Quo vadis: Hydrologic inverse analyses using high-performance computing and a D-Wave quantum annealer

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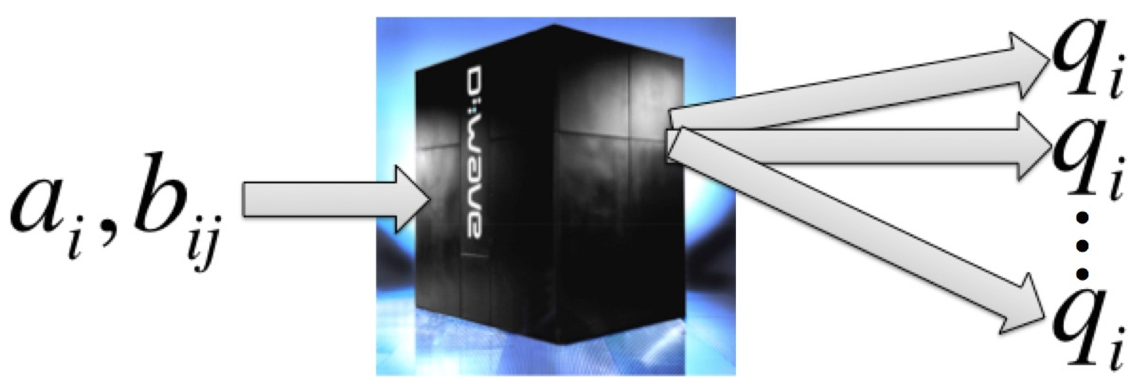
Quantum Annealing (QA)



$$f(\mathbf{q}) = \sum_{i=1}^{n} a_i q_i + \sum_{i=1}^{n} \sum_{j=1}^{i-1} b_{ij} q_i q_j$$

Returns $\mathbf{q}$'s that make $f(\mathbf{q})$ small.

Small 1D Inversion with QA

Finite difference equation: $0 = \nabla \cdot (k \nabla h)$

$$0 = k_1(h_1 - h_2) + k_2(h_3 - h_2)$$

Reformulate as a least squares problem

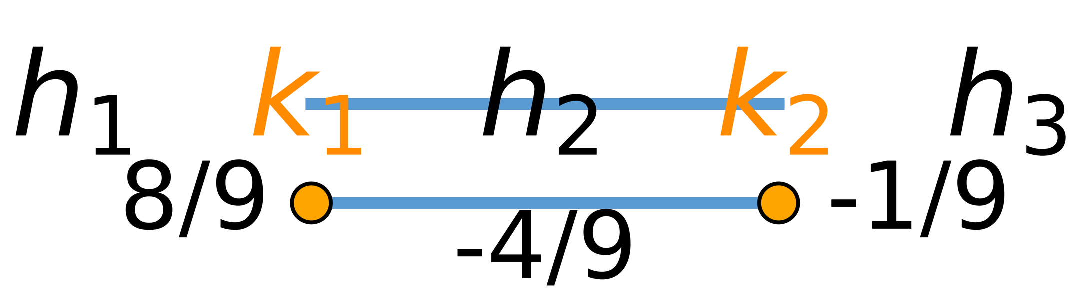
$$0 \approx [k_1(h_1 - h_2) + k_2(h_3 - h_2)]^2$$

Fill in, say, $h_1 = 1$, $h_2 = \frac{1}{3}$, $h_3 = 0$

$$0 \approx \left(\frac{2k_1}{3} - \frac{k_2}{3}\right)^2$$

Discretize $k_i = 1 + q_i$, $q_i \in \{0, 1\}$

$$0 \approx \left(\frac{2 + 2q_1}{3} - \frac{1 + q_2}{3}\right)^2 = \frac{8}{9}q_1 - \frac{1}{9}q_2 - \frac{4}{9}q_1 q_2 + \frac{1}{9}$$

