

Quantum Annealing Applied to Optimization Problems in Radiation Medicine



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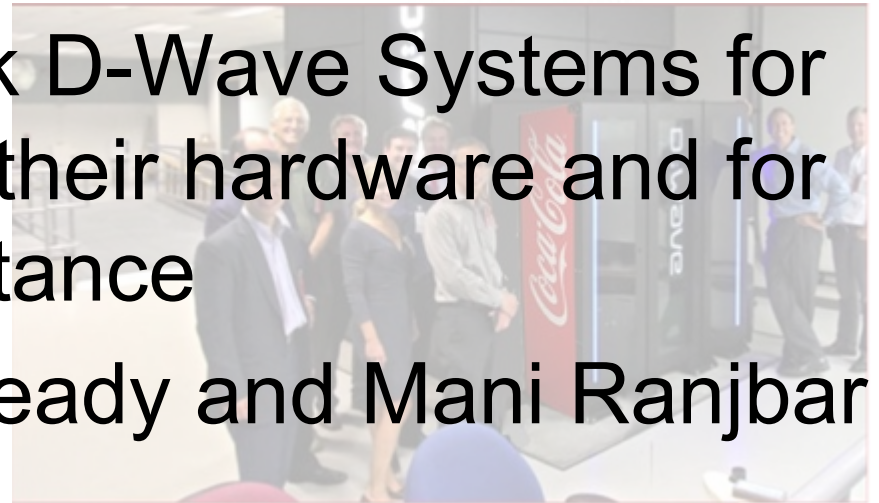
Acknowledgments

We would like to thank D-Wave Systems for providing access to their hardware and for computational assistance

In particular, Bill Macready and Mani Ranjbar

Jason Spaans

Tyler Papham



Cancer is one of the leading causes of morbidity and mortality worldwide

In 2012 there were 14 million new cases of cancer

There were 8.2 million cancer-related deaths

Number of new cases expected to rise by 70% over next 2 decades (WHO)



Cancer in the US:

In 2016 there will be an estimated 1.69 million new cases of cancer

There will be 596,000 cancer deaths

39.6% of people will be diagnosed with cancer in their lifetimes

Most common types: breast, lung, prostate, colon, bladder

Cancer is treated using three methods:

Surgery



Cancer is treated using three methods:
Chemotherapy

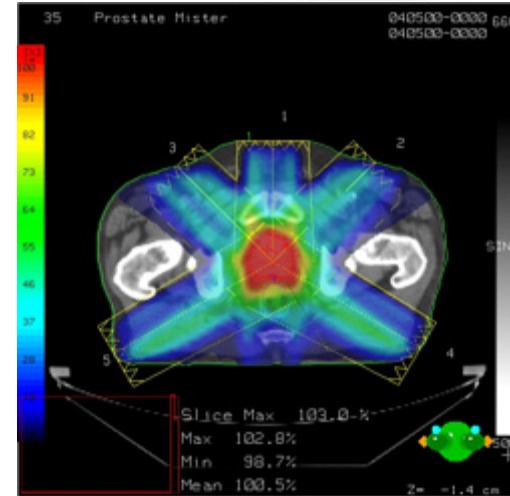


Cancer is treated using three methods:
Radiation Therapy



This is the subject of our work

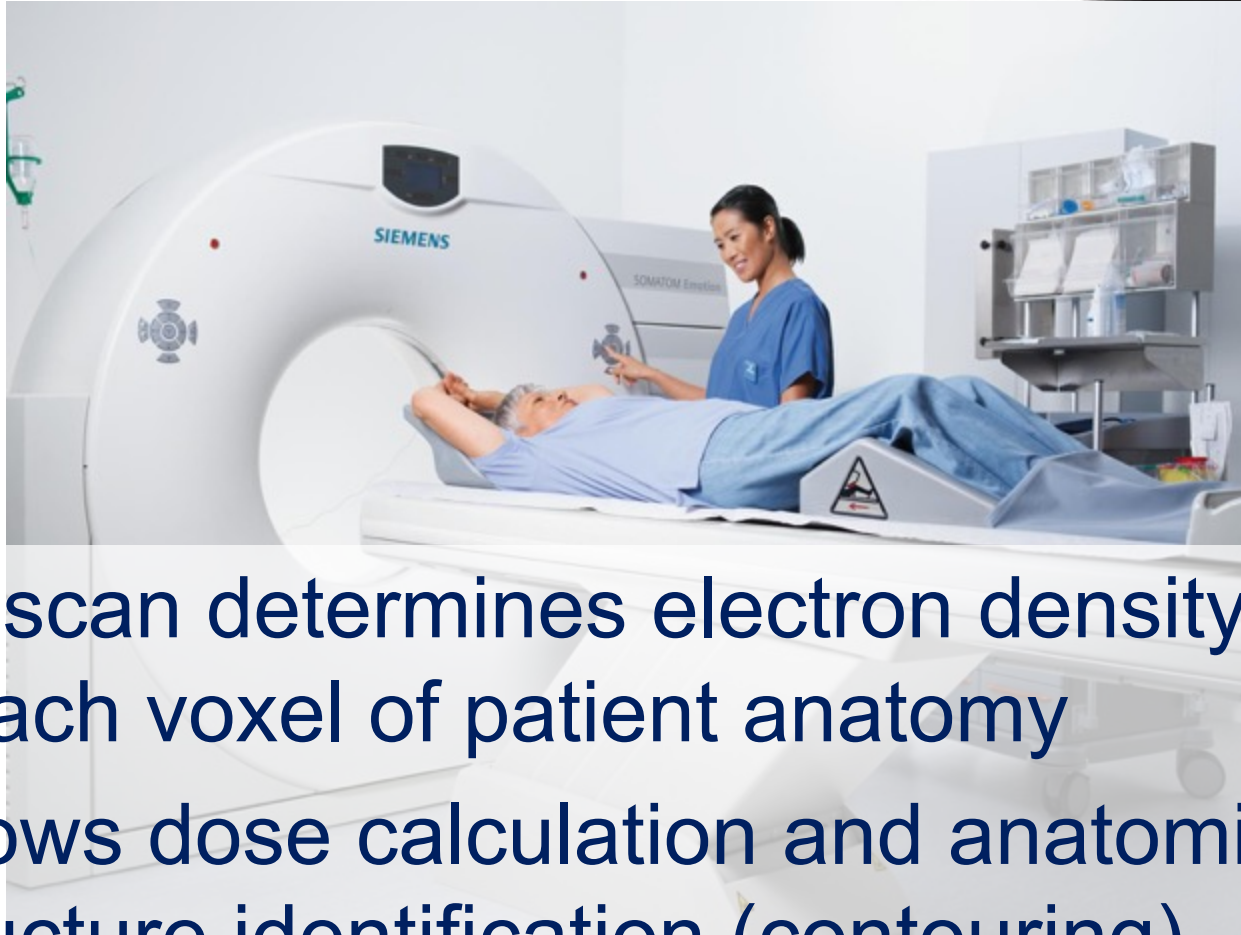
Radiation dose distribution



Absorbed dose measured in Gy (J/kg)

Calculated from well-known physics principles

Clinical calculations use FDA-approved software



CT scan determines electron density of each voxel of patient anatomy

Allows dose calculation and anatomic structure identification (contouring)

