

Parallel Algorithms - DNA computing

L24-1

Model of Computation (Implicit)

Sequential - if an operation (e.g., comparison) takes one time unit, n such operations take n time units
→ single processor hardware

Different hardware → different properties

Parallel - if an operation takes one time unit on one processor, n such independent operations take one time unit on n processors.

Think about decision problems - imagine a room full of people
SAT: ① Each person randomly assigns literals and checks whether it satisfies relations
② If satisfies, stand up.

→ Improvement: Instead of being random, I could assign them to ensure full coverage of all possibilities

→ Optimization Problem: Similar, but must find a way to compare costs (e.g. tour lengths) from each participant

→ Parallel computers exist, in many configurations

- Independent machines connected on a network (SOTI@home)
- Shared memory machines

↳ Could spend an entire semester on these architectures and alg. (breaking apart problem, communication, coordination)

There are, of course, radically different computer "architectures" with very different properties

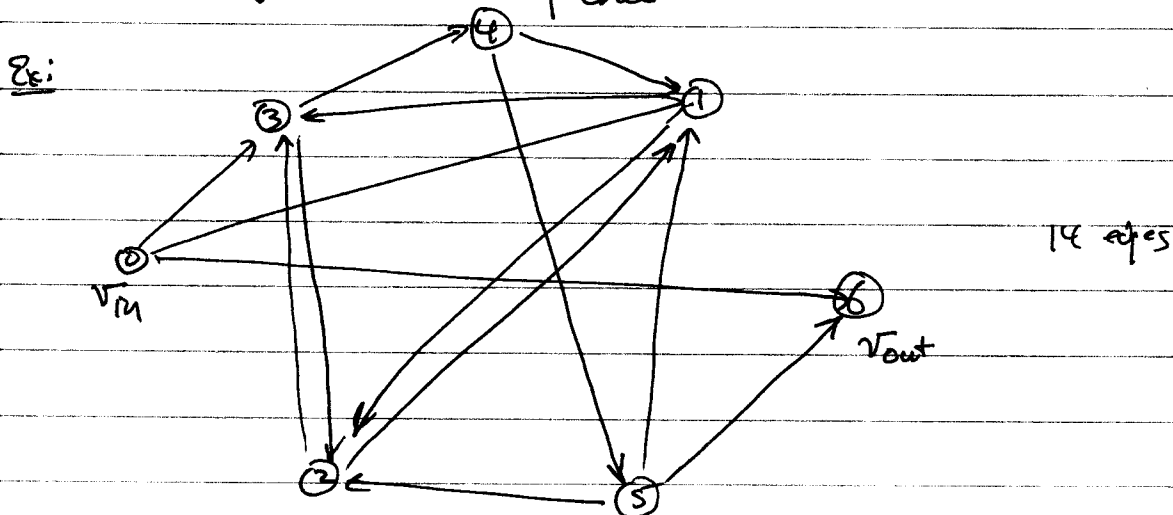
→ quantum computers — make use of superpositions of states and quantum properties

→ DNA computers — harnessing the power of molecular biology, ~~the natural~~ and the large number of molecules available in small volumes to do computation with molecules.

Hamiltonian Path Problem (~~1994~~ (Adleman, 1994))

Input: Directed graph $G(V, E)$ with two specific vertices v_{in} and v_{out}

Output: Decision (YES/NO) on whether there exists a path $v_{in} \rightarrow v_{out}$ that enters all vertices exactly once



Yes: $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5 \rightarrow 6$

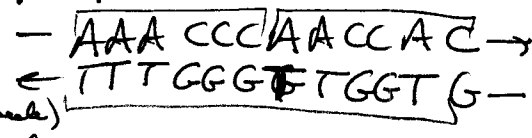
This problem is NP-complete

Consider the following Algorithm

- ① Generate random paths through graph ← hopefully complete
- ② Keep only those beginning at v_{in} & ending at v_{out}
- ③ Keep only those paths entering $|V|$ vertices
- ④ Keep only those paths entering each vertex (at least once)
- ⑤ If any paths remain \Rightarrow YES; otherwise \Rightarrow NO

