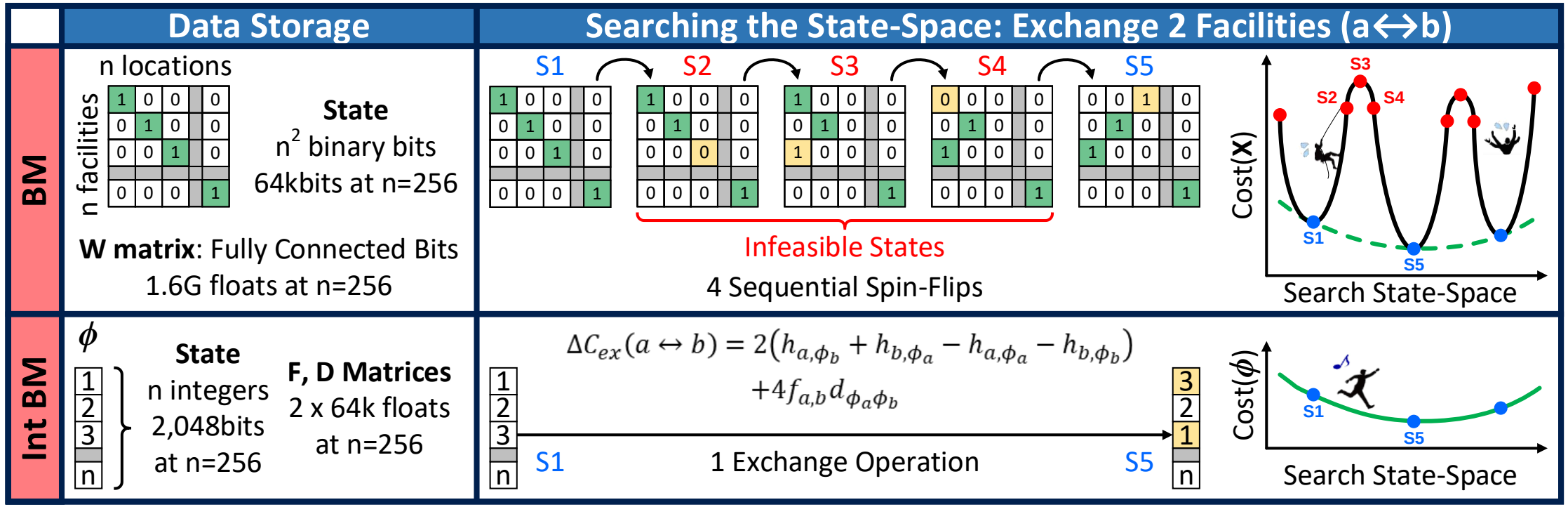


2D – $n \times n$ neurons



State Cost/ Energy	$C(\mathbf{X}) = -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} w_{i,j}x_i x_j - \sum_{i=1}^{N} b_i x_i$	(5)	$C(\mathbf{X}) = -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n} w_{i,j;k,l}x_{i,j}x_{k,l} - \sum_{i=1}^{n}\sum_{j=1}^{n} b_{i,j}x_{i,j}$	(7)
Neuron Local Fields	$h_i(\mathbf{X}) = \sum_{j=1}^{N} w_{i,j}x_i + b_i$	(6)	$h_{i,j}(\mathbf{X}) = \sum_{k=1}^{n}\sum_{l=1}^{n} w_{i,j;k,l}x_{k,l} + b_{i,j}$	(8)

BM vs Integer BM for QAP [2,3]