Medical Linear Accelerator



Linear Accelerator Part 1

Radiation Production

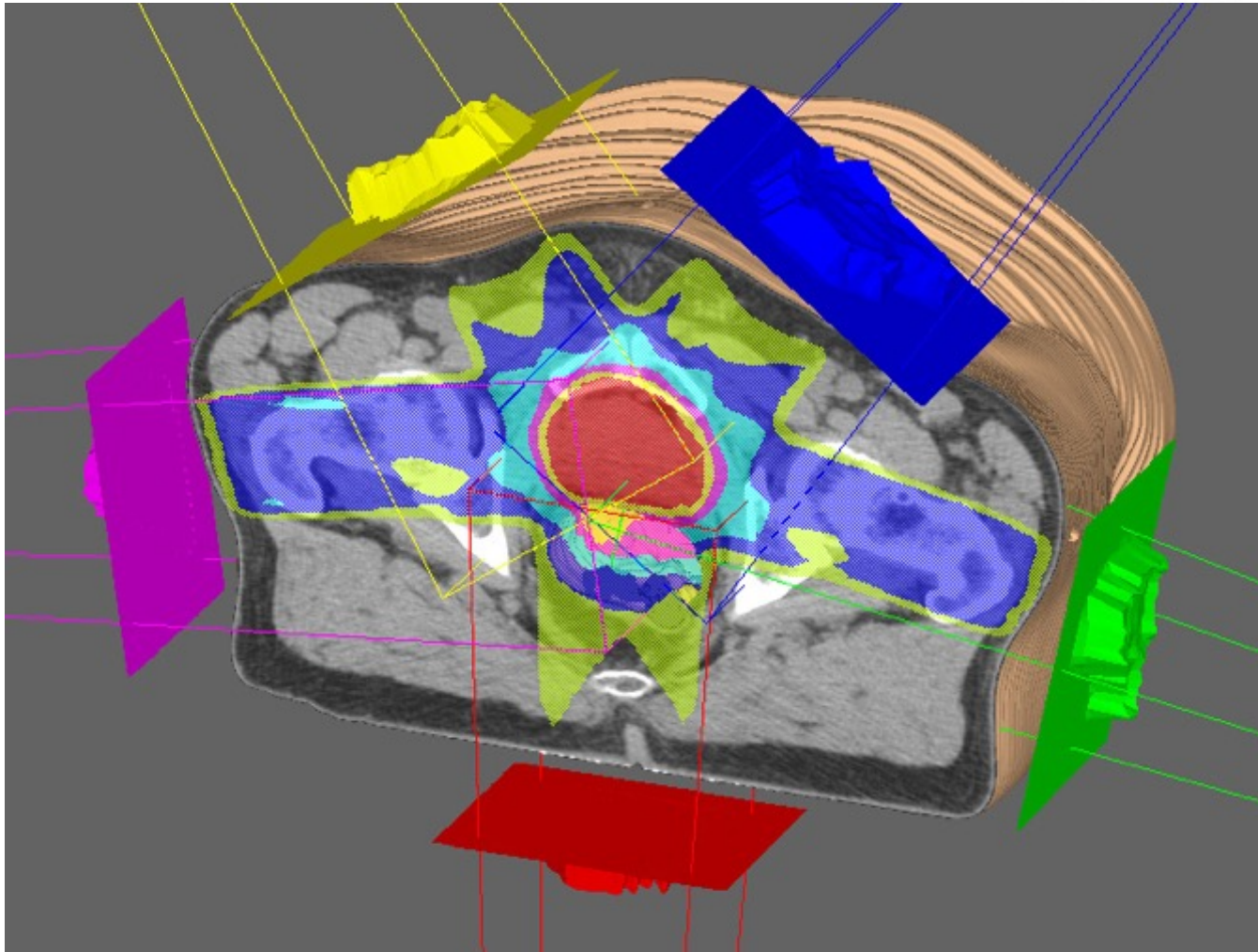


Linear Accelerator Part 2

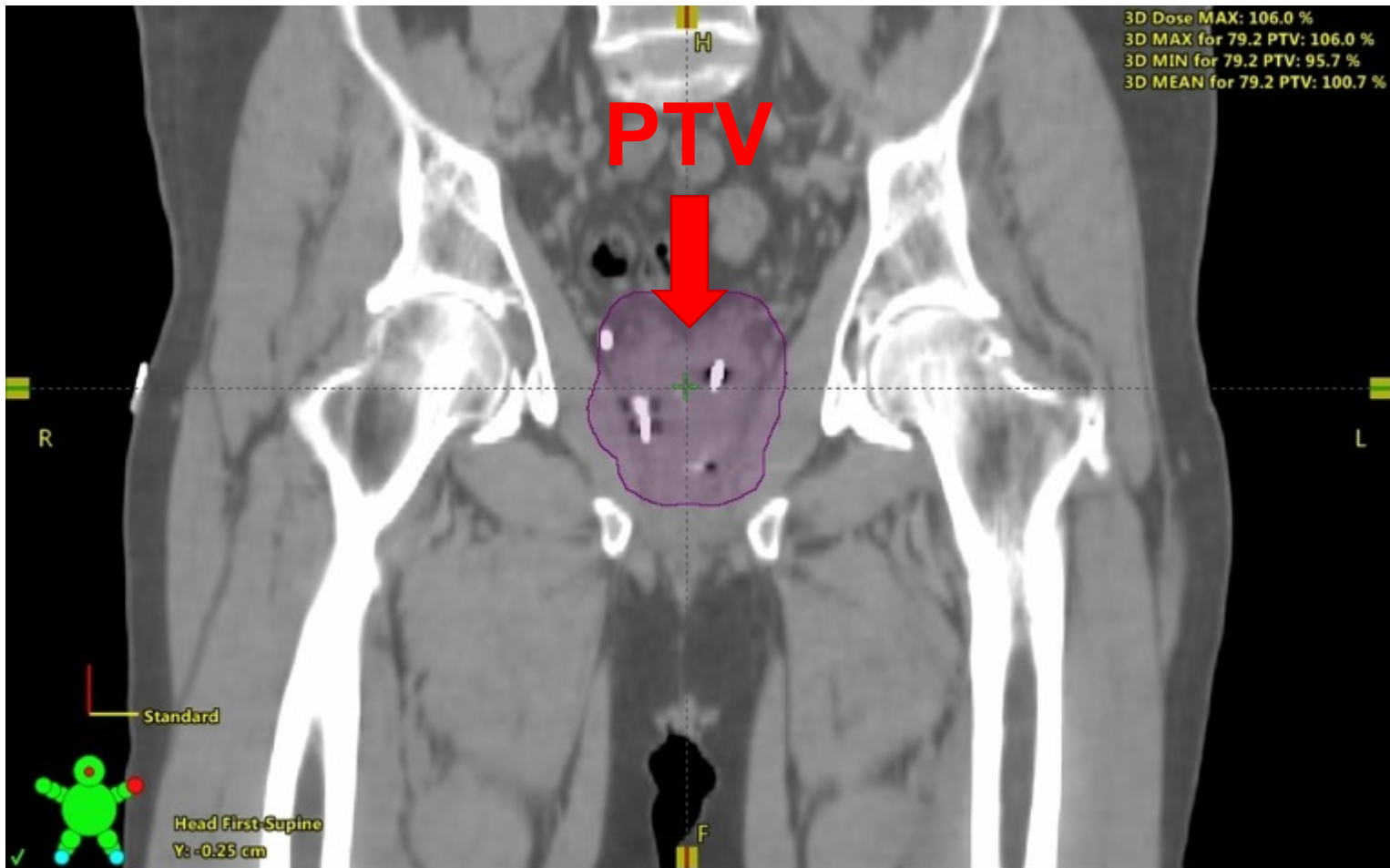
Energy ~ 6 MeV

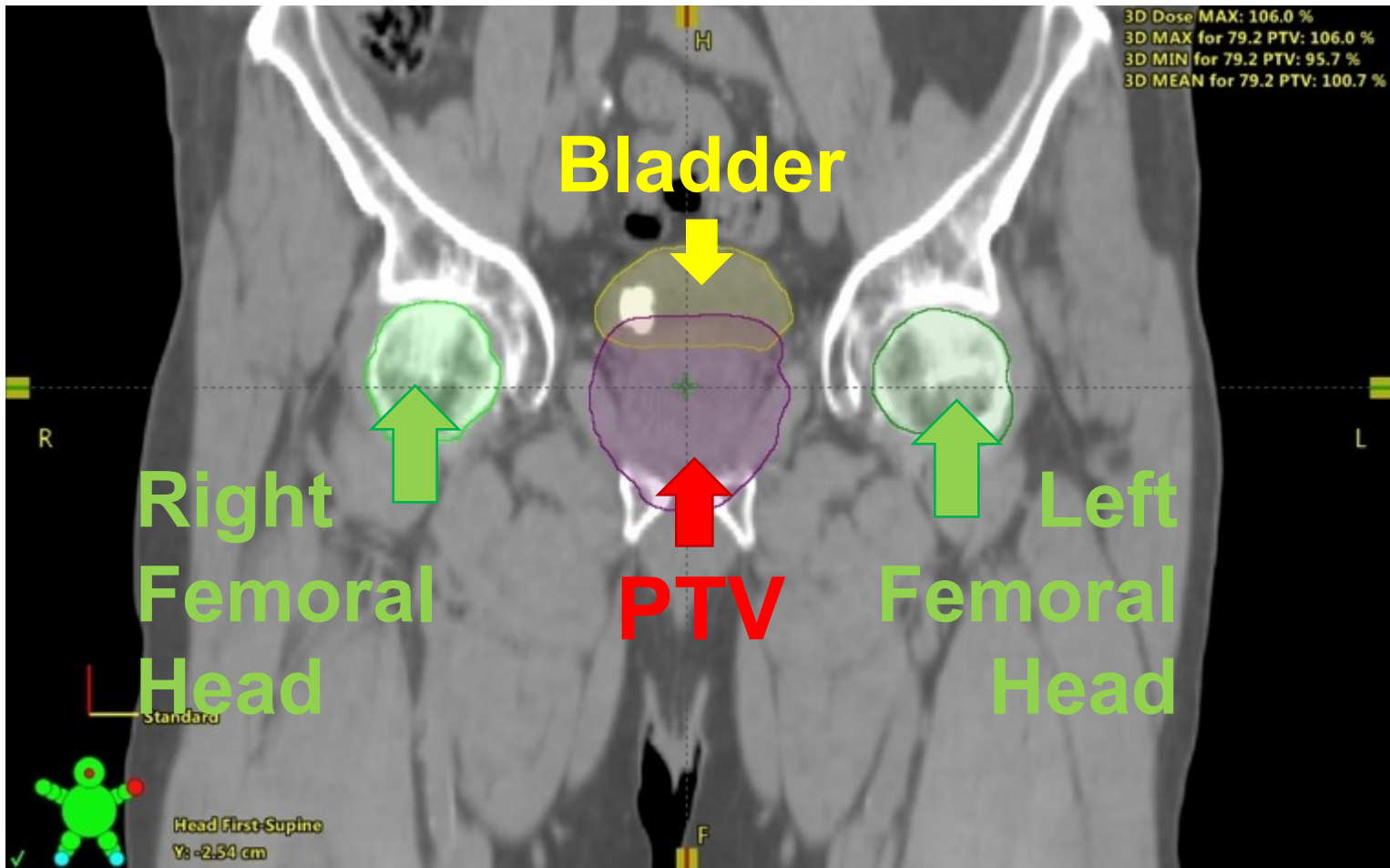


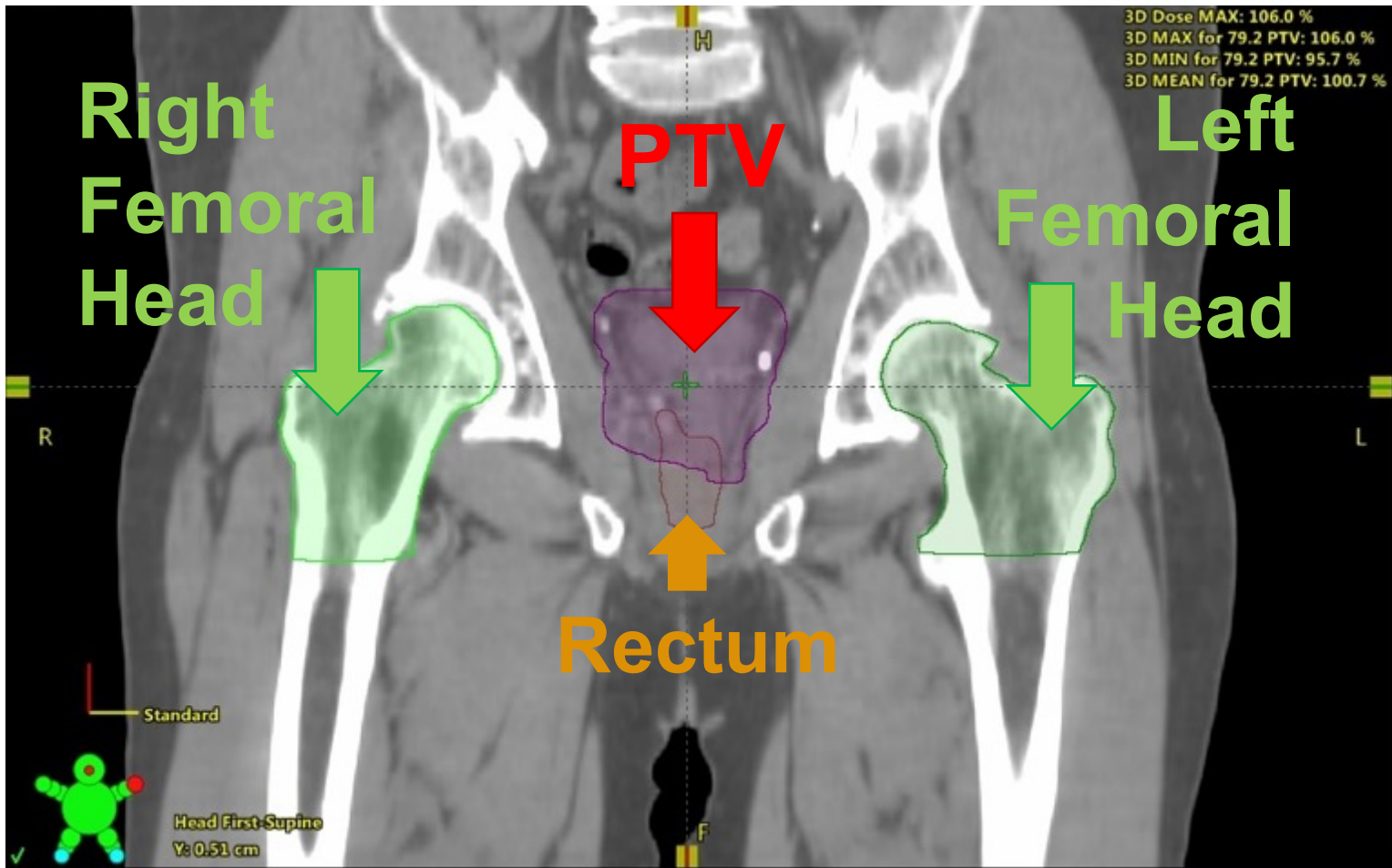
Linear Accelerator Part 3

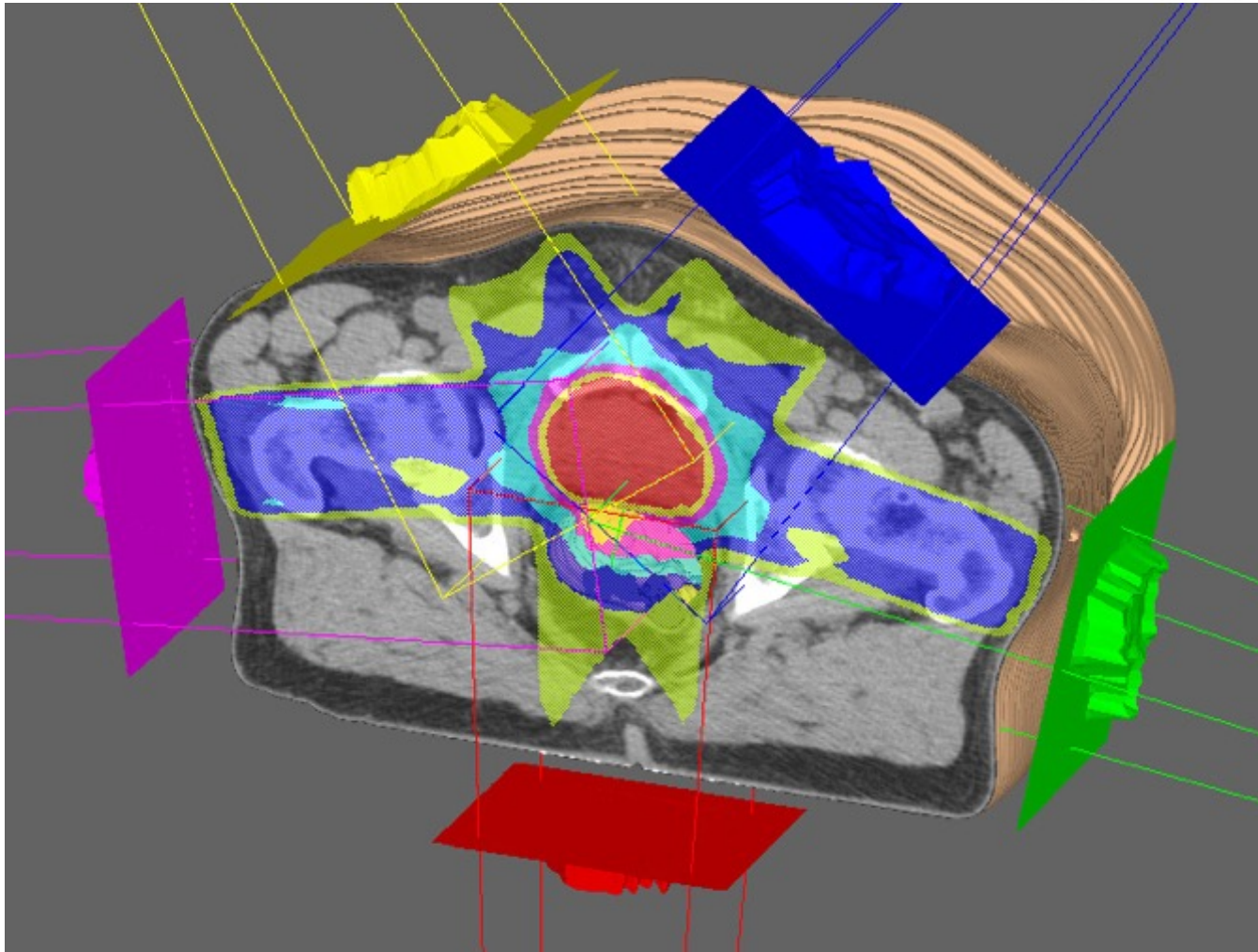


IMRT Treatment

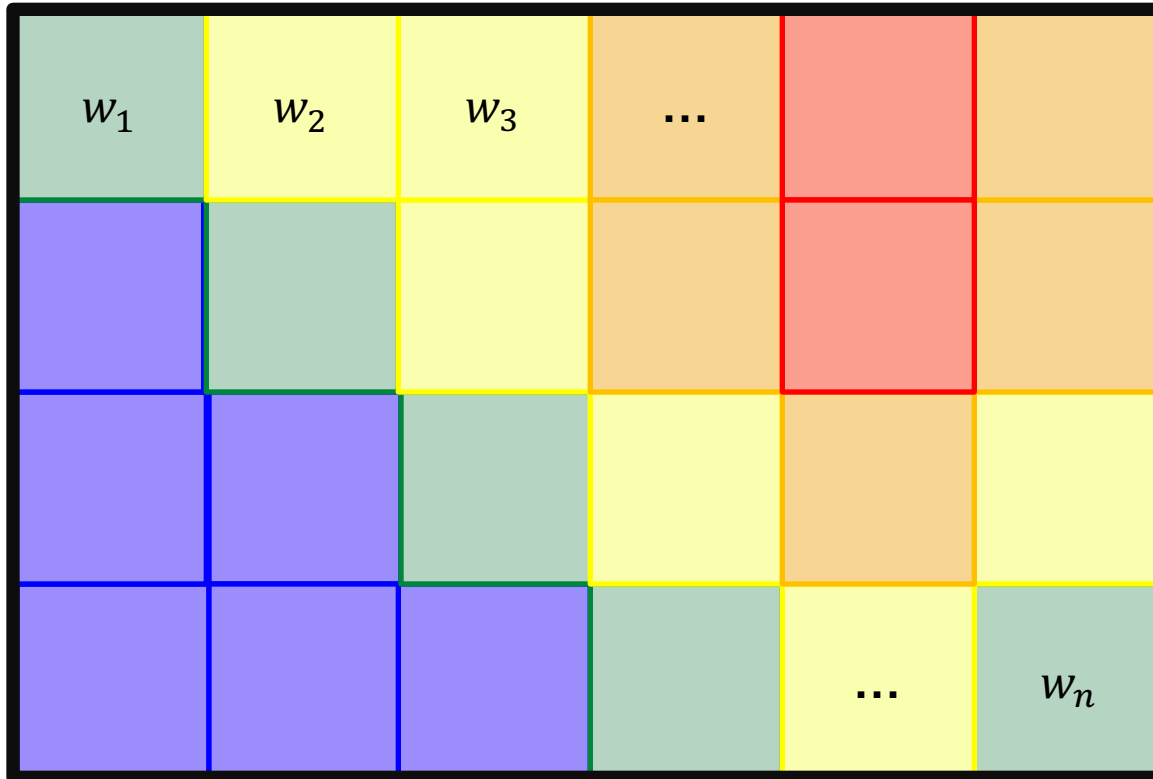






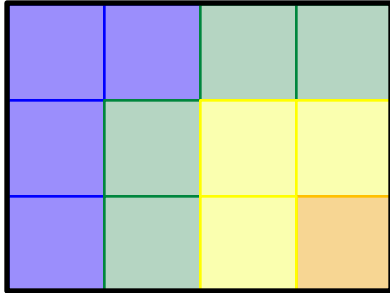


x-jaw

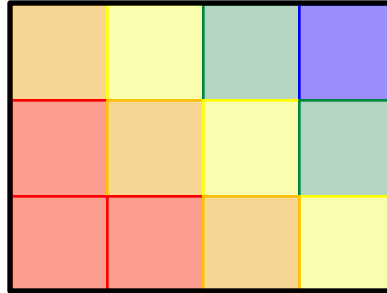


y-jaw

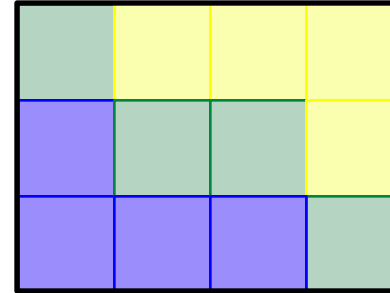
$$\mathbf{W}_{beam} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \cdot \\ \cdot \\ \cdot \\ w_n \end{pmatrix}$$