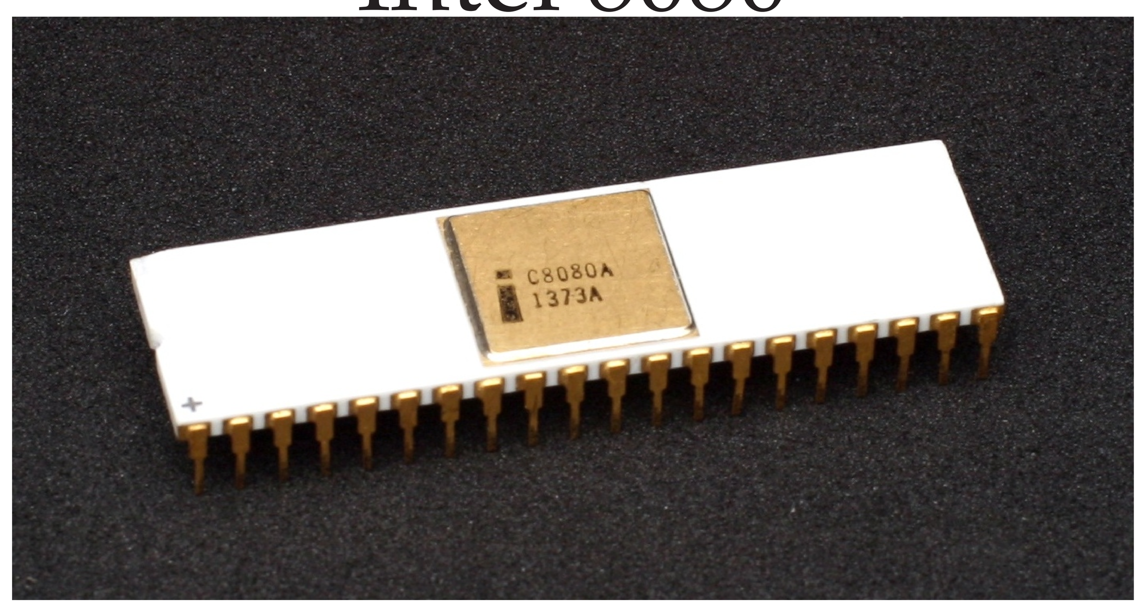


$$\begin{aligned} f(q_1, q_2) &= \frac{8}{9}q_1 - \frac{1}{9}q_2 - \frac{4}{9}q_1 q_2 + \frac{1}{9} \\ P(Q_1 = q_1, Q_2 = q_2) &\propto \exp\left[-\beta f(q_1, q_2)\right] \\ \beta &\approx 16.6 \end{aligned}$$

(q_1, q_2)	$f(\mathbf{q})$	$P(\mathbf{Q} = \mathbf{q})$	D-Wave probs.
$(0, 0)$	$\frac{1}{9}$	0.136	0.136
$(1, 0)$	1	5×10^{-8}	10^{-6}
$(0, 1)$	0	0.863	0.863
$(1, 1)$	$\frac{4}{9}$	0.0005	0.00018