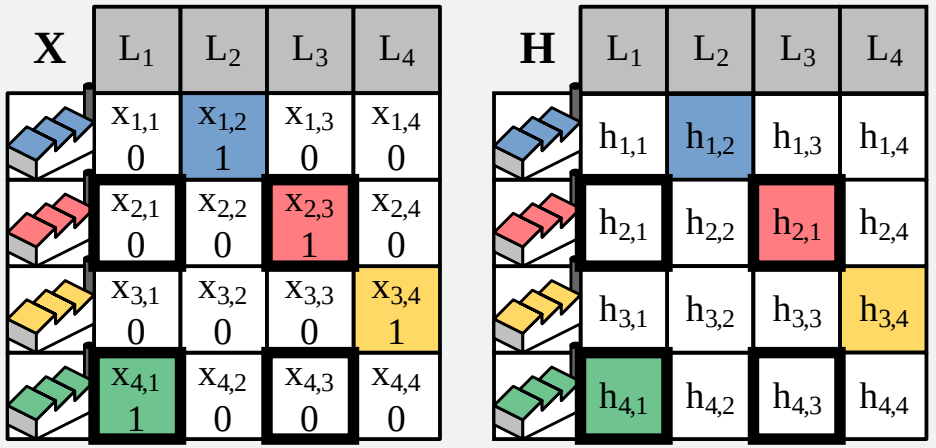


- 2D BM requires penalty terms to enforce one-hot constraints on rows/columns of **X**
- Using an Integer BM with intrinsic exchange moves (4-bit-flip equivalent) simplifies problem formulation and speeds up search, significantly reduces memory reqs.

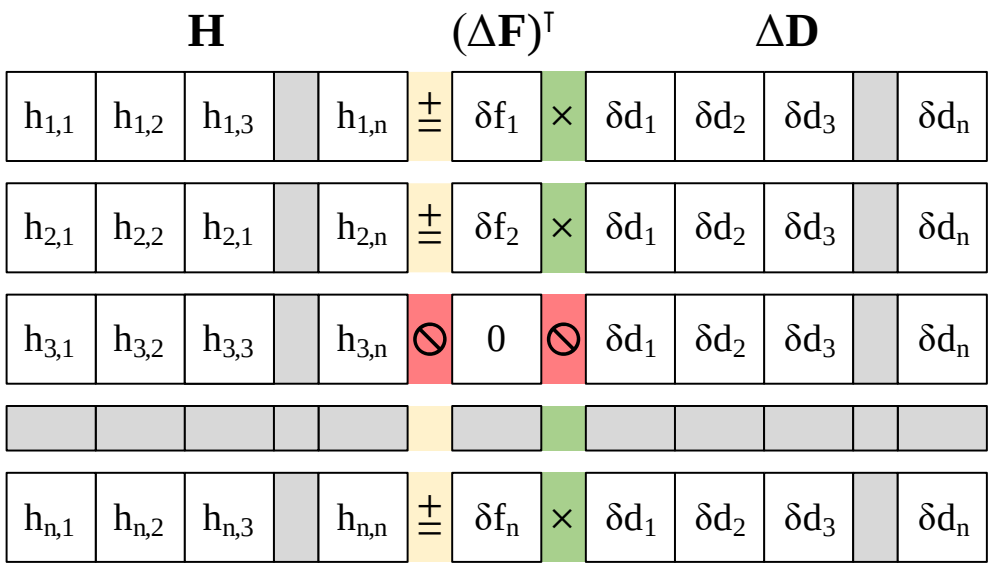
Int BM QAP Formulation

Notes	Formulation	#
• Remove conditions on the summation loop iterator	$\Delta C_{ex} = \sum_{i=1, i\neq a,b}^{n} 2(f_{b,i} - f_{a,i})(d_{\phi_a,\phi_i} - d_{\phi_b,\phi_i})$	(4)
• Introduces extra terms within the sum • Compensate via additional terms	$\Delta C_{ex} = \sum_{i=1}^{n} 2(f_{b,i} - f_{a,i})(d_{\phi_a,\phi_i} - d_{\phi_b,\phi_i}) + 4f_{a,b}d_{\psi_a\psi_b}$	(9)
• Create vector of flow row differences	$\Delta_a^b \mathbf{F} = \mathbf{F}_{b,*} - \mathbf{F}_{a,*}$	(10)
• Create vector of permutation ordered distance row differences	$\Delta_{\phi_b}^{\phi_a} \mathbf{D}^{\mathbf{X}} = \left(\mathbf{D}_{\phi_a,*} - \mathbf{D}_{\phi_b,*}\right)\mathbf{X}^{\intercal}$	(11)
• Reformulate using a dot product	$\Delta C_{ex} = 2\Delta_a^b \mathbf{F} \cdot \Delta_{\phi_b}^{\phi_a} \mathbf{D}^{\mathbf{X}} + 4f_{a,b}d_{\phi_a\phi_b}$	(12)