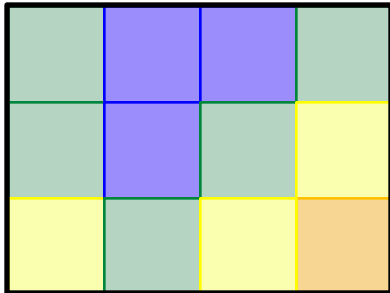
Beam 1



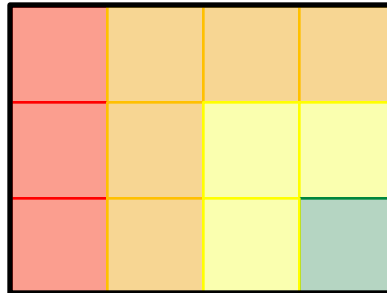
Beam 2



Beam 3



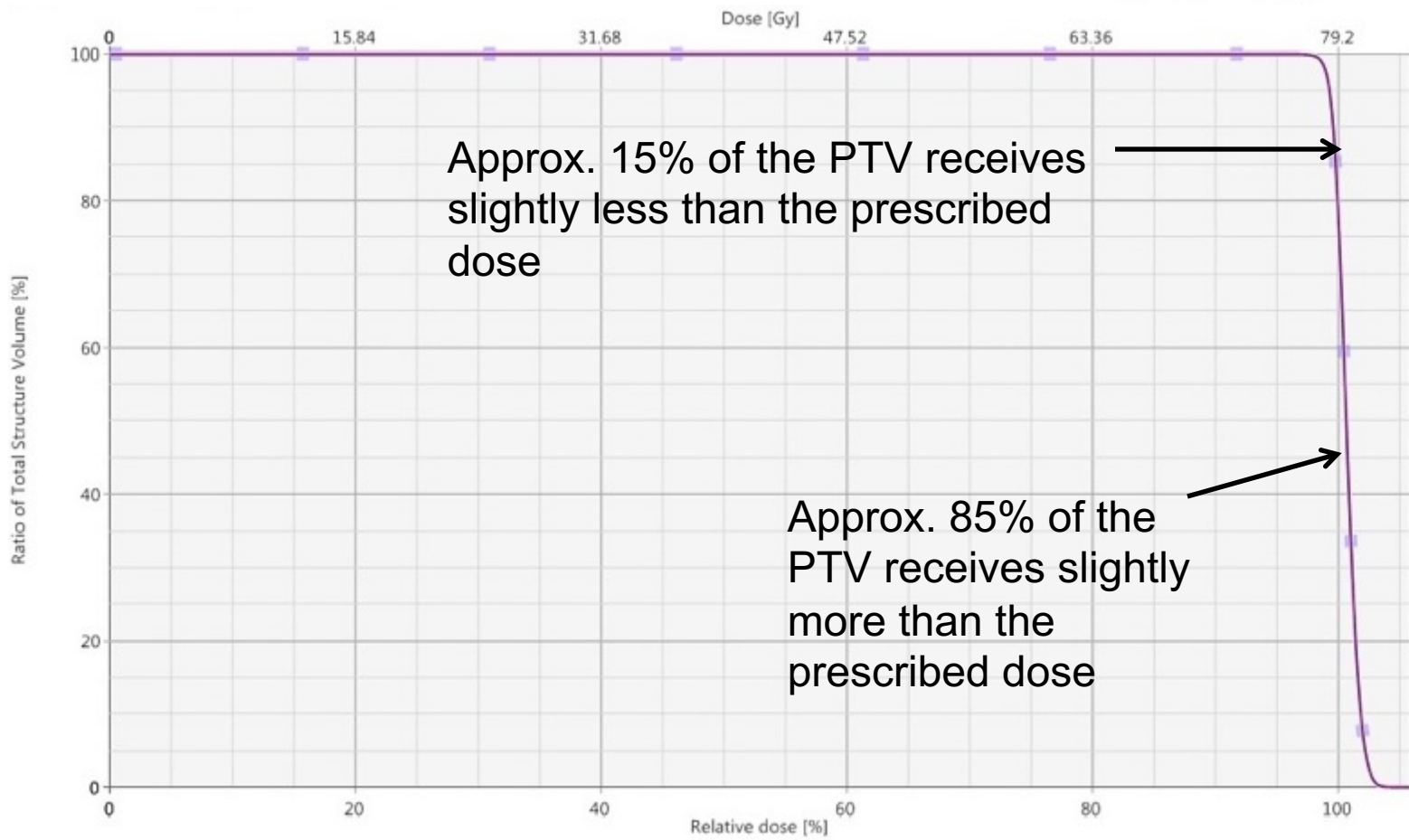
Beam 4



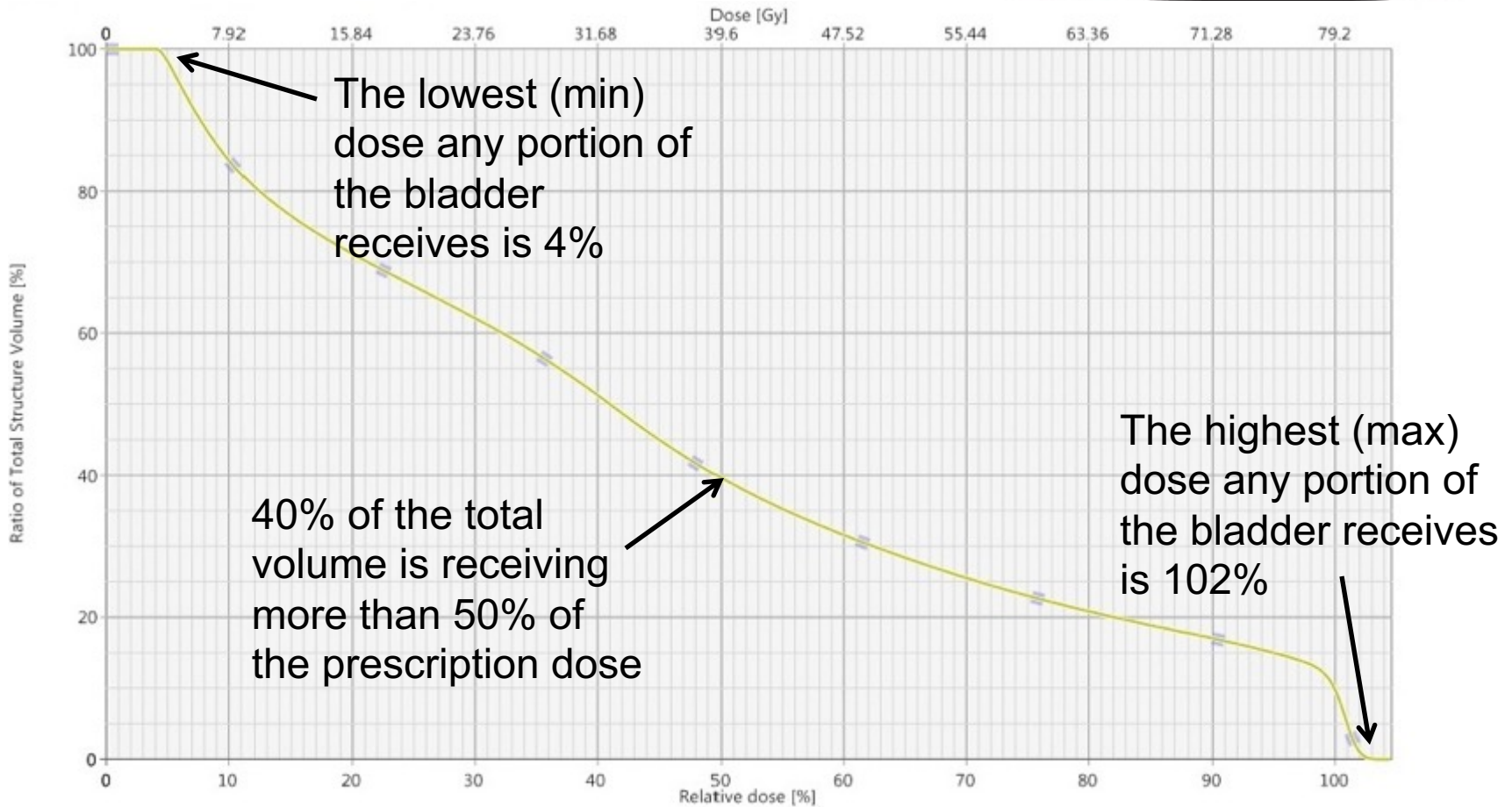
Beam 5

$$\mathbf{W} = \begin{pmatrix} \mathbf{w}_{beam\ 1} \\ \mathbf{w}_{beam\ 2} \\ \mathbf{w}_{beam\ 3} \\ \mathbf{w}_{beam\ 4} \\ \mathbf{w}_{beam\ 5} \end{pmatrix}$$

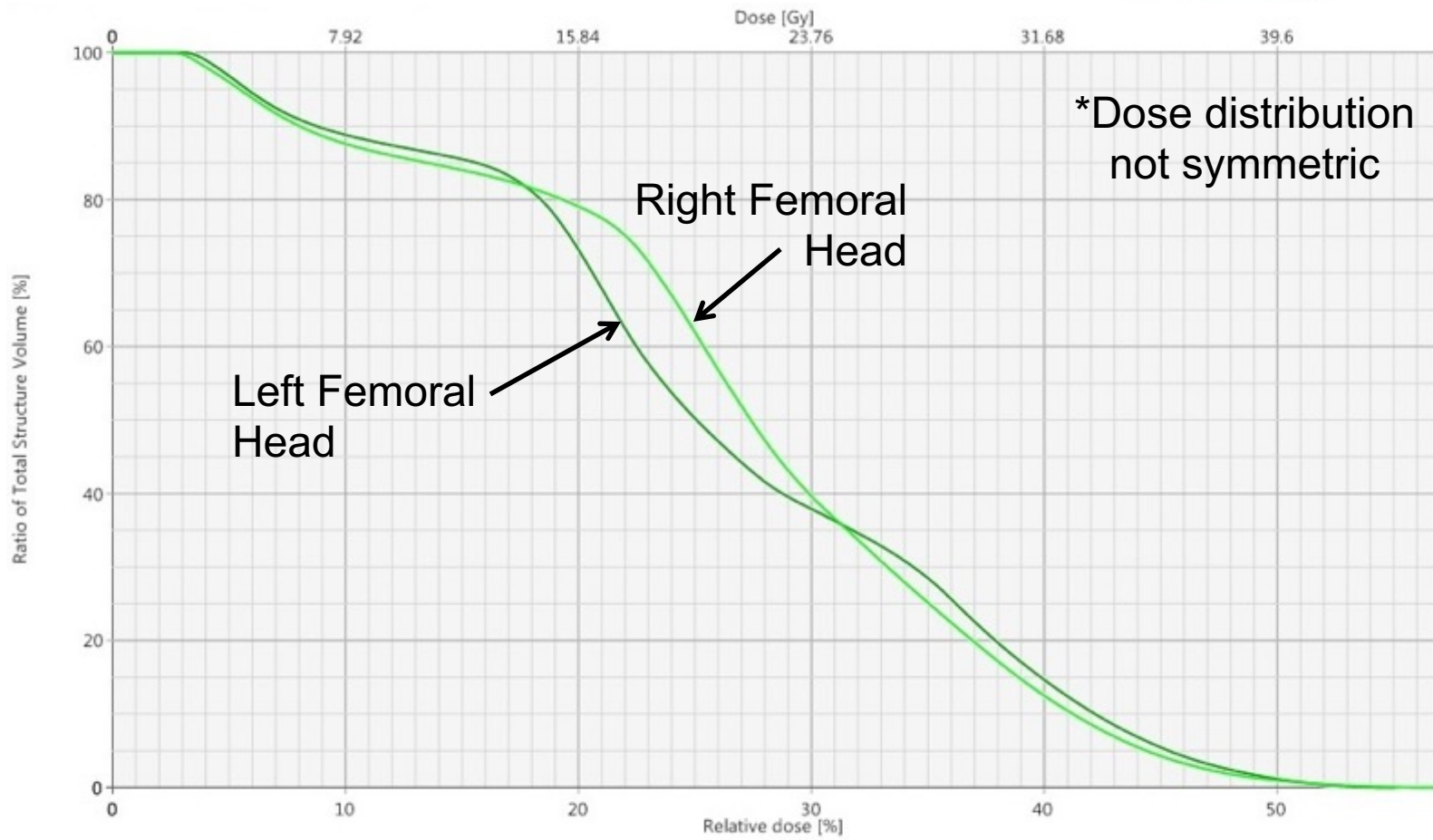
- A Dose-Volume Histogram (DVH) is a graphical representation of the percentage of dose received by a portion of the volume
- For a given treatment plan, the PTV and each organ has an associated DVH
- Is critical to defining the objective function



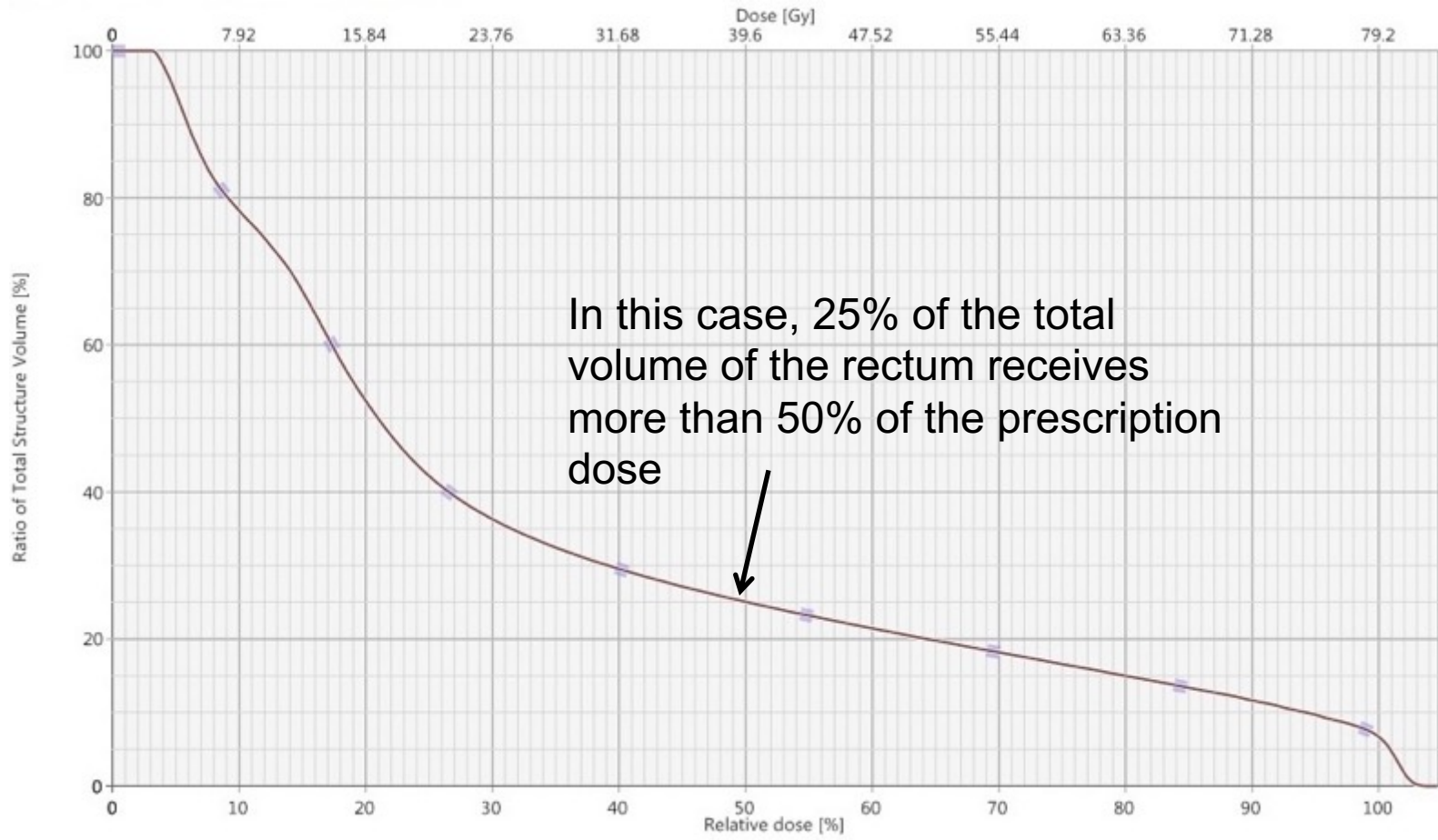
Bladder DVH



Fem. Heads DVH



Rectum DVH



The Objective Function

$$F(\mathbf{w}) = \alpha(P_v - D_v(\mathbf{w}))^2 + \sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$

\mathbf{w} is a vector of beamlet weights or intensities

Minimizing $F(\mathbf{w})$ results in optimal IMRT treatment plan

The Target

$$F(\mathbf{w}) = \alpha(P_v - D_v(\mathbf{w}))^2 + \sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$

α =Priority of target dose (How important is it that this dose is fully administered?)