DNA Primer

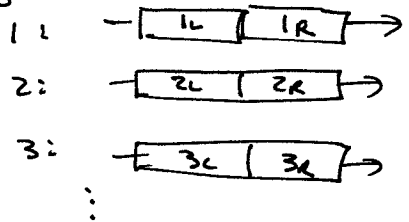
- a) There are four "bases" $A \leftrightarrow T$ $C \leftrightarrow G$
- b) A string of bases (synthesized as a contiguous polymer) binds tightly to its complement



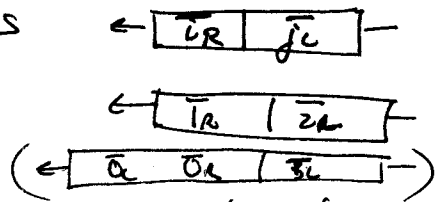
Actually did this experimentally (manually)
 DNA length variation
 Make random paths

- c) ligation glues adjacent strands into contiguous piece
- d) gel electrophoresis separates by size (equal-length)
- e) PCR amplification from desired endpoints
- f) digest single stranded DNA

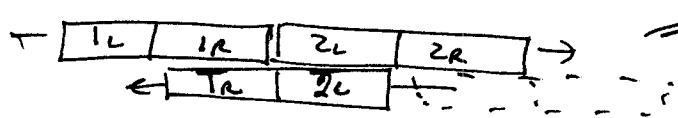
① Each vertex of graph represented by unique string (20-mer)



Each edge (i, j) represented as

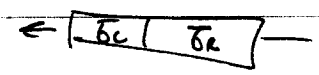
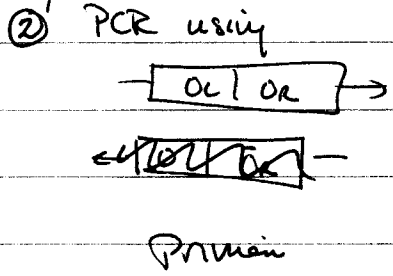


50 μ m of DNA representing all edges and all vertices mixed (3×10^{13} copies of each)



Produce paths through the graph
 Use ligation to chemically lock the paths

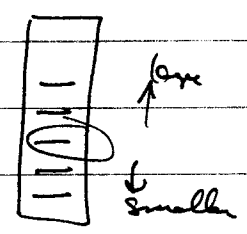
Keep only paths starting at $v_{in}=0$ & ending at $v_{out}=6$



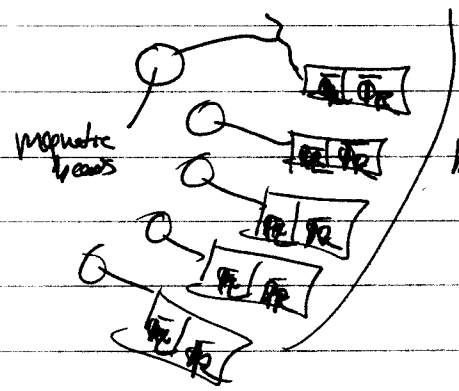
→ Amplifies (make copies of) chains starting with $v_{in}=0$ & ending with $v_{out}=6$. Others are diluted to negligible level

③ Pass through each vertex (V) vertices
Separate DNA based on length (gel electrophoresis) and excise 140 bp lengths, purify.

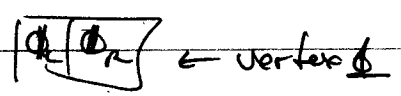
20x7



④ Pass through each vertex at least once



binds strands single strands containing



Repeat for 2, 3, 4, 5
(0 & 6 covered by PCR)

⑤ ~~HTS~~ Do any paths remain?

— Run on a gel and look for ~~dup~~ → reveal only one

Summary:

one week of work

most time ("a whole day") on Step 4 (cognitive load)

↳ time is linear in # of vertices \Rightarrow PLY TIME,
but on 'unequal architecture'

Can actually read out the path,
though difficult to decode superposition
of many solus.