3rd Generation Intel

Intel 8080



24 head nodes
48 parameters

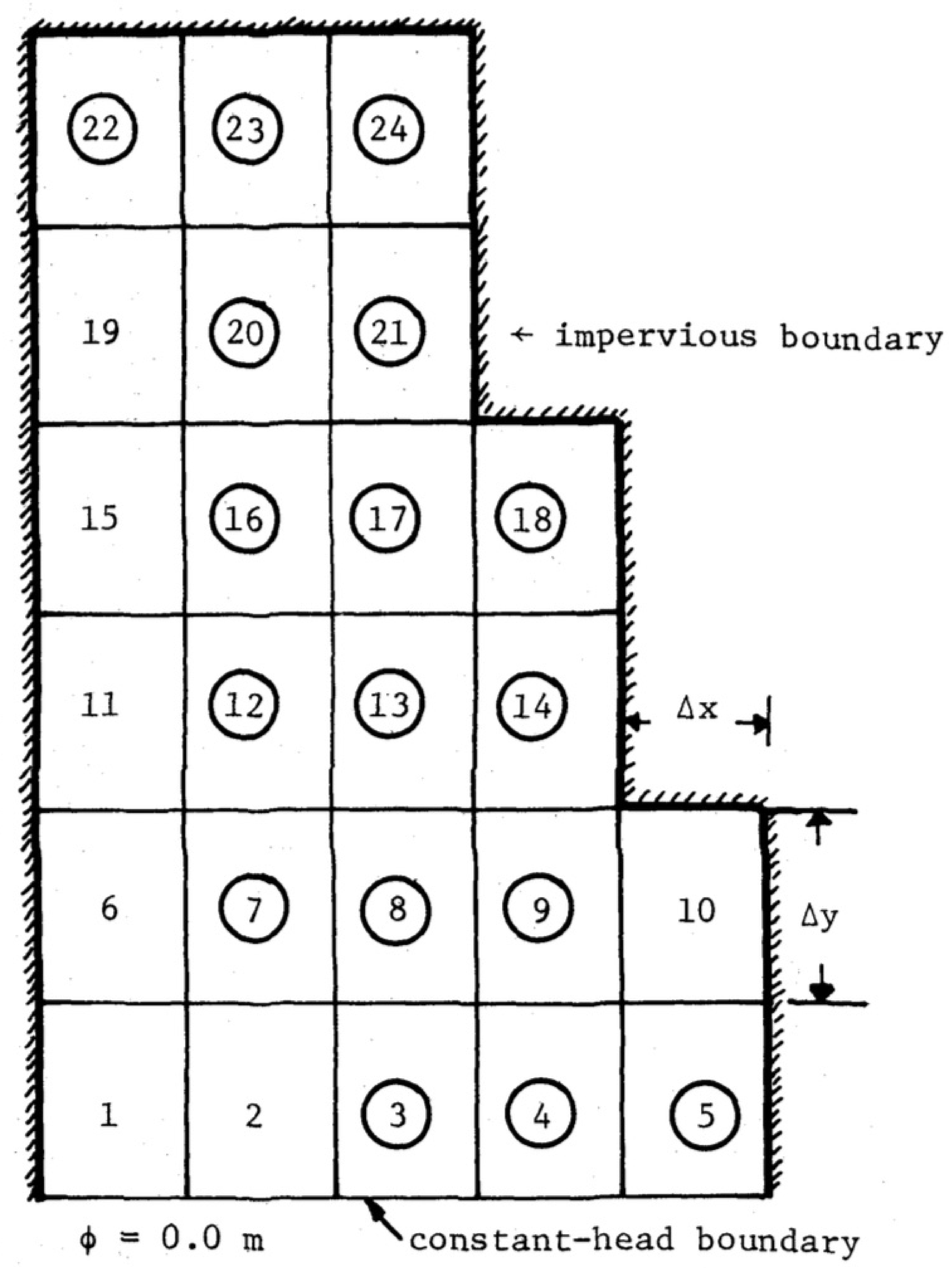
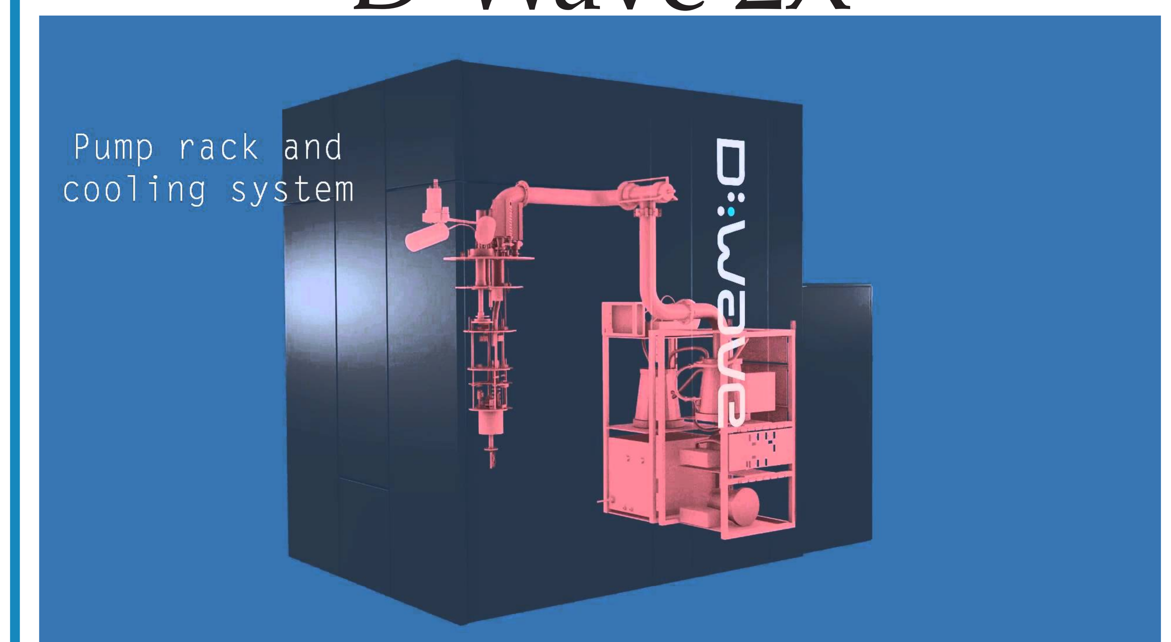