P_v =Dose prescribed to a given volume, v , of the target

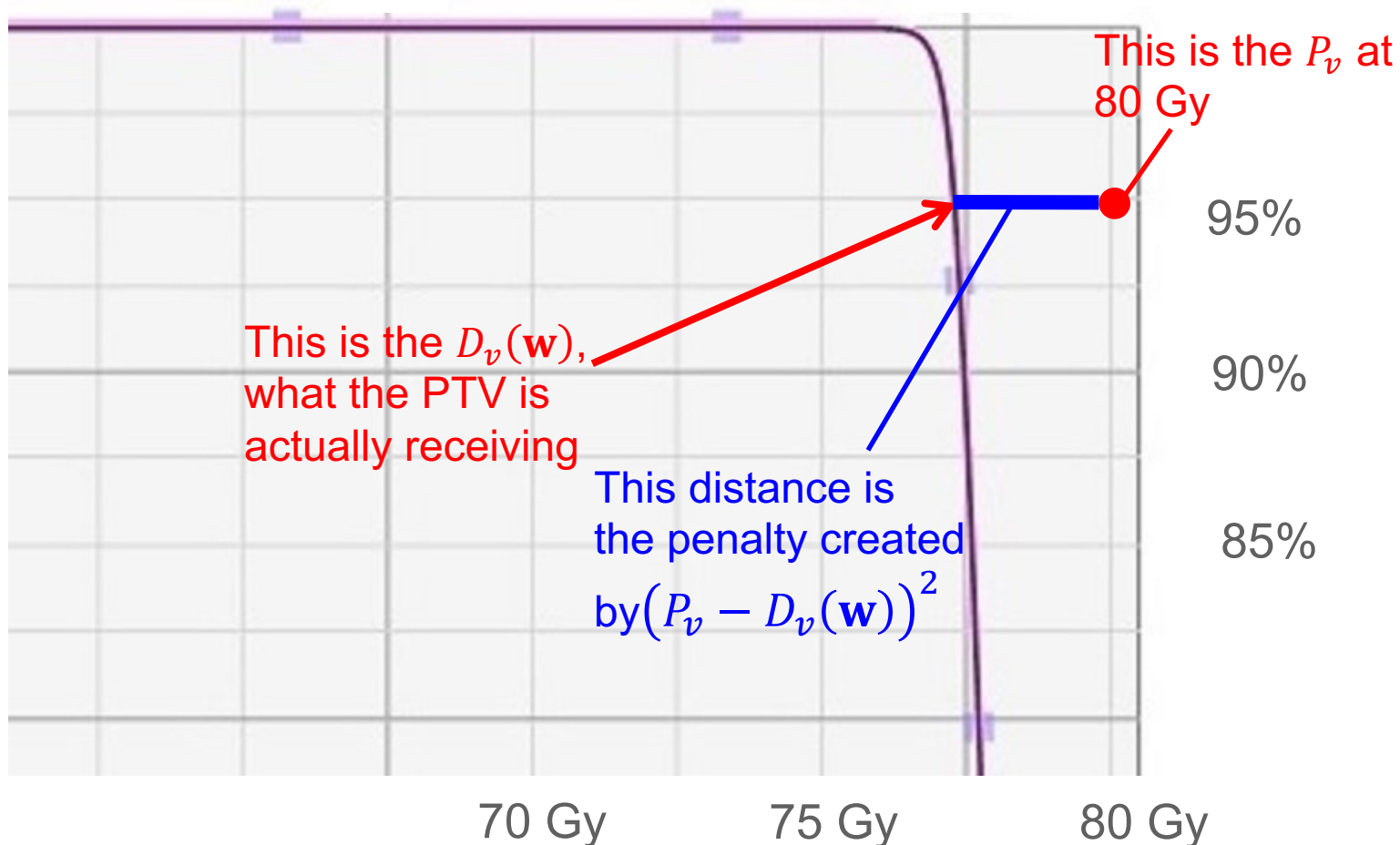
$D_v(\mathbf{w})$ =Dose actually received by volume v for weight vector \mathbf{w}

The Target

$$\alpha(P_v - D_v(\mathbf{w}))^2$$



$$\alpha(P_v - D_v(\mathbf{w}))^2$$



$$\alpha(P_v - D_v(\mathbf{w}))^2$$

- In clinical terms, this ensures that the dose received by the target is as close as possible to the dose prescribed

Organs at Risk (OARs)

$$F(\mathbf{w}) = \alpha(P_v - D_v(\mathbf{w}))^2 + \sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$

\sum_i = Sum over each OAR, eg. bladder = 1

\sum_j = Sum over multiple objectives for a given OAR

β_i = Priority of OAR

C_{ij} = Objective dose

D_{ij} = Actual dose received by OAR

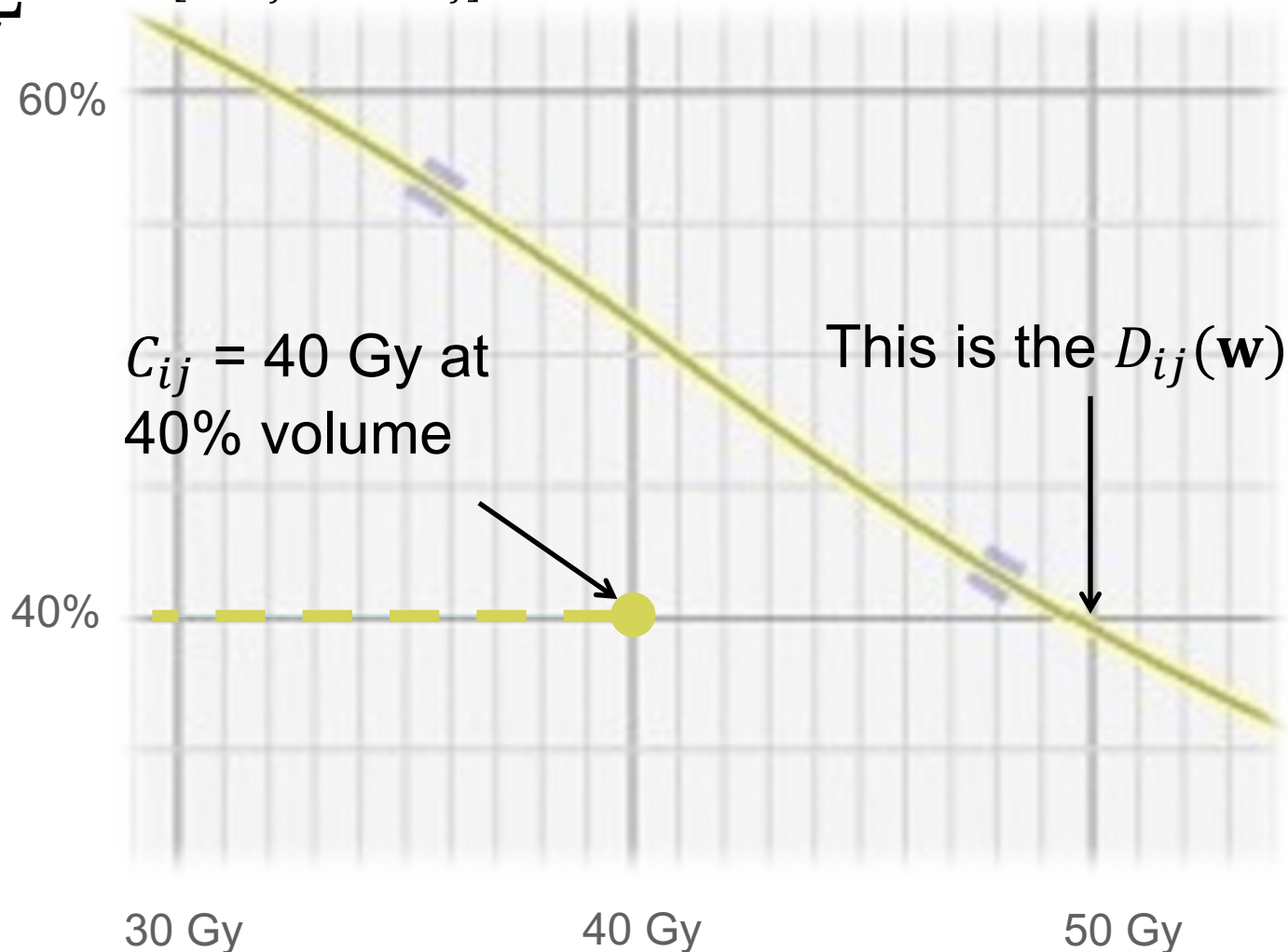
Organs at Risk (OARs)

$$\sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$



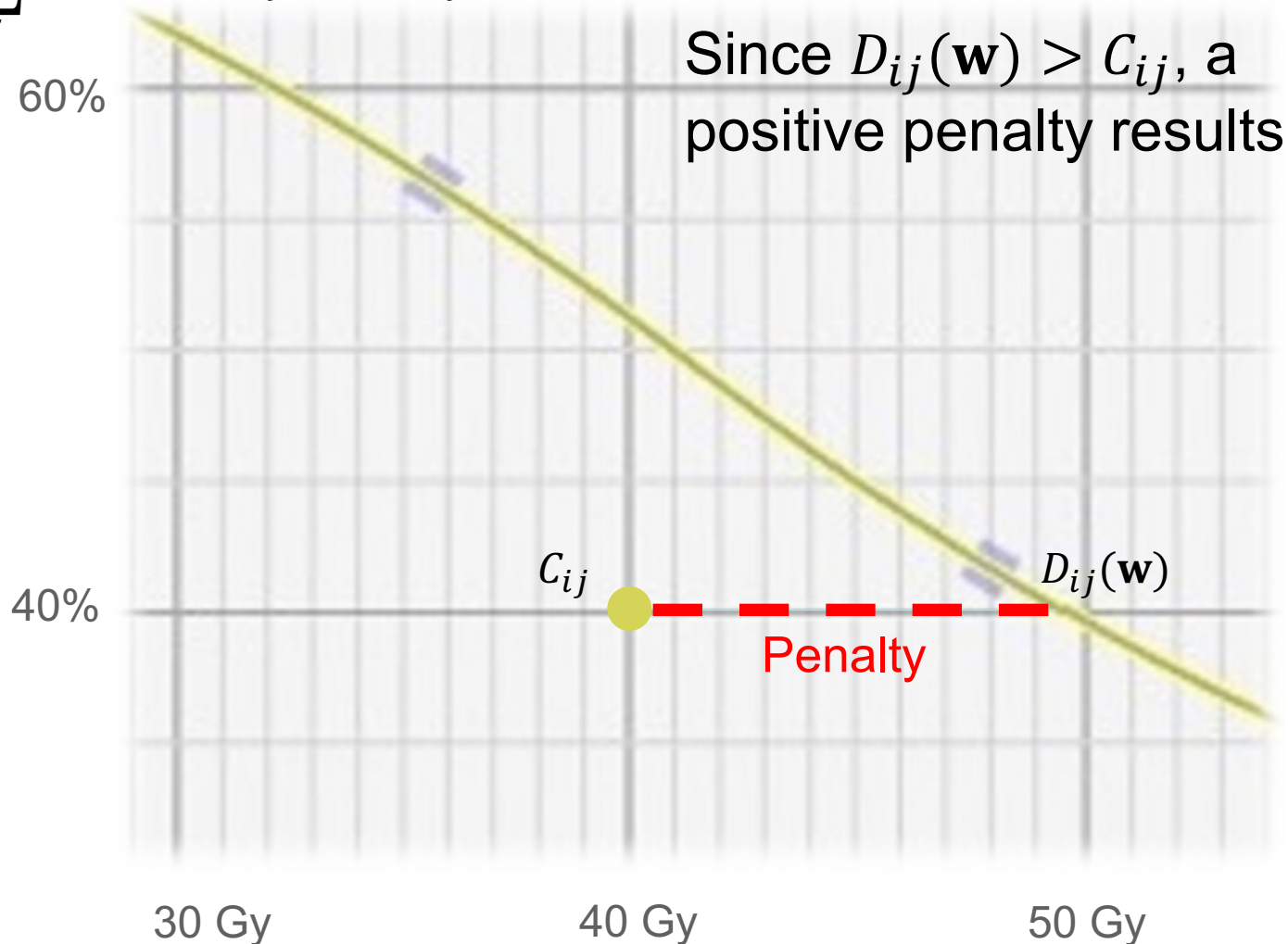
Organs at Risk (OARs)

$$\sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$



Organs at Risk (OARs)

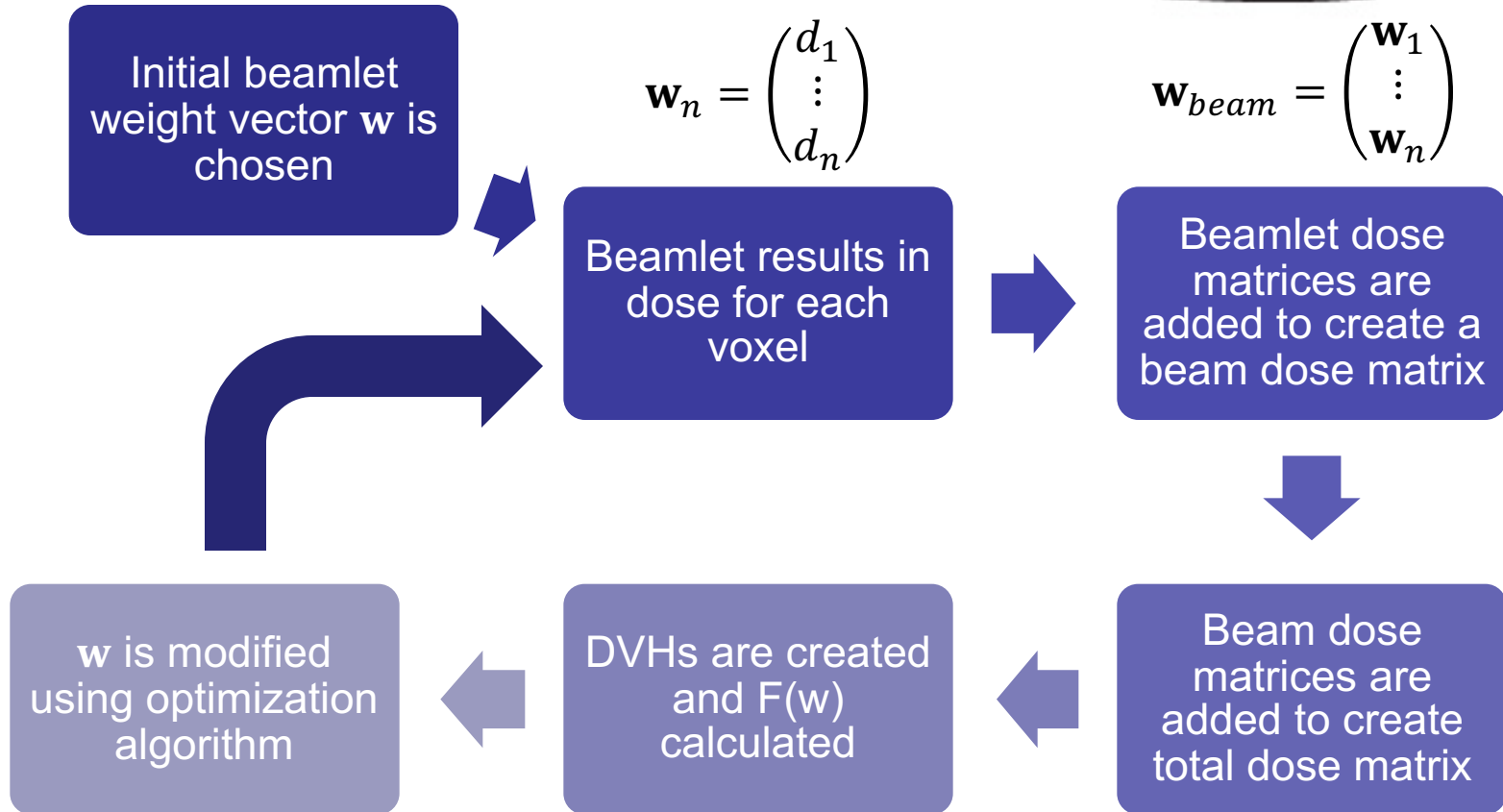
$$\sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$



$$\sum_i \sum_j \beta_i (\max[0, D_{ij}(\mathbf{w}) - C_{ij}])^2$$

- There is no reward for $D_{ij}(\mathbf{w}) < C_{ij}$ because there is negligible clinical benefit to administering less than the objective dose to the OAR