Integer BM: Local Fields

Notes	Formulation	#
• Generate cache values at start of search in $\mathcal{O}(n^3)$ time	$\mathbf{H} = \mathbf{F}(\mathbf{D}^{\mathsf{T}}\mathbf{X}) = (h_{r,c}) \in \mathbb{R}^{n \times n}$	(13)
• Elements in $\mathbf{H}$ correspond to bits in $\mathbf{X}$ • Element $h_{r,c}$ is cost of assigning a facility r to location c		
• Reformulate dot product as sum of 4 $\mathbf{H}$ elements taking $\mathcal{O}(1)$ time	$\Delta_a^b \mathbf{F} \cdot \Delta_{\phi_b}^{\phi_a} \mathbf{D}^{\mathbf{X}} = h_{a,\phi_b} + h_{b,\phi_a} - h_{a,\phi_a} - h_{b,\phi_b}$	(14)
$\Delta C_{ex} = 2\Delta_a^b \mathbf{F} \cdot \Delta_{\phi_b}^{\phi_a} \mathbf{D}^{\mathbf{X}} + 4 f_{a,b} d_{\phi_a \phi_b}$ →	$\Delta C_{ex} = 2(h_{a,\phi_b} + h_{b,\phi_a} - h_{a,\phi_a} - h_{b,\phi_b}) + 4 f_{a,b} d_{\phi_a \phi_b}$	(15)

Int BM: Local Field Updates



$$\mathbf{H} \mathrel{+}= \left(\Delta_a^b \mathbf{F}\right)^{\intercal} \otimes \Delta_{\phi_b}^{\phi_a} \mathbf{D} \qquad (16)$$

- Update local fields 1 row at a time using floating point fused-multiply-adds
  - $\mathcal{O}(n^2)$
- Can skip rows corresponding to 0 elements in $\Delta\mathbf{F}$
- Significant speed-ups if $\mathbf{F}$ is sparse or has a particular pattern that leads to sparse $\Delta\mathbf{F}$ vectors

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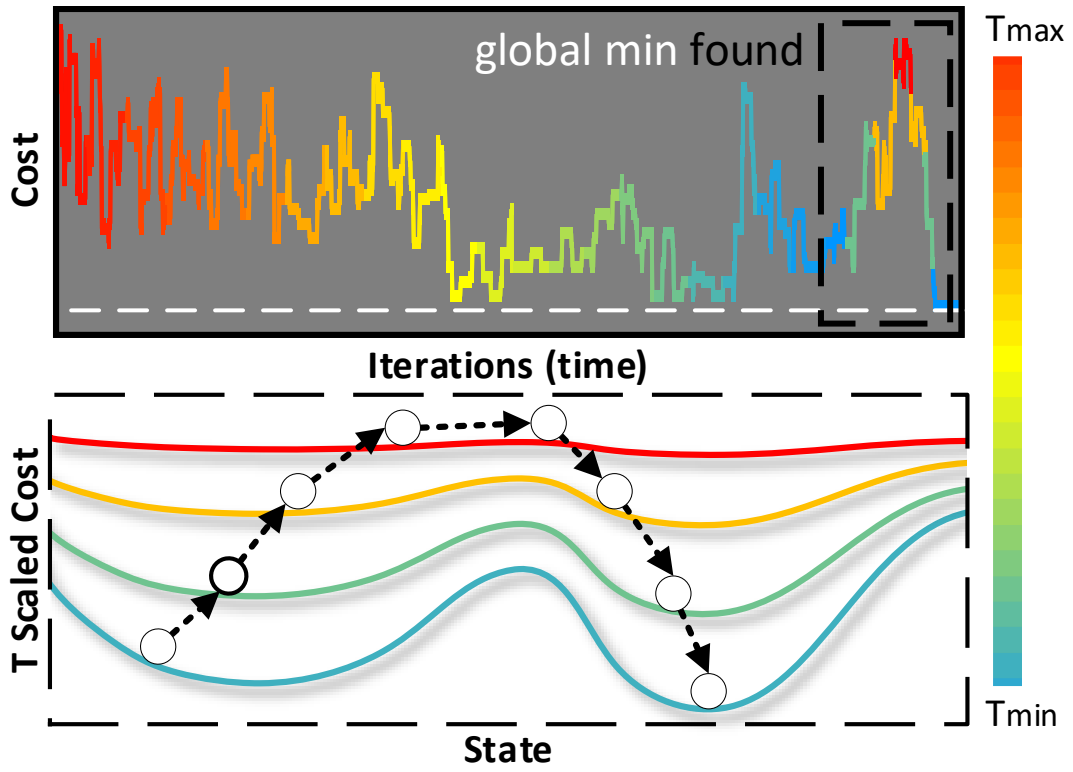
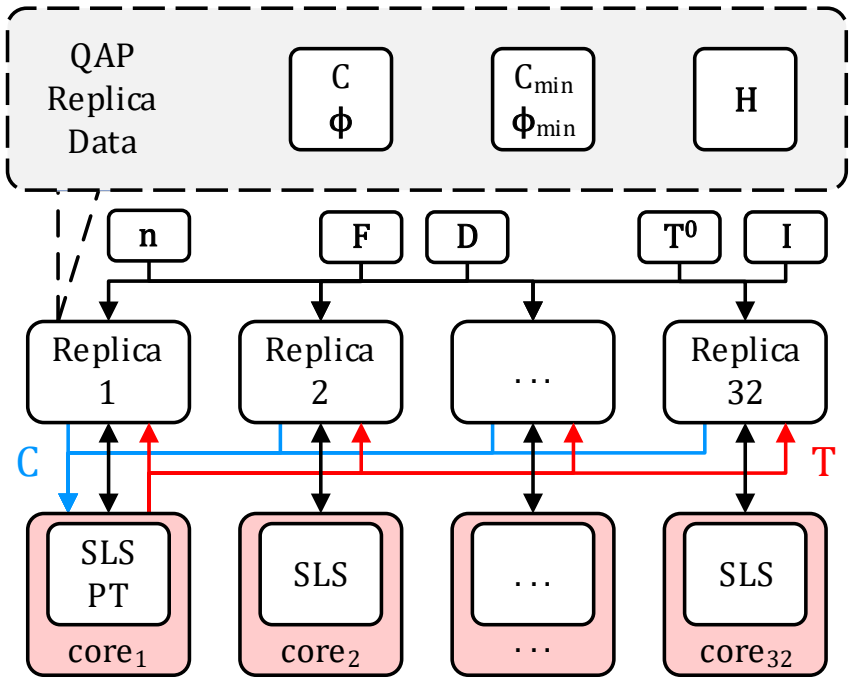
Parallel Tempering