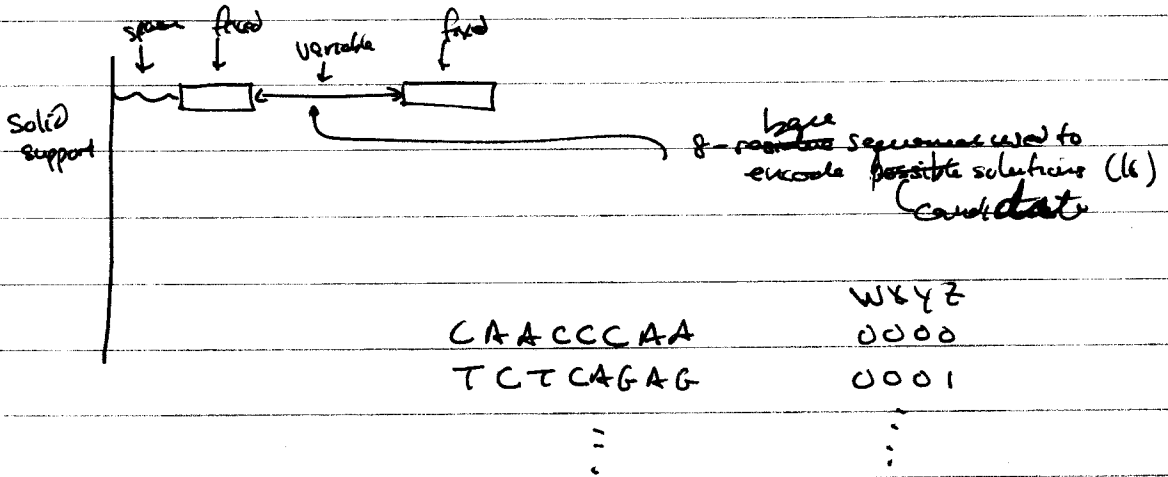
Problem - scaling up to interesting size problems
(70 vertices) would require 10^{25} kg of material.

↑
~ weight of Earth

SAT: (Liu et al., 2000)

$$(W V X V Y) \wedge (W V \bar{Y} V Z) \wedge (\bar{X} V Y) \wedge (\bar{W} V \bar{Y})$$

4 binary vars $\Rightarrow 2^4 = 16$ candidate solutions



① Synthesize all and attach to surface

② Remove those incompatible with clause 1 ($W V X V Y$)

\Rightarrow 0000 & 0001 are the only incompatible

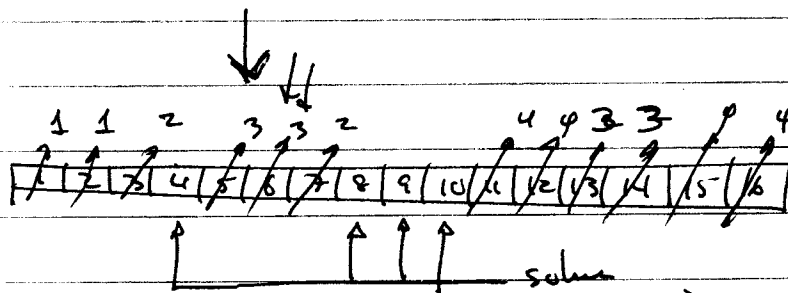
\Rightarrow So other 14 complements added, hybridized (to protect), direction of single-stranded w/ exonuclease

\Rightarrow wash to de-hybridize

Protect Mask \rightarrow

Destroy \rightarrow

Protect Unmasked \rightarrow

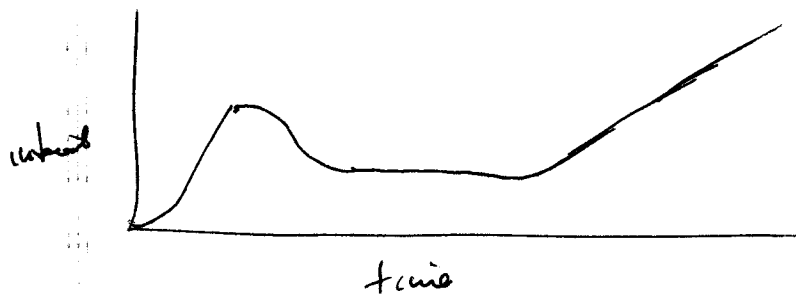


2: 0 & 10
3: w 1 0 z
4: 1 x 1 z

4 solutions
0011
0111
1000
1001

\rightarrow identify by PCR & hybridize to addressable array.

\propto (# of mask & destroy operations grows polynomially in # of variables)



- Holds non-linear potential; still has problems (scale-up).
- Algorithm are very inefficient:
 - Make all possible solutions and destroy members of search space and destroy ourselves.
 - Improvements that create only a small part of the space presented to contain the solve would scale much better.