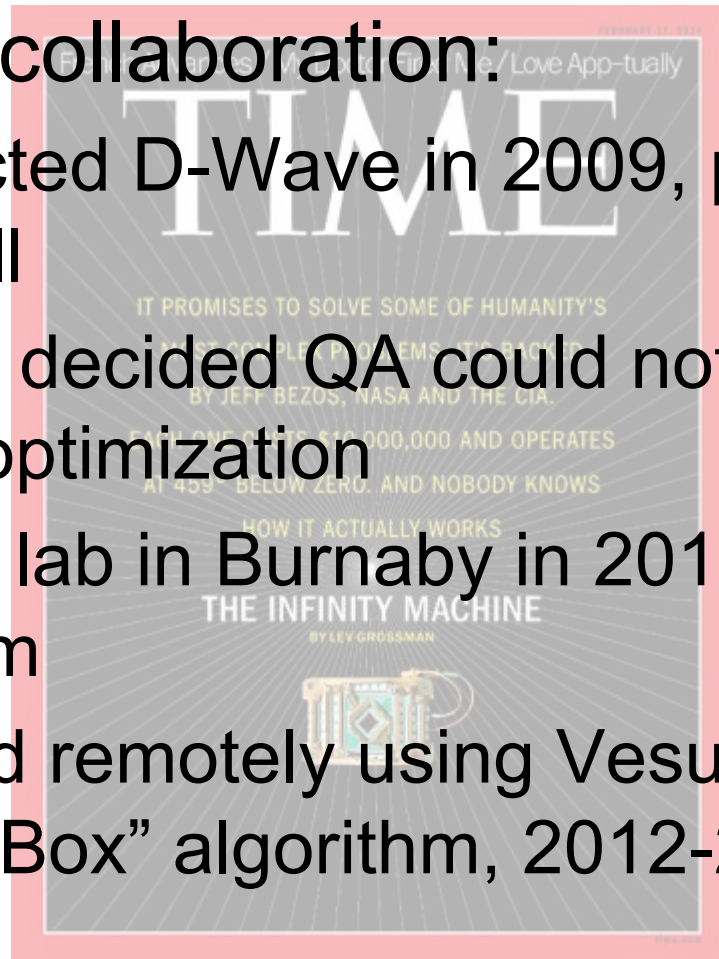
The Process



$$w_{total} = \begin{pmatrix} w_{beam\ 1} \\ \vdots \\ w_{beam\ n} \end{pmatrix}$$

History of collaboration:

- Contacted D-Wave in 2009, put in touch with Bill
- Initially decided QA could not support IMRT optimization
- Visited lab in Burnaby in 2011 and revisited problem
- Worked remotely using Vesuvius chip and “Black Box” algorithm, 2012-2014



First application of quantum annealing to IMRT beamlet intensity optimization

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CrossMark

Abstract

Optimization methods are critical to radiation therapy. A new technology, quantum annealing (QA), employs novel hardware and software techniques to address various discrete optimization problems in many fields. We report on the first application of quantum annealing to the process of beamlet intensity optimization for IMRT.

We apply recently-developed hardware which natively exploits quantum mechanical effects for improved optimization. The new algorithm, called

Vesuvius chip supported ~ 512 qubits

Weight variables discretized to 7-digit binary variables

Therefore, 70 beamlet weights (non-negative, continuous) were included

Actual clinical case would require 600-1000 beamlet weights

Conventional simulated annealing (SA) features:

- Minimize function that is combo of original plus entropy
- Entropy is weighted by temp parameter T
- T is slowly reduced from large values (search space exploration) to 0 (solution)
- Can attain global minimum if cooling slow enough (but exponentially long)

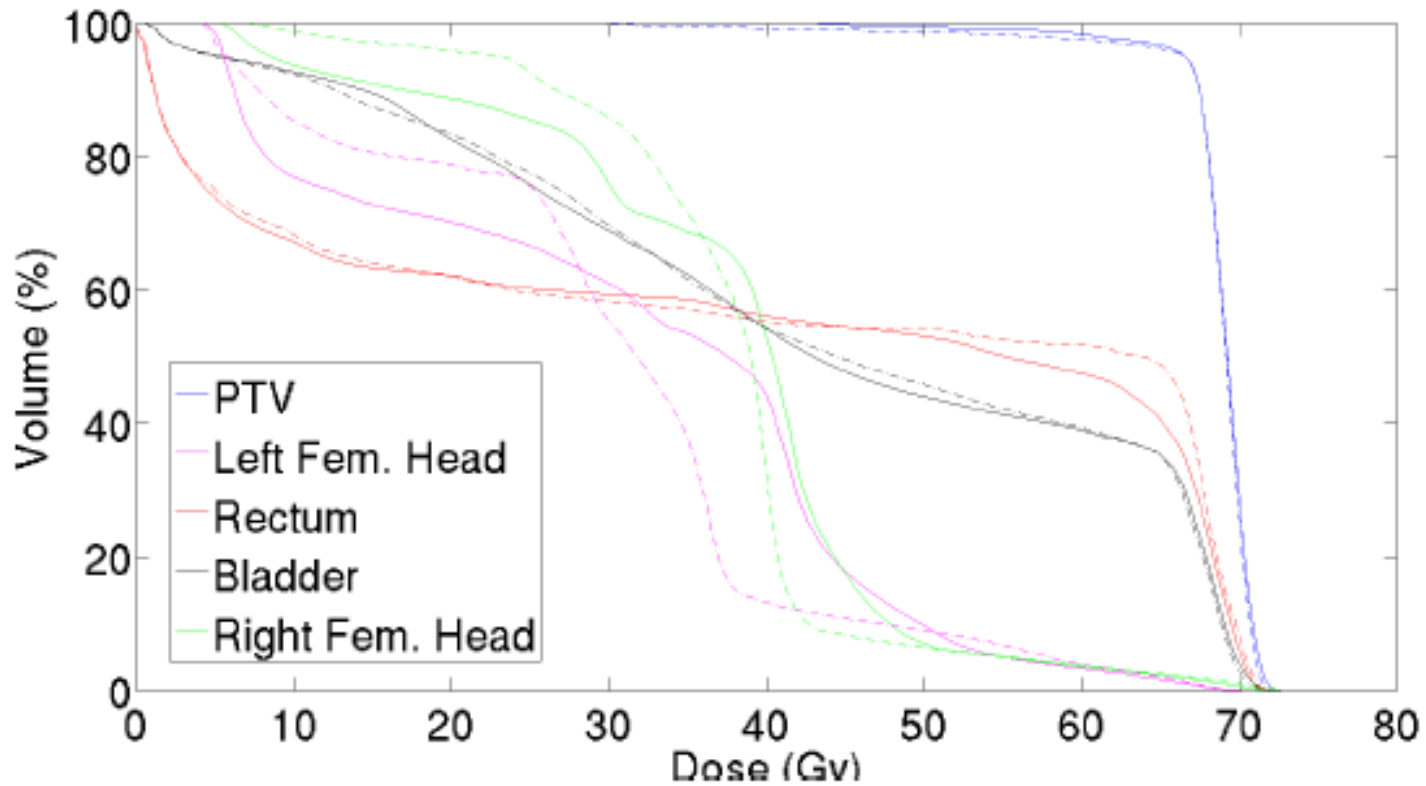
Three methods compared:

- Quantum annealing
- Simulated annealing
- Tabu search: popular heuristic used in combinatorial optimization

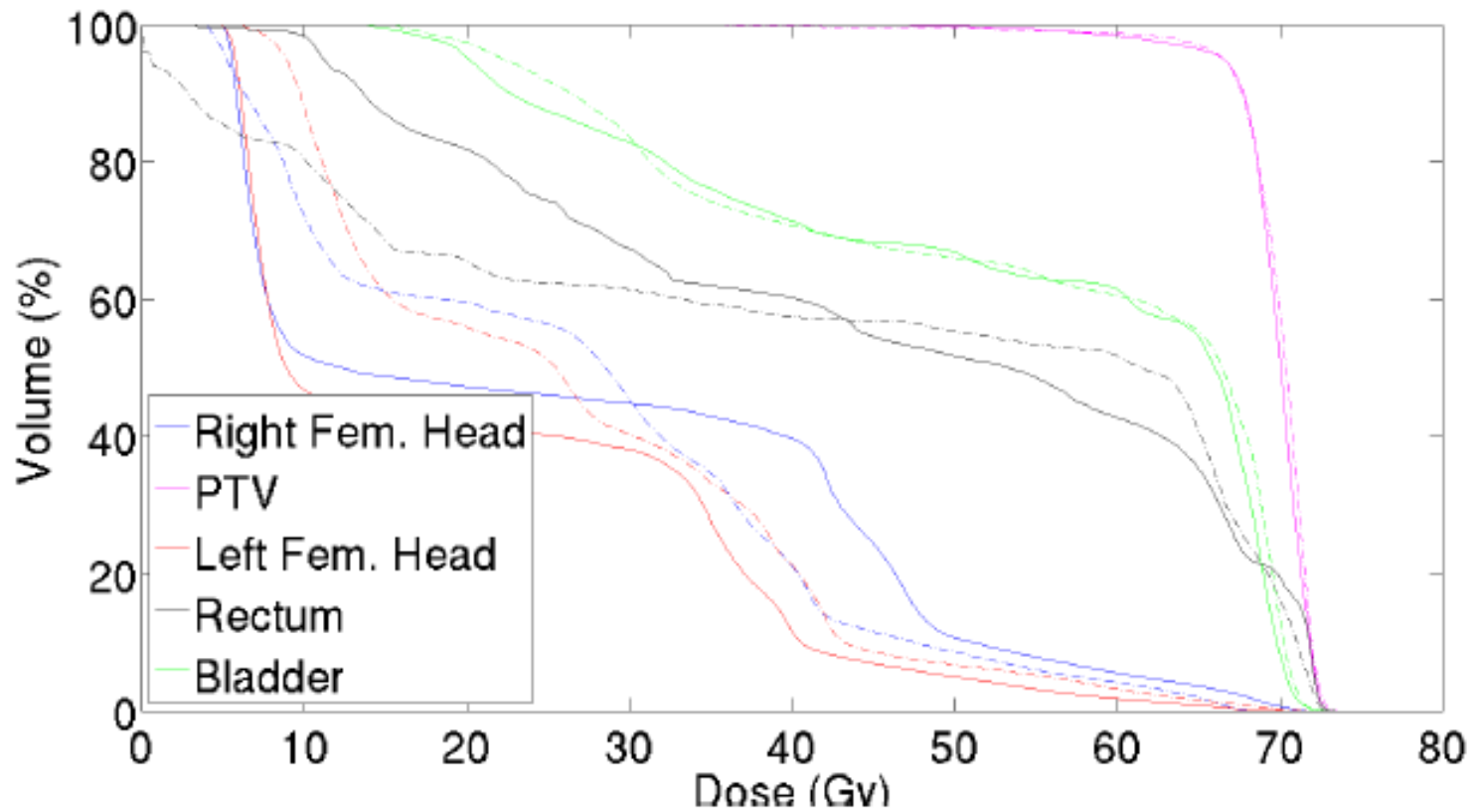
Methods were used to determine beamlet weights for two prostate bed cases

Each was run for 10^7 function evaluations and compared for speed and score

Patient	Method	Evals/sec /core	Final Score
1	QA	9.3	16.9
1	SA	9.6	6.7
1	Tabu	4.3	10.0
2	QA	15.4	70.7
2	SA	17.4	22.9
2	Tabu	6.3	120.0



QA (solid) and SA (dashed) for Patient 1



QA (solid) and Tabu (dashed) for Patient 2

Wall Clock Time



Patient	Method	Time
1	QA	1.00
1	SA	2.89
1	Tabu	3.23

2	QA	1.00
2	SA	2.67
2	Tabu	3.67

Results Summary

SA produced best score for both patients

QA was second, third

QA was fastest, by factors of 2.7 – 3.7

DVHs were compared and similar

Plans were not clinically viable due to small number of beamlets



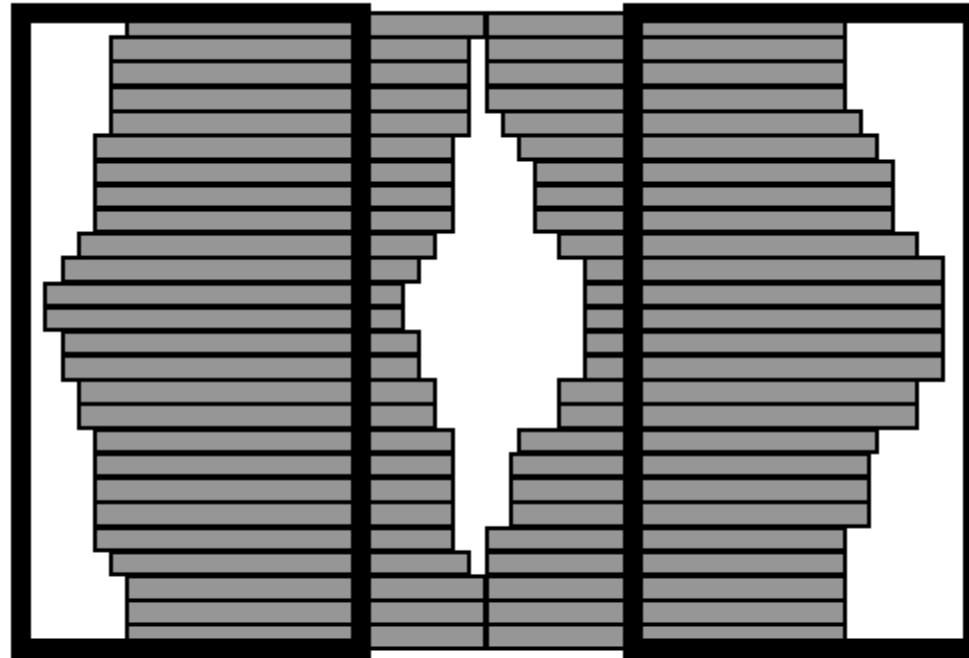
Future Work – VMAT



VMAT

VMAT Treatment

VMAT Optimization



This is first application of QA to IMRT optimization

Compared QA to SA and Tabu

Evaluated using clinical DVH-based objective functions

QA hardware will rapidly scale in size

Further research on application of QA to VMAT may offer promising returns

Thank You!

YouTube Embeds

[Linear Accelerator](#)

[IMRT Treatment](#)

[VMAT Treatment](#)

Thoughts and Experiences

Five years of Quantum Programming



Pre-history: Conversation with Geordie Rose

- Sometime in the fall of 2011, after flubbing my first phone interview with GR, I was granted a second chance.
- I remember two questions that he asked:

What is a support vector machine?



What are the odds that a book appearing on the New York Times best seller list in the next ten years will have been written by a machine?