- Uses M unique search-states/replicas with unique temperatures, $T = (T_k) \in R^M$
- Replicas perform Local Search at their assigned temperature
  - Can swap temperatures with other replicas with probability calculated via (17)
  - Allows for an escape mechanism from local minima

$$SAP = min\left\{1, \exp\left(\left(\frac{1}{T_k} - \frac{1}{T_{k+1}}\right)(C_k - C_{k+1})\right)\right\} \quad (17)$$

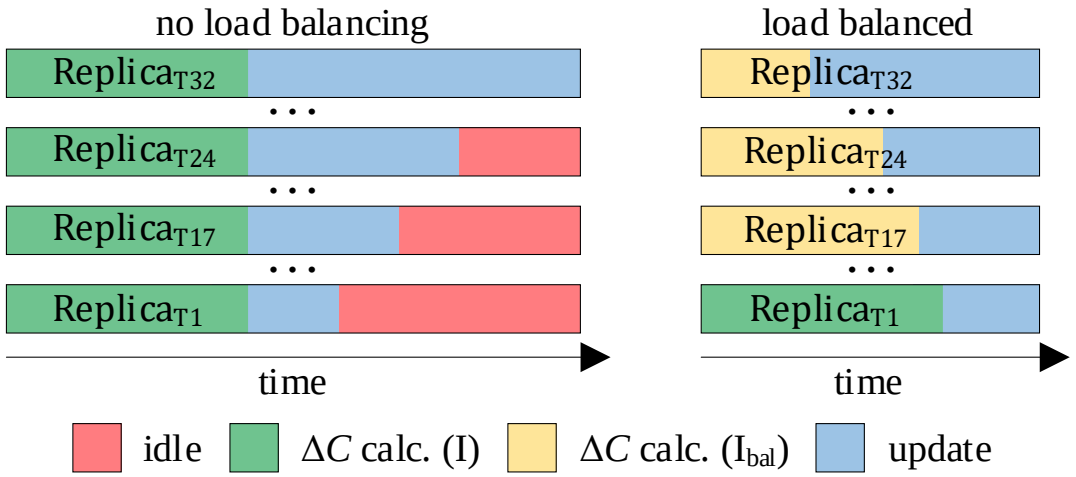
Parallel Tempering Solver System



32 Replica PT Engine

- Experimental setup:
  - 64-Core AMD 3990X CPU with AVX2 support
  - Coded in C++ and compiled with GCC-9
- Float32 used to store $\mathbf{F}, \mathbf{D}, \mathbf{H}$
  - Allows for Fused-Multiply-Add instructions
- Each engine uses 32 replicas in combination with a PT controller
  - Each replica is run on a dedicated CPU core
  - 2 engines are run in parallel to utilize all 64 cores
  - Runs until a target cost is found or a 5-minute time-out limit is reached