Fig. 3. The model studied in example 1.

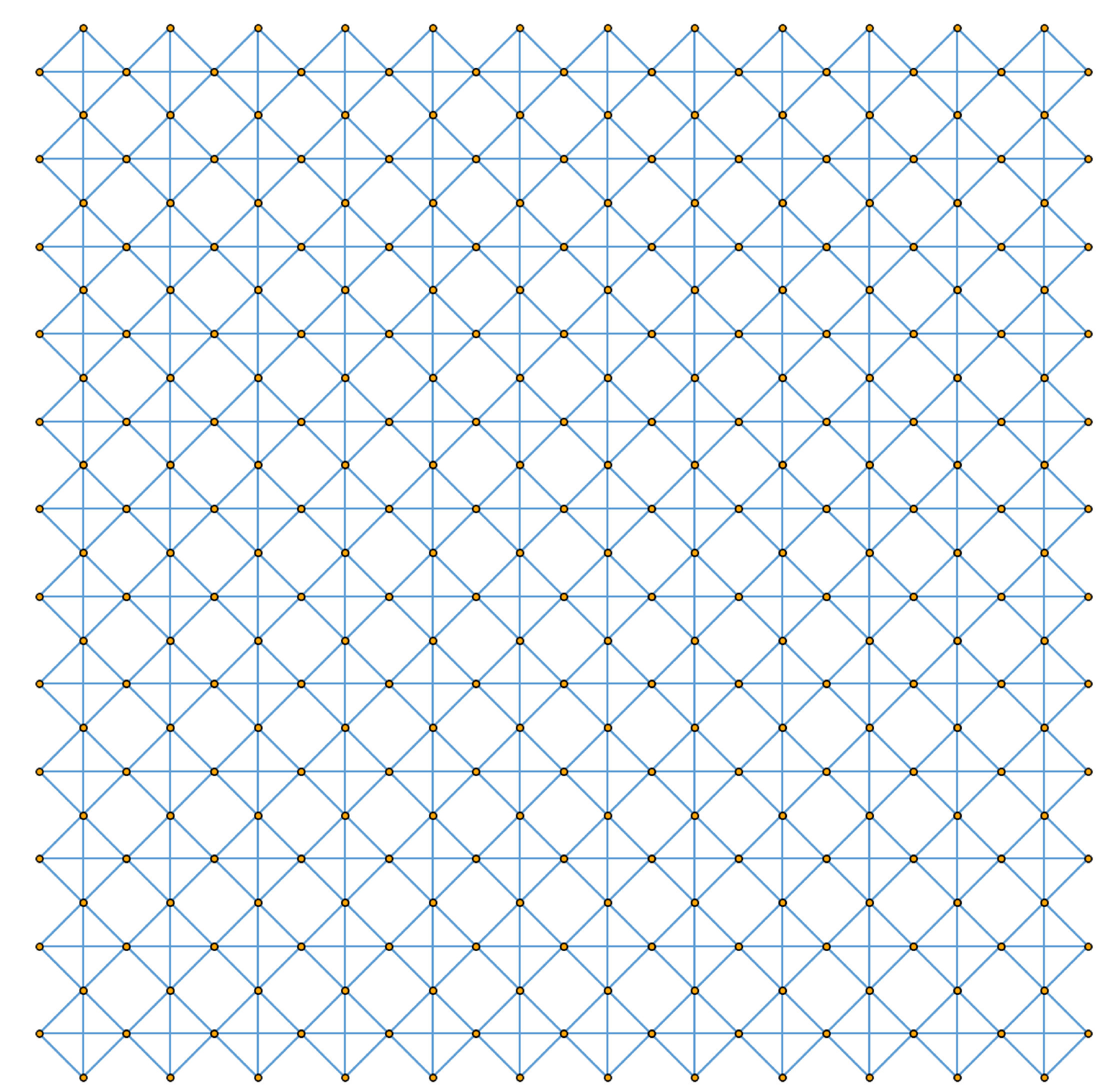
"The identification problem as stated in the present work is solved as a linear or a **quadratic programming problem**. The solution in the latter case is much more complicated, whereas the solution of the linear programing problem is based on readily available computer programs."[1]