Day 1

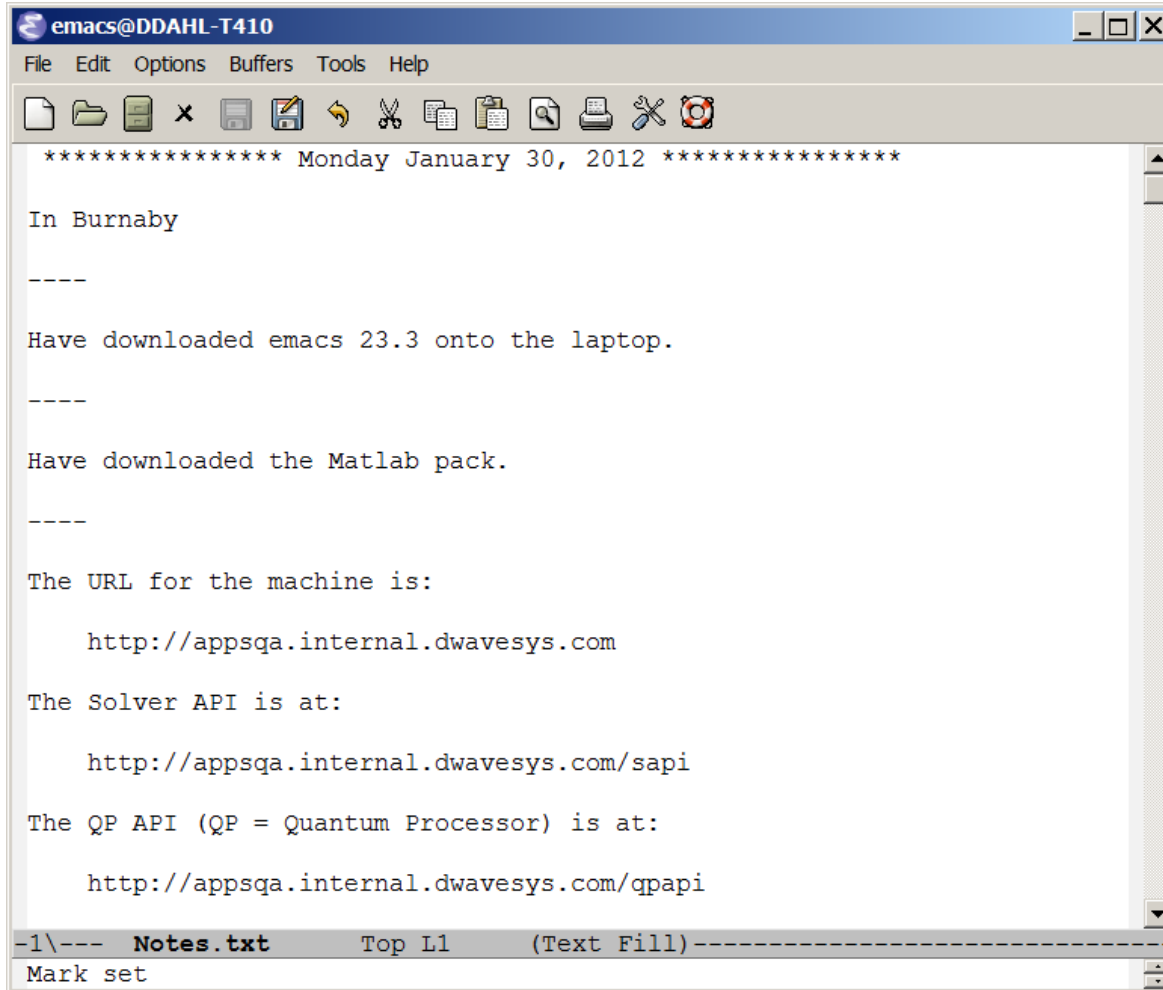


First NASA Quantum Future Technologies Conference

January 17–21, 2012

NASA Ames Research Center • Moffett Field, California

Day 14: First things first



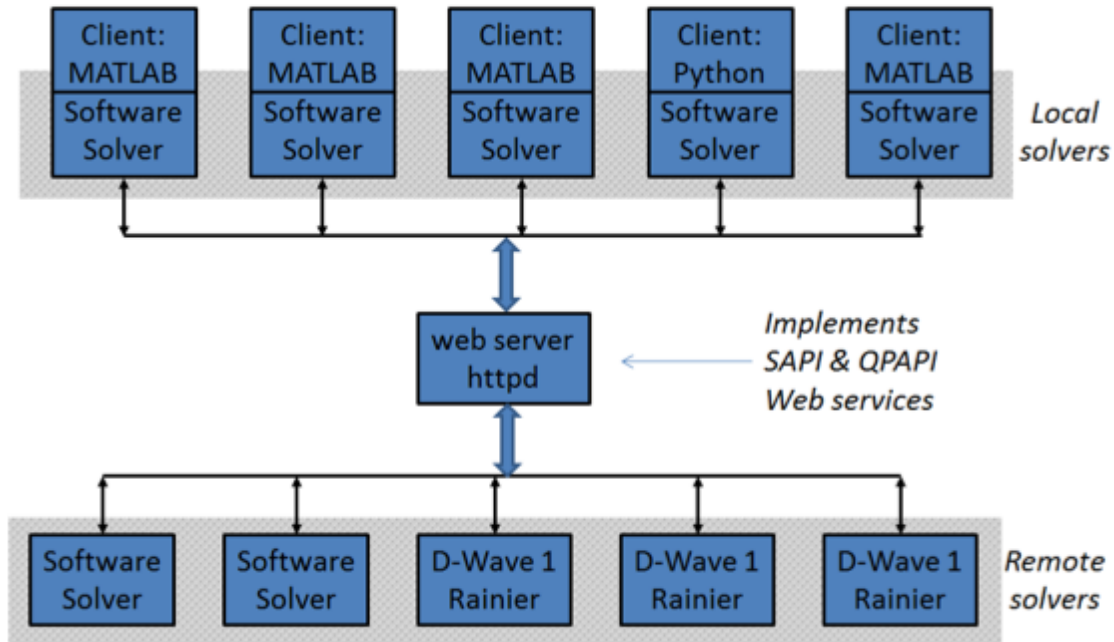
The screenshot shows an Emacs window titled 'emacs@DDAHL-T410'. The menu bar includes 'File', 'Edit', 'Options', 'Buffers', 'Tools', and 'Help'. The toolbar contains icons for file operations like opening, saving, and printing. The main text area contains the following content:

```
***** Monday January 30, 2012 *****  
  
In Burnaby  
-----  
Have downloaded emacs 23.3 onto the laptop.  
-----  
Have downloaded the Matlab pack.  
-----  
The URL for the machine is:  
  
    http://appsqa.internal.dwavesys.com  
  
The Solver API is at:  
  
    http://appsqa.internal.dwavesys.com/sapi  
  
The QP API (QP = Quantum Processor) is at:  
  
    http://appsqa.internal.dwavesys.com/qpapi
```

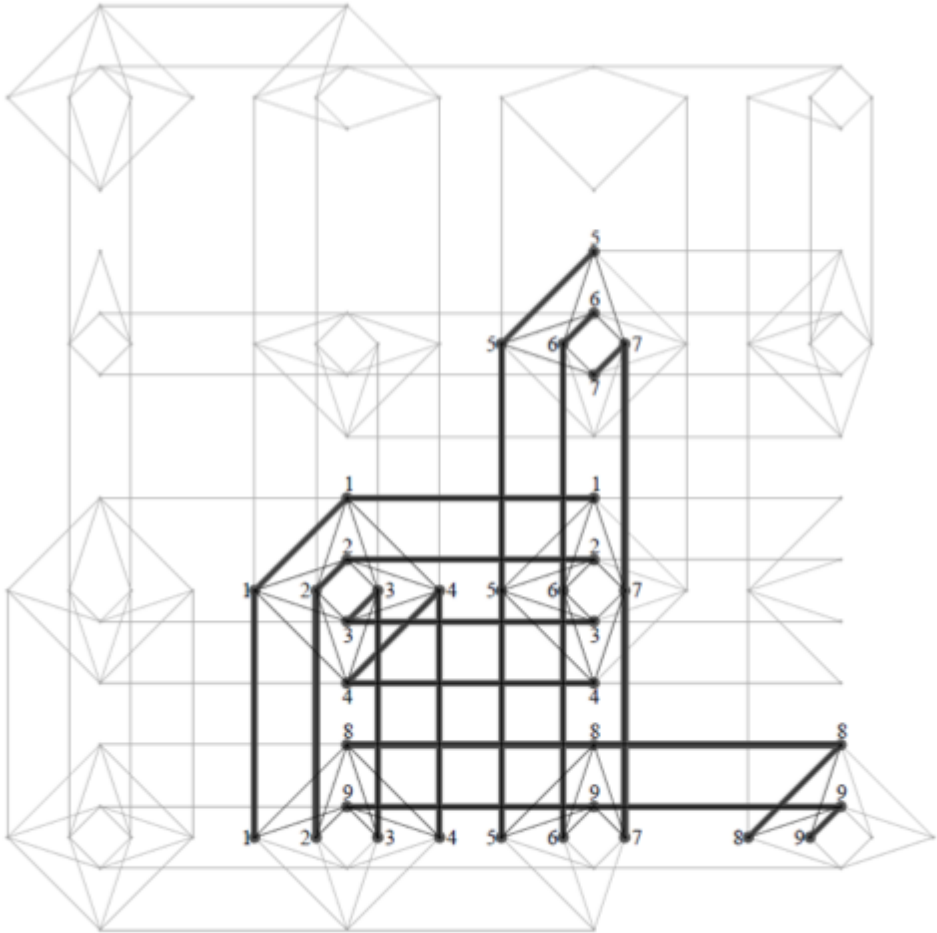
The status bar at the bottom shows the current file path as '-1\--- Notes.txt', the cursor position as 'Top L1', and the buffer type as '(Text Fill)'. Below the status bar, it indicates 'Mark set'.

Day 15: Early software architecture

D-Wave Software Stack

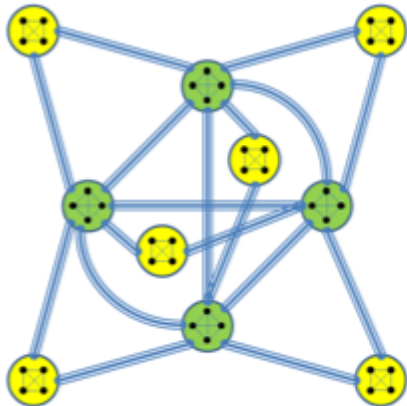






Day 15: Chimera, circa 2012



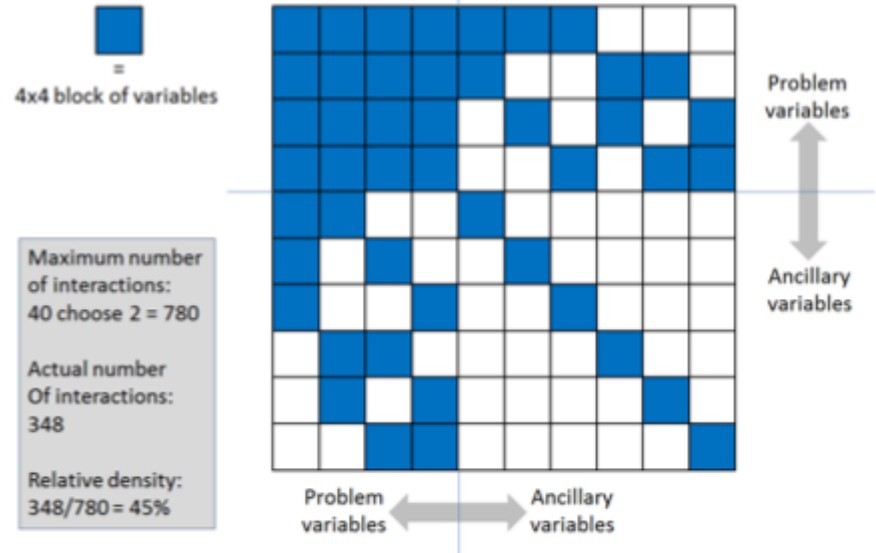
Day 21 – 22: Hadamard matrices, manually

4x4 Hadamard: QUBO interactions



Problem variables		4 vars
Ancillary variables		4 vars
Quadratic interactions		16 terms
		6 terms
Totals:		
Variables : $4 \times 10 = 40$		
Interactions : $18 \times 16 + 10 \times 6 = 348$		

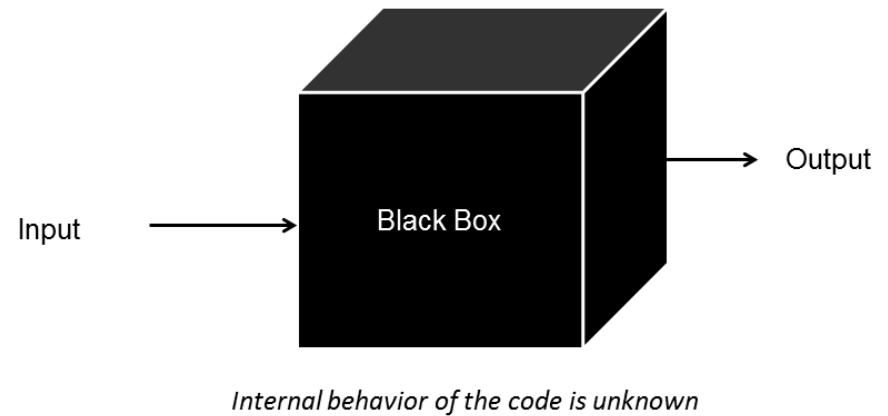
Block structure of QUBO



Day 23: Depression sets in

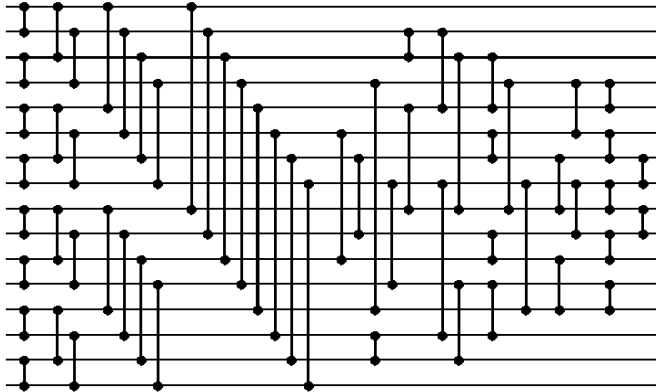


Day 24: BlackBox restores hope

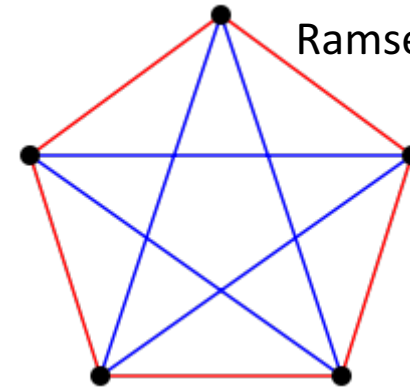


Day 25 – ∞ : Problems. Lots of Problems.

sorting networks



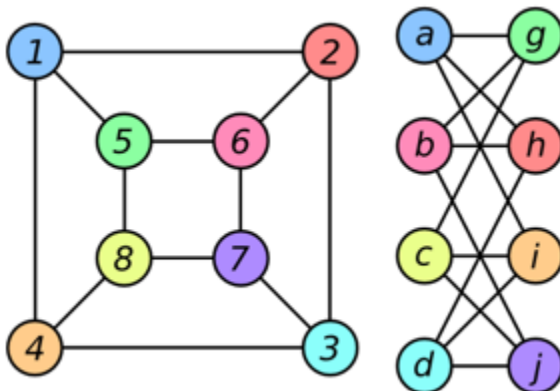
Ramsey theory



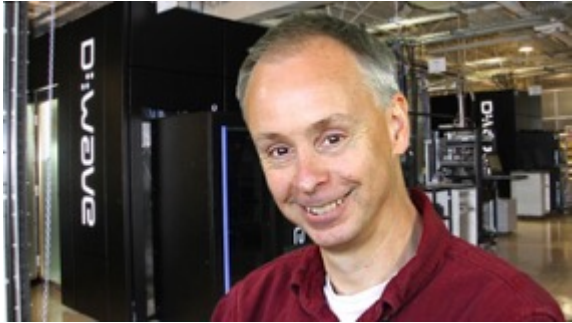
travelling salesman problem



graph isomorphism



Day 210 – 212: Learning from the Master

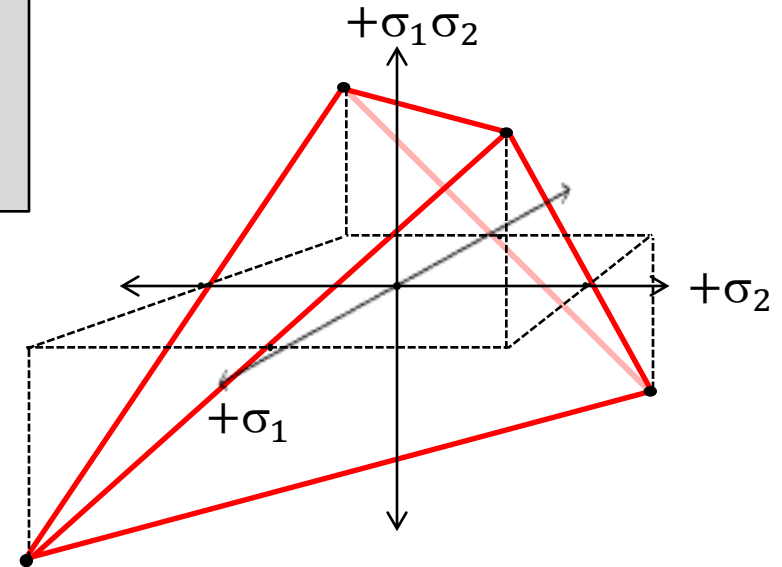


Day 250: Polytopes for Adiabatic QC

Chimeratope(1,1,1)