Load Balancing Threads



- Varying proposal acceptance rates of replicas at different temperatures causes thread imbalance when using Parallel Tempering
- Track average time-per-iteration at each temperature and scale iterations at each temperature to try to equalize thread run-times

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QAP Benchmark Results

TABLE I: QAP TtS Across Solvers (values in seconds)

Instance	ParEOTS	Int BM + PT	Speed-Up
dre42	0.7	0.10 ± 0.01	7.00×
dre56	5.6	0.99 ± 0.07	5.66×
dre72	26.0	5.23 ± 0.31	4.97×
Inst50	17.0	3.58 ± 0.27	4.75×
Inst60	67.0	2.00 ± 0.16	33.5×
Inst70	127.0	6.24 ± 0.98	20.35×
Inst80	116.0	19.36 ± 1.75	5.99×
sko81	22.4	0.13 ± 0.01	172.31×
sko90	92.0	0.26 ± 0.01	353.85×
sko100a	69.0	0.27 ± 0.01	255.56×
sko100b	45.0	0.19 ± 0.01	236.84×
sko100c	56.0	0.29 ± 0.02	193.1×
sko100d	37.0	0.38 ± 0.02	97.37×
sko100e	47.0	0.21 ± 0.01	223.81×
sko100f	57.0	0.24 ± 0.01	237.5×
tai60b	4.6	0.14 ± 0.01	32.86×
tai80b	53.0	0.43 ± 0.01	123.26×
tai100b	71.0	0.36 ± 0.02	197.22×
wil100	97.0	0.46 ± 0.02	210.87×
Geometric Mean Speedup			**57.09×**

- Avg. Time-to-Solution (TtS) across 100 independent, randomly seeded, runs with 99% confidence interval for 19 difficult QAP instances
  - Instances from [4,5,6]
- ParEOTS [7]: Parallel Extremal Optimization + Tabu Search
  - Best performing published QAP solver
  - 128 cores on CPU cluster 8 x 16–core AMD 6376 CPU
  - TtS reported as average across 10 runs with 5-minute time-out
- 57x faster than ParEOTS on average
  - Max speed-up of 353x

Conclusion

- Extended BMs to support for integer variables with one-hot constraints
  - Remove need for penalty tuning on user side
- Added support for weight-generation using submatrices for problem topologies such as QAP
  - Larger problem support due to lower memory requirements
- Integer BM based CPU solution displays performance that is orders of magnitude faster than competing solvers across difficult QAP instances

Future Work

- Accelerate search relative to high-performance multi-core CPU system through dedicated hardware

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Thank You!

Looking forward to your questions at the live session

References

- [1] Lawler, E.L.: The quadratic assignment problem. Manage. Sci. 9(4), 586–599 (1963).
- [2] M. Bagherbeik, P. Ashtari, S. F. Mousavi, K. Kanda, H. Tamura, and A. Sheikholeslami, "A permutational boltzmann machine with parallel tempering for solving combinatorial optimization problems," in *International Conference on Parallel Problem Solving from Nature*. Springer, 2020, pp. 317–331
- [3] M. Bagherbeik and A. Sheikholeslami, "Caching and vectorization schemes to accelerate local search algorithms for assignment problems," in *IEEE Congress on Evolutionary Computation (to appear)*, 2021.
- [4] Burkard, R.E., Karisch, S.E., Rendl, F.: QAPLIP-a quadratic assignment problem library. J. Global Optim. 10(4), 391–403 (1997).
- [5] Palubeckis, G.: An algorithm for construction of test cases for the quadratic assignment problem. Informatica Lith. Acad. Sci. 11, 281–296 (2000)
- [6] Drezner, Z., Hahn, P.M., Taillard, E.D.: Recent advances for the quadratic assign- ´ ment problem with special emphasis on instances that are difficult for metaheuristic methods. Ann. Oper. Res. 139(1), 65–94 (2005).
- [7] Munera, Danny, Daniel Diaz, and Salvador Abreu. "Hybridization as cooperative parallelism for the quadratic assignment problem." *International Workshop on Hybrid Metaheuristics*. Springer, Cham, 2016.