3rd Generation D-Wave

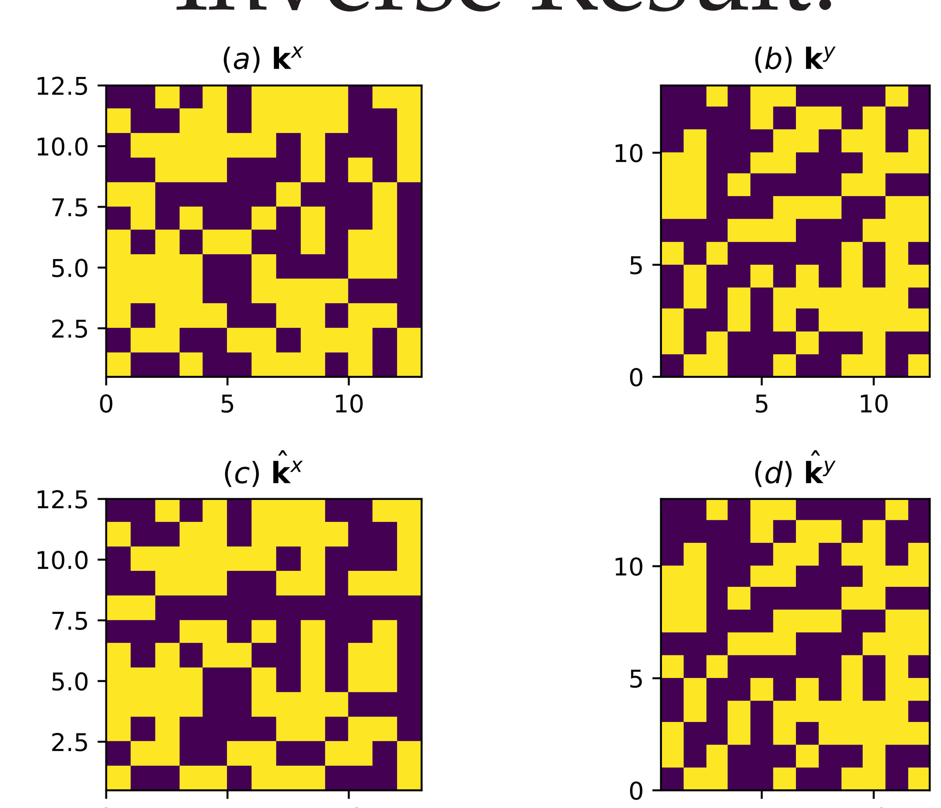
D-Wave 2X



196 head nodes
312 parameters

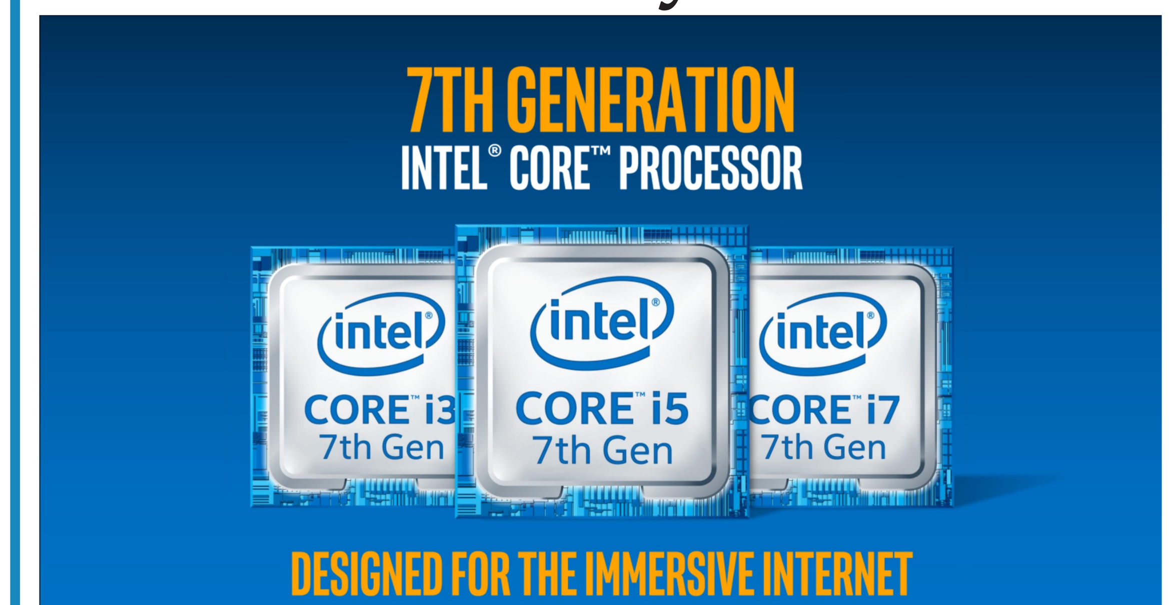


Inverse Result:[2]