Chimeratope(L,M,N) –or– CH(L,M,N)

- L = half number of spins in the unit cell
- M = number of rows
- N = number of columns



Day 270: Automorphism Groups of Chimera

tiling	size	factorization	group
1x1	1152	$2^7 * 3^2$	$S(2) \times S(4) \times S(4)$
1x2	27648	$2^{10} * 3^3$	$S(2) \times S(4) \times S(4) \times S(4)$
1x3	663552	$2^{13} * 3^4$	$S(2) \times S(4) \times S(4) \times S(4) \times S(4)$
1x4	15925248	$2^{16} * 3^5$	$S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
2x1	27648	$2^{10} * 3^3$	$S(2) \times S(4) \times S(4) \times S(4)$
2x2	2654208	$2^{15} * 3^4$	$D(4) \times S(4) \times S(4) \times S(4) \times S(4)$
2x3	31850496	$2^{17} * 3^5$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
2x4	764411904	$2^{20} * 3^6$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
3x1	663552	$2^{13} * 3^4$	$S(2) \times S(4) \times S(4) \times S(4) \times S(4)$
3x2	31850496	$2^{17} * 3^5$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
3x3	1528823808	$2^{21} * 3^6$	$D(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
3x4	1.8345885696e10	$2^{23} * 3^7$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
4x1	15925248	$2^{16} * 3^5$	$S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
4x2	764411904	$2^{20} * 3^6$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
4x3	1.8345885696e10	$2^{23} * 3^7$	$S(2) \times S(2) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$
4x4	8.8060251341e11	$2^{27} * 3^8$	$D(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4) \times S(4)$

Day 574: Conquering the Unit Cell

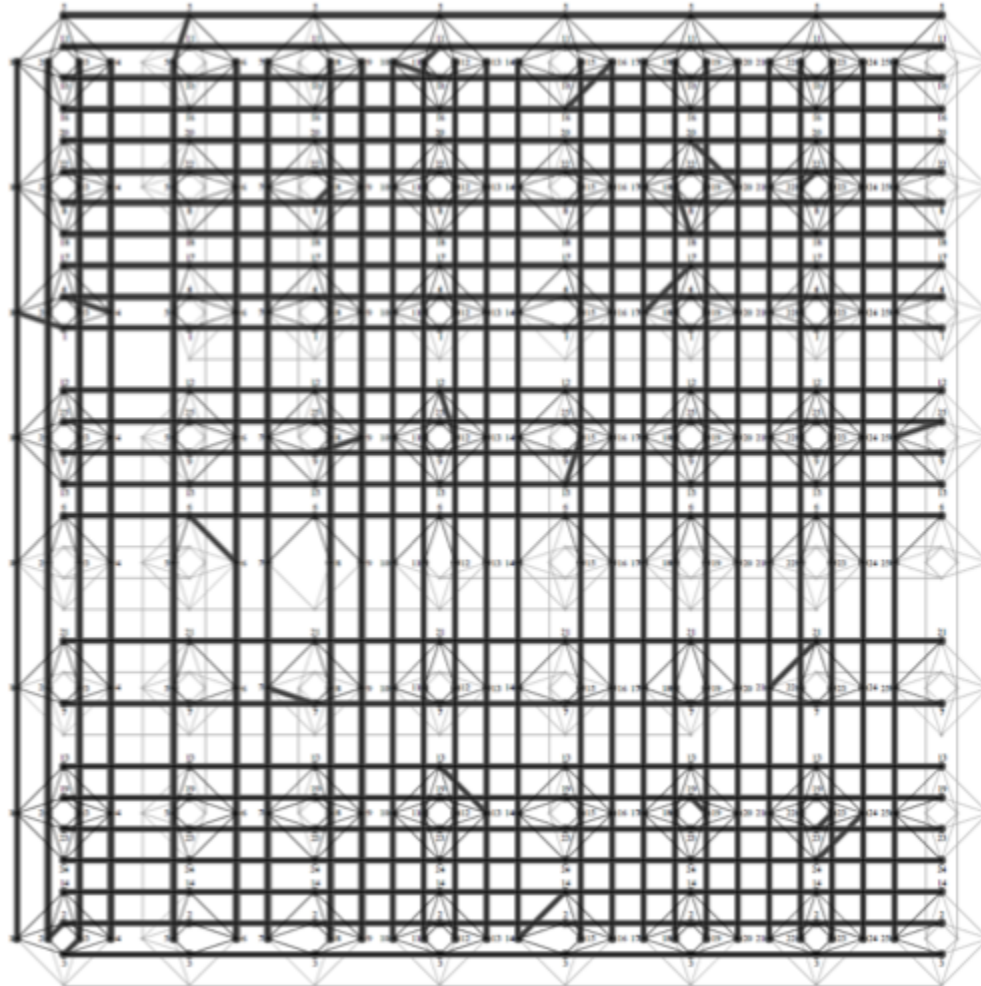
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--(Unix)--- ListOrbitEXT4 Top L1 (Fundamental)-----
End of buffer
```



Mathieu Dutour Sikiric



Day 370: Vesuvius



Day 395: Big B



Day 455 – ∞: Training



D-Wave Quantum Computer Training

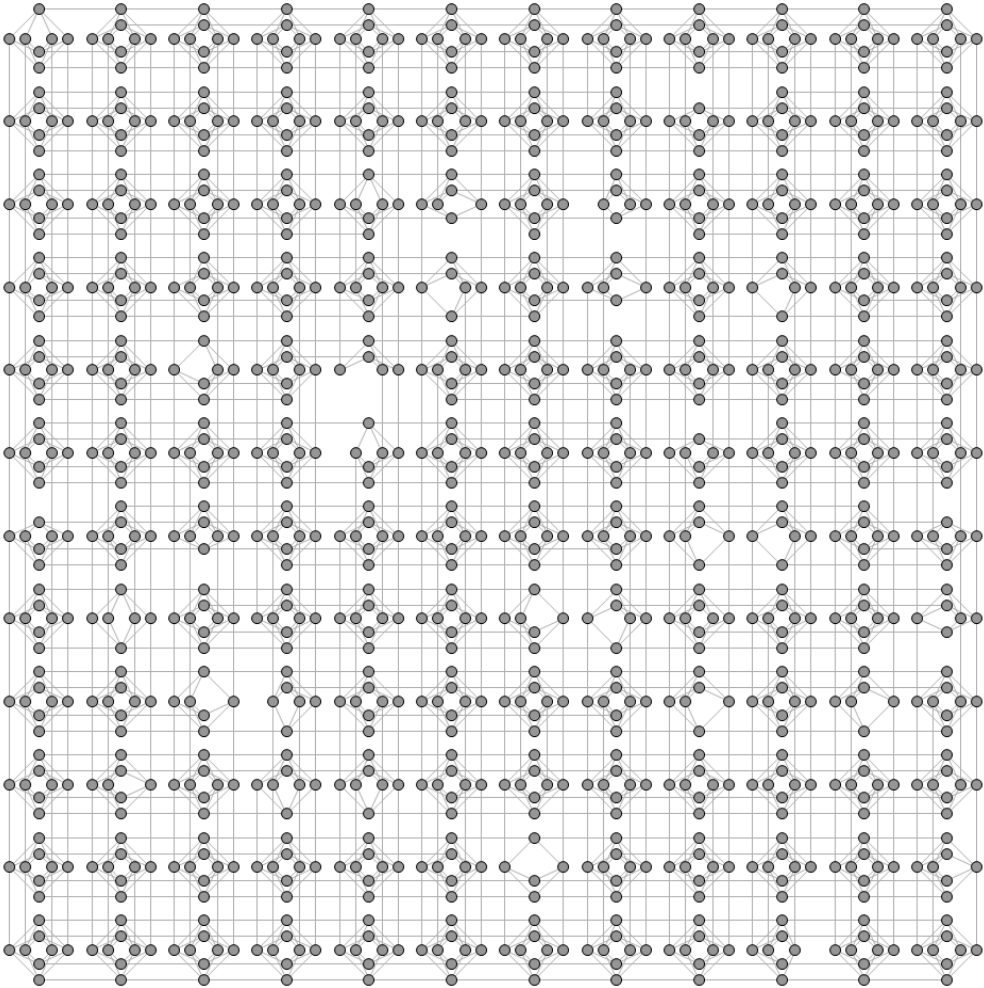
April 3 -5, 2013

Location: University of Southern California, Information Sciences Institute (ISI)
4676 Admiralty Way, Suite 1001
Marina del Rey, CA 90292

Attendees: Various Australian Small-Medium Enterprises



Day 720: Washington



Day –8760: Archaeology of Map Coloring



Neural Network Algorithm for an NP-Complete Problem: Map and Graph Coloring

Edward Denning Dahl, L-298

Lawrence Livermore National Laboratory
P. O. Box 808
Livermore, CA 94550

1. Introduction

The four color conjecture¹ states that any map drawn on a plane or sphere can be colored with four colors so that no two countries which share a border have the same color. The proof of this appealing conjecture took more than one hundred years, and on the order of 10^{10} computer operations.² Unfortunately, the proof of this conjecture is not constructive. In fact, there is no algorithm which is guaranteed to color an arbitrary planar map without essentially resorting to exhaustive search. The absence of such an algorithm extends to a class of problems which generalizes the task of coloring a planar map with four colors. In the general problem, the map is not necessarily planar, but may lie on a more complicated surface such as a torus with several holes. To complete the specification of the general problem, pick a positive integer K which sets the number of colors available for use in coloring the map. The problem is to decide whether a K -coloring of the map exists: that is, an assignment of colors to regions on the map so that regions sharing a border receive different colors.

Since 1971 and the proof of Cook's Theorem,³ the notion of NP-Completeness has been made precise. For a problem to be NP-Complete it is required that one be able to find the solution to the problem in an amount of time polynomial in the problem size, provided one uses the very special model of computation represented by a non-deterministic Turing Machine. Secondly, an NP-Complete problem is at least as hard as any problem which satisfies the first criteria. Deciding whether a non-planar map is K -colorable is an NP-Complete Problem.⁴

John Hopfield has demonstrated⁵ that a Neural Network can provide a heuristic technique for solving the Traveling Salesman Problem (TSP). In one version of the Traveling Salesman Problem one is given some number of cities, the pairwise distances between all the cities, and some fixed length L . One must then decide whether there is some tour through the cities which visits each one once, and has total length less than the bound L . This problem is NP-Complete,⁶ and thus equivalently difficult to the Map K -colorability problem.

It is natural to wonder whether a Neural Network solution exists for the Map K -colorability problem, given that both it and the TSP are equivalently hard and that a Neural Net solution exists for the latter problem. We demonstrate that a Neural Network solution does exist for the Map K -colorability problem. The connectivity of the neurons in the net follows simply from the connectivity of the regions in the map. The dynamics of the

* Work performed under the auspices of the U. S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

¹ K. O. May, *The Origin of the Four Color Conjecture*. Isis, vol. 56, pp. 346-348 (1965).

² T. L. Saaty and P. C. Kalinen, *The Four-Color Problem*. McGraw-Hill, Inc. (1977).

³ S. A. Cook, *Proc. 3rd Ann. ACM Symp. on Theory of Computing*. New York, 151-158 (1971).

⁴ R. M. Karp, *Complexity of Computer Computations*. R. E. Miller and J. W. Thatcher (eds.), Plenum Press, New York, 85-103 (1972).

⁵ J. J. Hopfield and D. W. Tank, *Biol. Cyber.*, Vol. 52, 141 (1985).

⁶ M. R. Garey and D. S. Johnson, *Computers and Intractability*. Freeman and Company, San Francisco (1979).

Day 580: Map coloring on a quantum computer

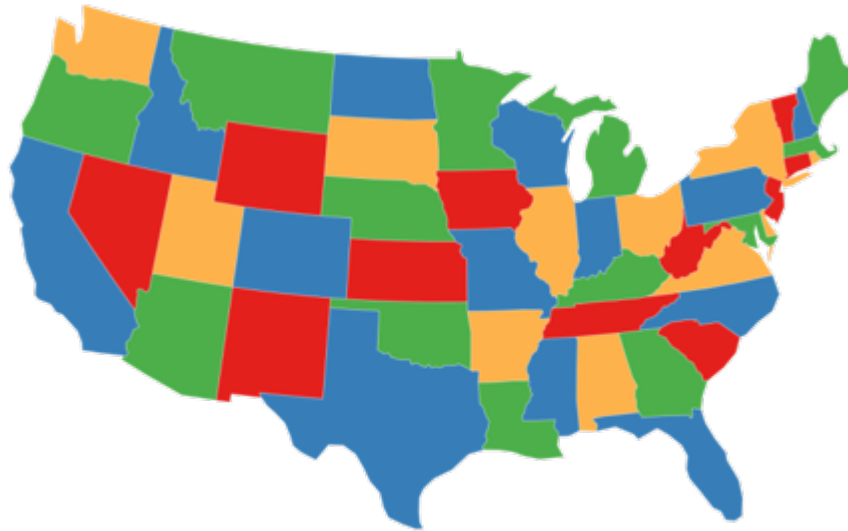
Canada regions/shell script



# of colors	Needle	Haystack	N/H
3	1728	$3^{13} = 1.6 \times 10^6$	0.0011
4	653184	$4^{13} = 6.7 \times 10^7$	0.0097

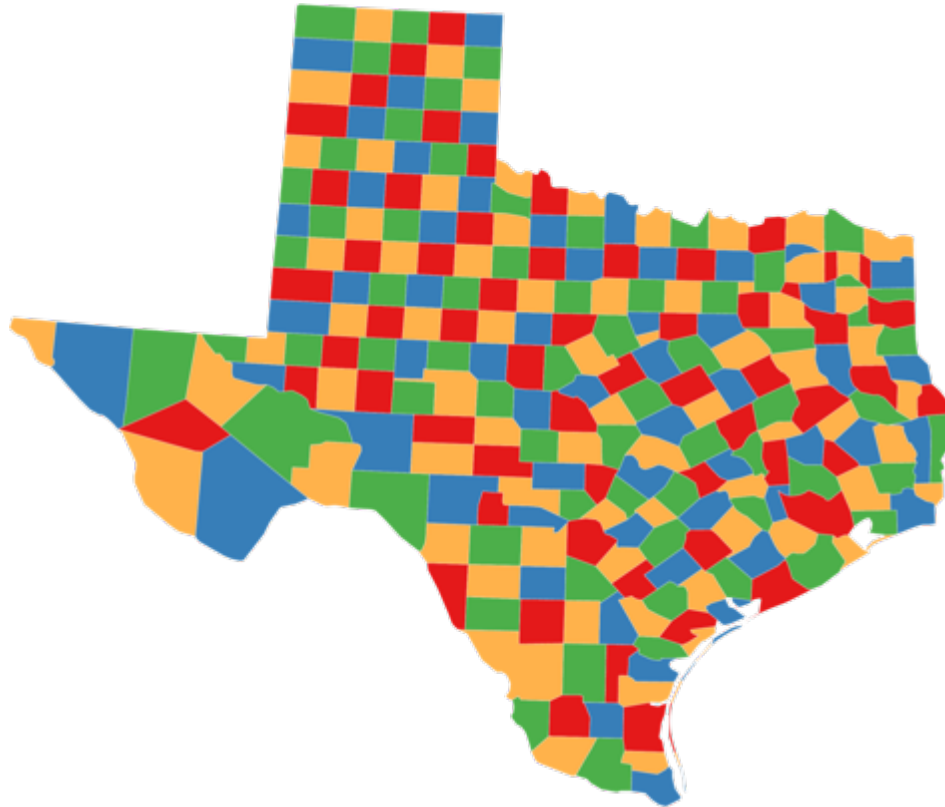
Day 610: Static decomposition

US states/MATLAB



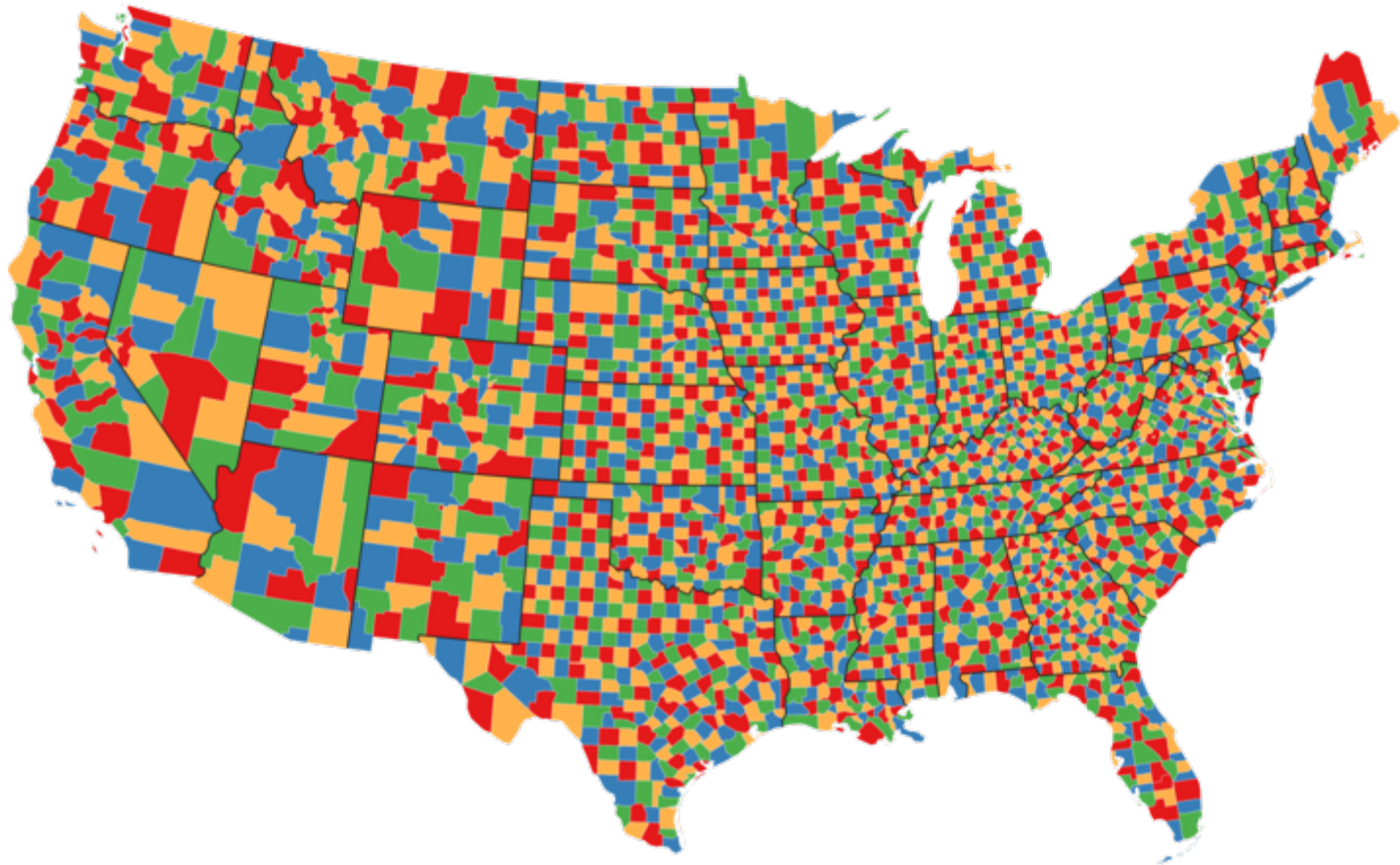
# of colors	Needle	Haystack	N/H
3	0	$3^{49} = 2.4 \times 10^{23}$	0
4	25623183458304	$4^{49} = 3.2 \times 10^{29}$	8×10^{-17}

Day 720: Dynamic decomposition / qbsolv



254 counties in Texas

Day 900: Dynamic decomposition / qbsolv



3108 US counties

Day 735: DEQO – the predecessor of ToQ

Deqo: A Direct Embedding Quantum Optimizer

E. D. Dahl, D-Wave Systems

January 24, 2014

Abstract

Deqo is a prototype compiler for the D-Wave System. It implements a simple language designed for constraint satisfaction problems (CSP) defined over both boolean and small integer variables. Deqo assumes its CSP has locality: in other words, it consists of a set of constraints each of which involves a small number of available variables. The compilation model proceeds by applying a sequence of transformations which move the problem representation closer to the native quantum machine instruction (QMI) of the D-Wave System. Each transformation is described in the context of a simple example. We conclude by discussing possible extensions to the compilation model.

Day 950 : Map coloring made easy / ToQ

C

```
void setup_unit_cell(int row, int col)
{
    int i, j;

    if (cell_region[row][col] == UNDEF)
        return;

    /* STEP 1: turn on one of C qubits */

    for (i=0; i<C; ++i)
    {
        weight[DW_QUBIT(row,col,'L',i)] += -0.5;
        weight[DW_QUBIT(row,col,'R',i)] += -0.5;
    }

    for (i=0; i<C; ++i)
        for (j=0; j<C; ++j)
            if (i != j)
                strength[DW_INTRACELL_COUPLER(row,col,i,j)] += 1;

    /* STEP 2: create chains */

    for (i=0; i<C; ++i)
    {
        weight[DW_QUBIT(row,col,'L',i)] += 1;
        weight[DW_QUBIT(row,col,'R',i)] += 1;
        strength[DW_INTRACELL_COUPLER(row,col,i,i)] += -2;
    }
}
```

Snippet (28 of 596 LOC)

ToQ

```
mbool: 1, 4, @AB
mbool: 1, 4, @BC
mbool: 1, 4, @MB
mbool: 1, 4, @NB
mbool: 1, 4, @NL
mbool: 1, 4, @NS
mbool: 1, 4, @NT
mbool: 1, 4, @NU
mbool: 1, 4, @ON
mbool: 1, 4, @QC
mbool: 1, 4, @SK
mbool: 1, 4, @YT

assert: @AB != @BC
assert: @AB != @NT
assert: @AB != @SK
assert: @BC != @NT
assert: @BC != @YT
assert: @MB != @NU
assert: @MB != @ON
assert: @MB != @SK
assert: @NB != @NS
assert: @NB != @QC
assert: @NL != @QC
assert: @NT != @NU
assert: @NT != @SK
assert: @NT != @YT
assert: @ON != @QC
```

entire program

QMI :



Day 1165: Sudoku

		3		9	2			
4				3			1	
2	7							
	1		3					8
	5		1	6	7		3	
3					8		6	
							5	3
	3			8				9
			6	2		1		

```
bash
Documents> qbsolv -h

qbsolv -i infile [-o outfile] [-m] [-T] [-n] [-S SubMatrix] [-w]
        [-h] [-v verbosityLevel] [-V] [-q]

DESCRIPTION
qbsolv executes a quadratic unconstrained binary optimization
(QUBO) problem represented in a file, providing bit-vector
result(s) that minimizes (or optionally, maximizes) the value of
the objective function represented by the QUBO. The problem is
represented in the QUBO(5) file format and notably is not limited
to the size or connectivity pattern of the D-Wave system on which
it will be executed.
The options are as follows:
-i infile
  The name of the file in which the input QUBO resides. This
  is a required option.
-o outfile
  This optional argument denotes the name of the file to
  which the output will be written. The default is the
```

```
emacs@DDAHL-T410
File Edit Options Buffers Tools Sh-Script Help
#####
#!/bin/bash

sudoku=$1

if [[ -z $sudoku ]]
then
  echo "usage: driver.bash <sudoku-file>"
  exit 1
fi

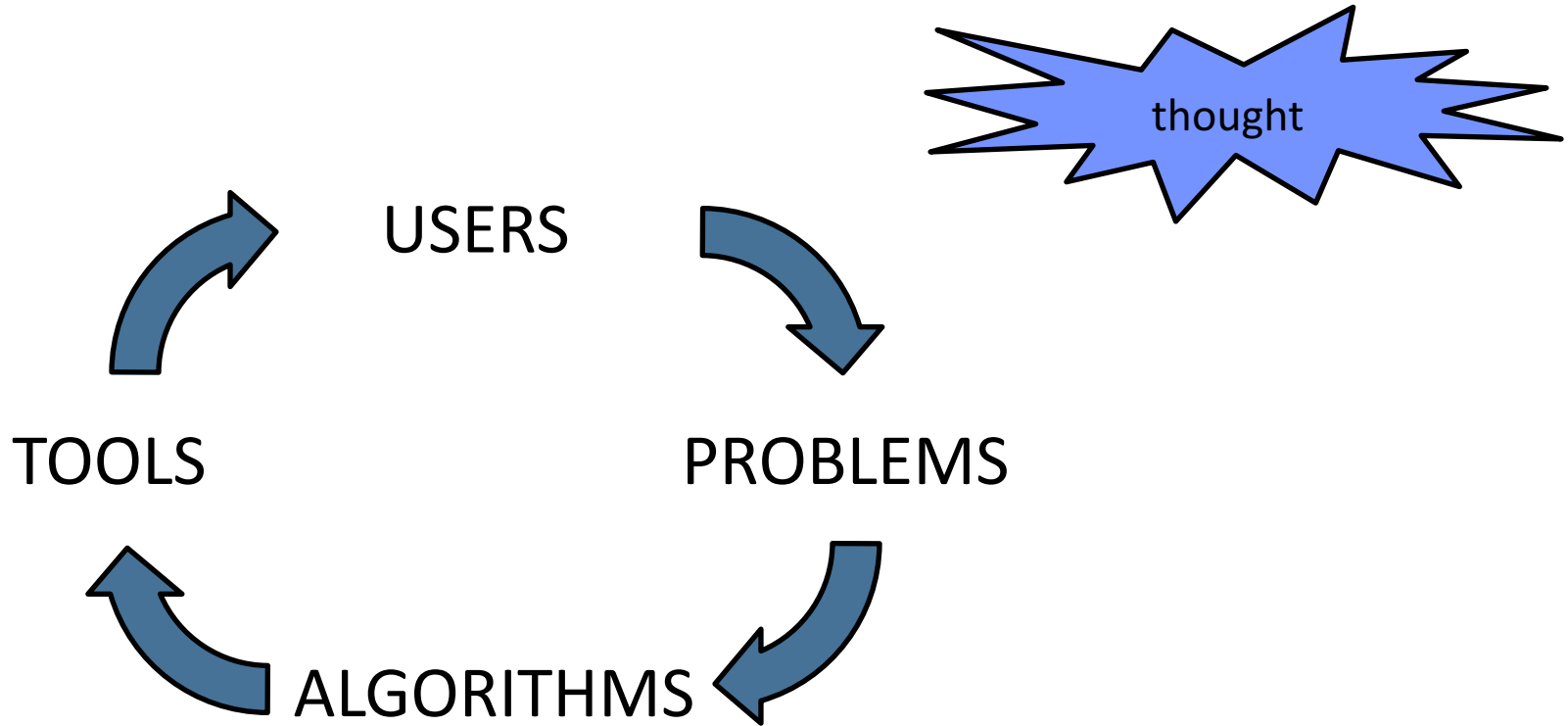
echo "***** Create QUBO for blank grid *****"
s1.bash > s1.out

echo "***** Identify fixed variables *****"
s2.bash < $sudoku > s2.out

echo "***** Compute reduced QUBO *****"
s3.bash > s3.out

echo "***** Identify free variables ; Enumerate variables *****"
s4.bash < s3.out > s4.out
--\--- driver.bash Top L1 (Shell-script[bash])-----
Indentation setup for shell type bash
```

Day $\pi * 365$: The Virtuous Cycle



Day 1642: Virtual Full Yield

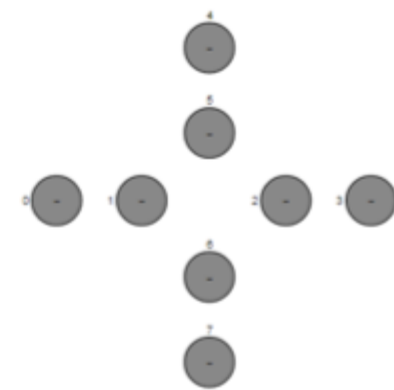
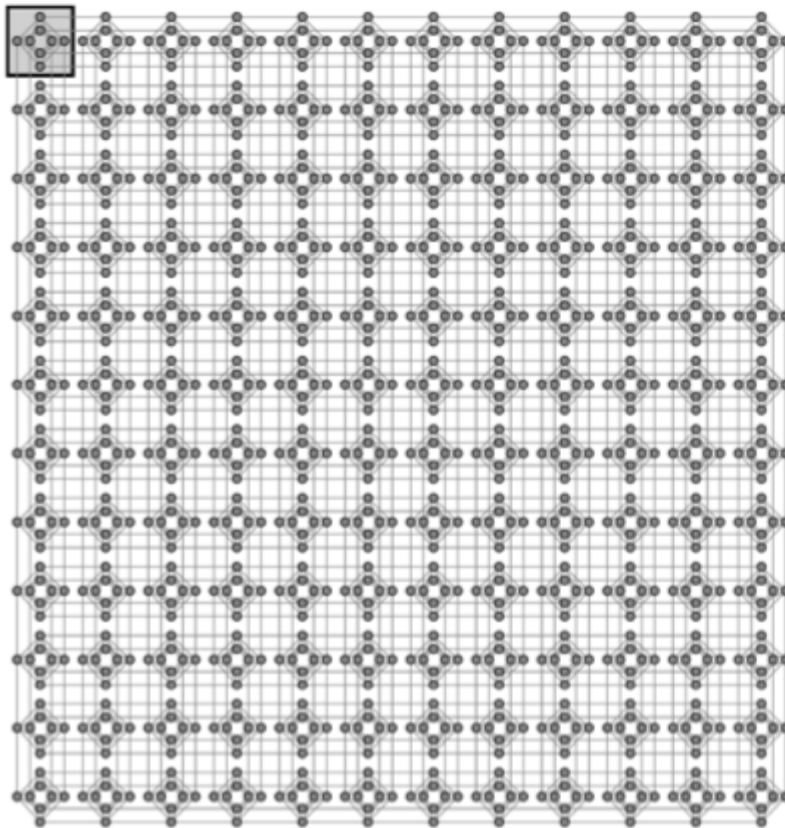
Submit Problem

Submit problem to DW2X_VFYC

Configure

Options

Graph Data Solutions



Any Day, All Day

Problem	Technique
Hadamard matrices	Direct embedding
Ramsey lower bounds & more	BlackBox (Qsage)
Travelling Salesman Problem	BlackBox, QUBO, Parallel Update
Quadratic Assignment Problem	BlackBox, QUBO
Cyclic Ordering	Blackbox / Sorting network
Graph Isomorphism	Blackbox / Sorting network
Map Coloring	Various
Hello World	SAPI
Sudoku	qbsolv
Factoring	qbsolv

Perspectives about what might work best

STONEBRAKER ALGORITHM

Code section 2.

```
Until (it works) {  
    Come up with a new idea;  
    Prototype it with the help of superb computer scientists;  
    Persevere, fixing whatever problems come up; always remembering that it is never too late to throw  
    everything away;  
}
```



Likely copyright violation
DOI:10.1145/2869958

The D-Wave Trinity

Optimization & Constraint Satisfaction Problems

Machine Learning

Sampling

Day 1721: Today