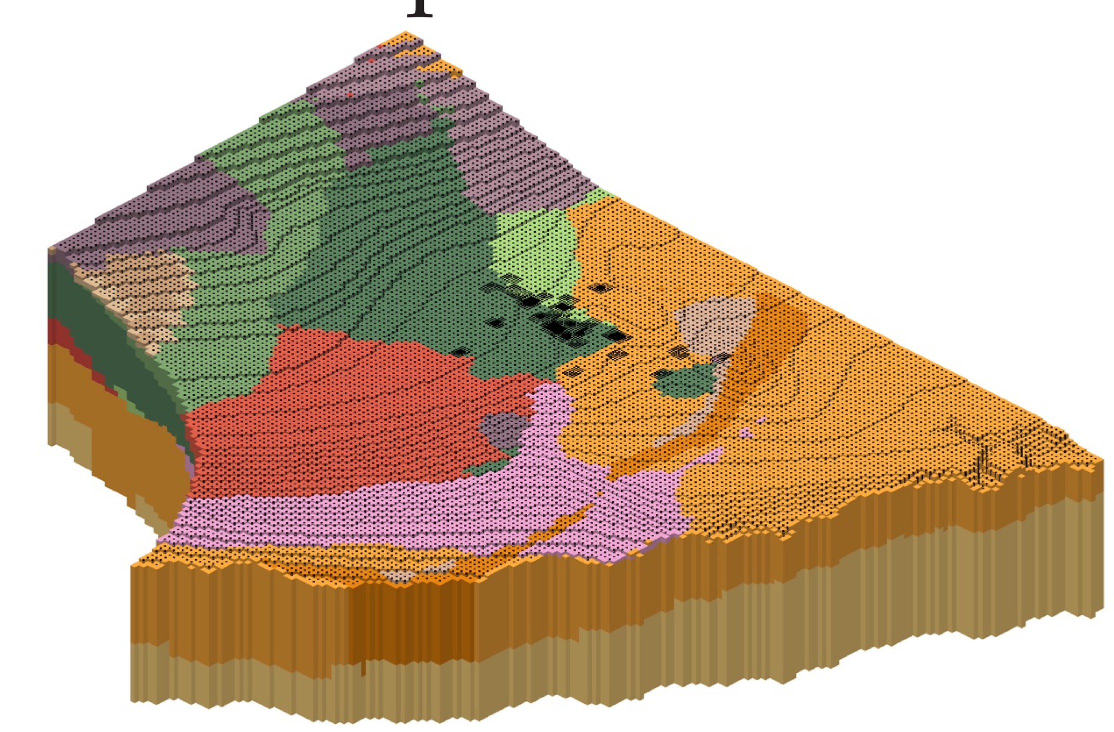


20th Generation Intel

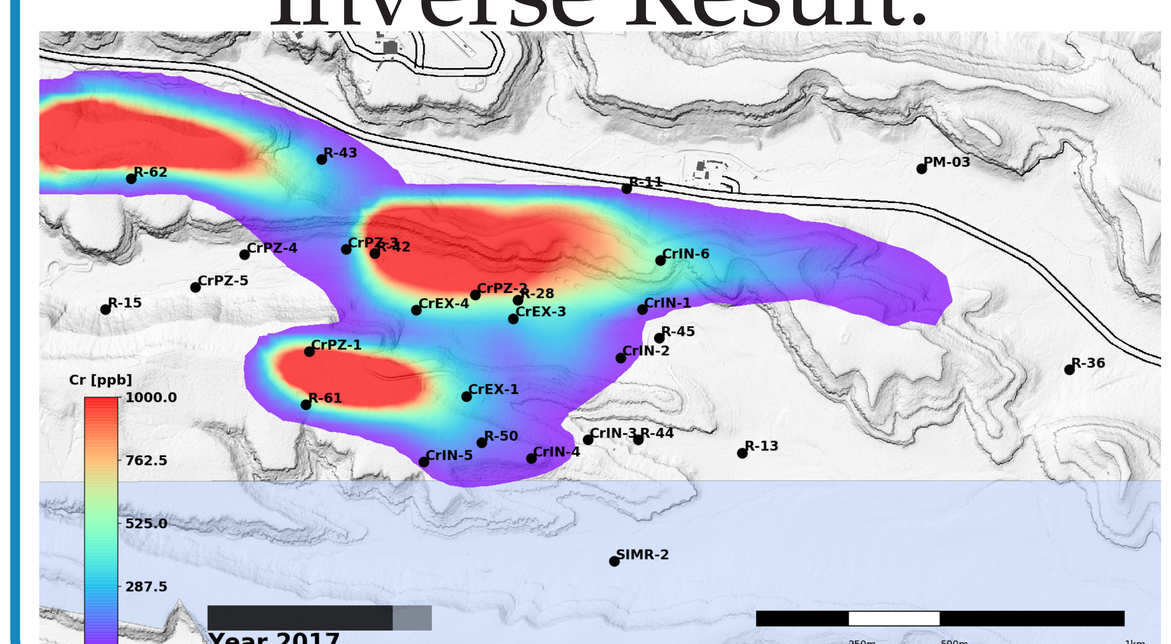
Intel Kaby Lake



766,283 head nodes
252 parameters



Inverse Result:



References

1: Hefez, E., Shamir, U., & Bear, J. (1975). Identifying the parameters of an aquifer cell model. *Water Resources Research*, 11(6), 993-1004.
2: O'Malley, D. (2017) Quantum-computational hydrologic inverse analysis. *In submission*.