Quantum Bio...

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Benasque workshop 2010

Quantum bio?

Why?   Trendy?   Useful?   Funded?   Interesting?

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Started with single photon detection in locust eyes (Lillywhite 1977)

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--> most biophysics is not quantum – a case of

“everything looks like a nail to a hammer”?

Quantum bio?

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--> most biophysics is not quantum – a case of

"everything looks like a nail to a hammer"?

soft condensed matter contributes far more to understanding of biological processes...

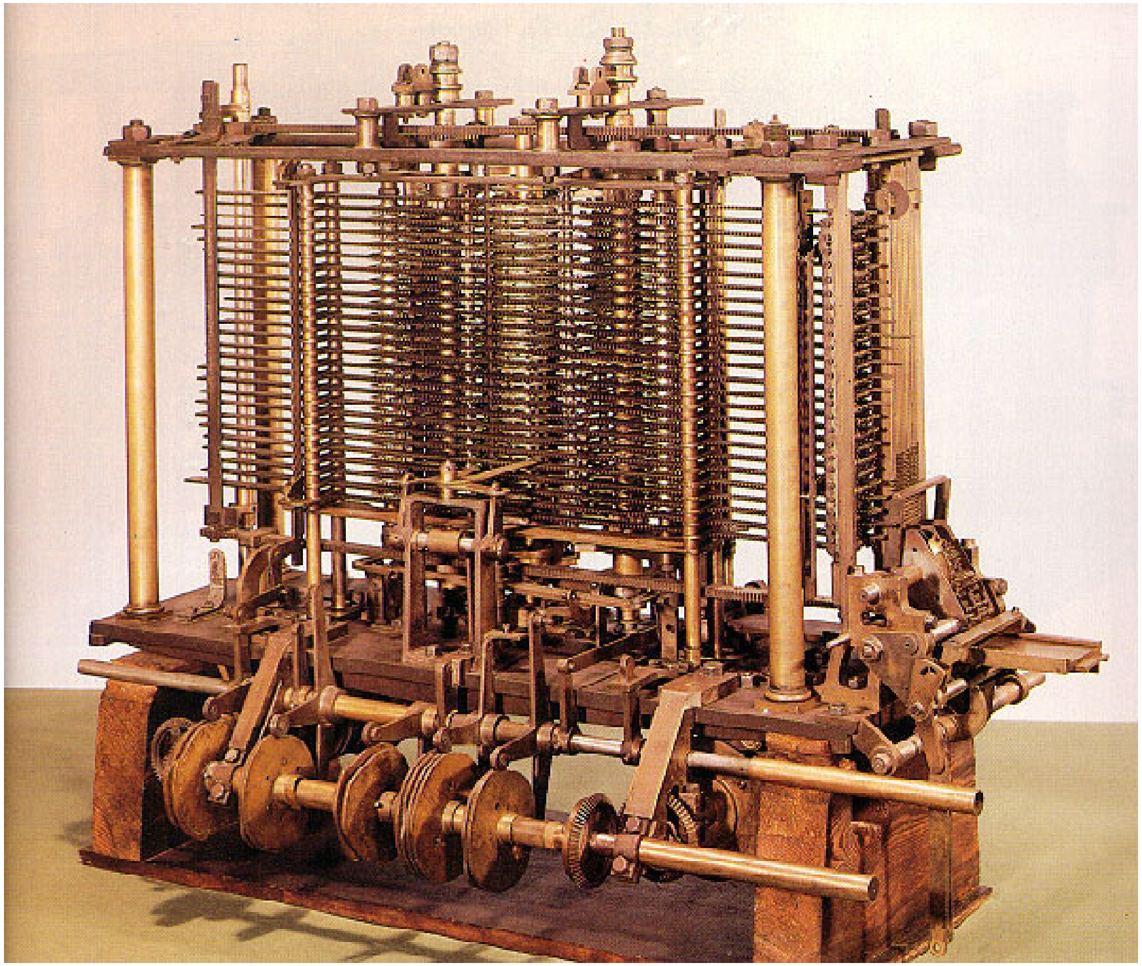
Quantum bio?

- in the spirit of

"if I was going there
I wouldn't start from here"

Computational science...

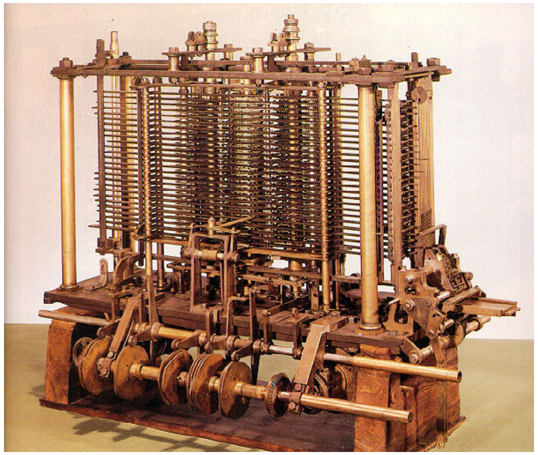
numerical simulation
computational modelling

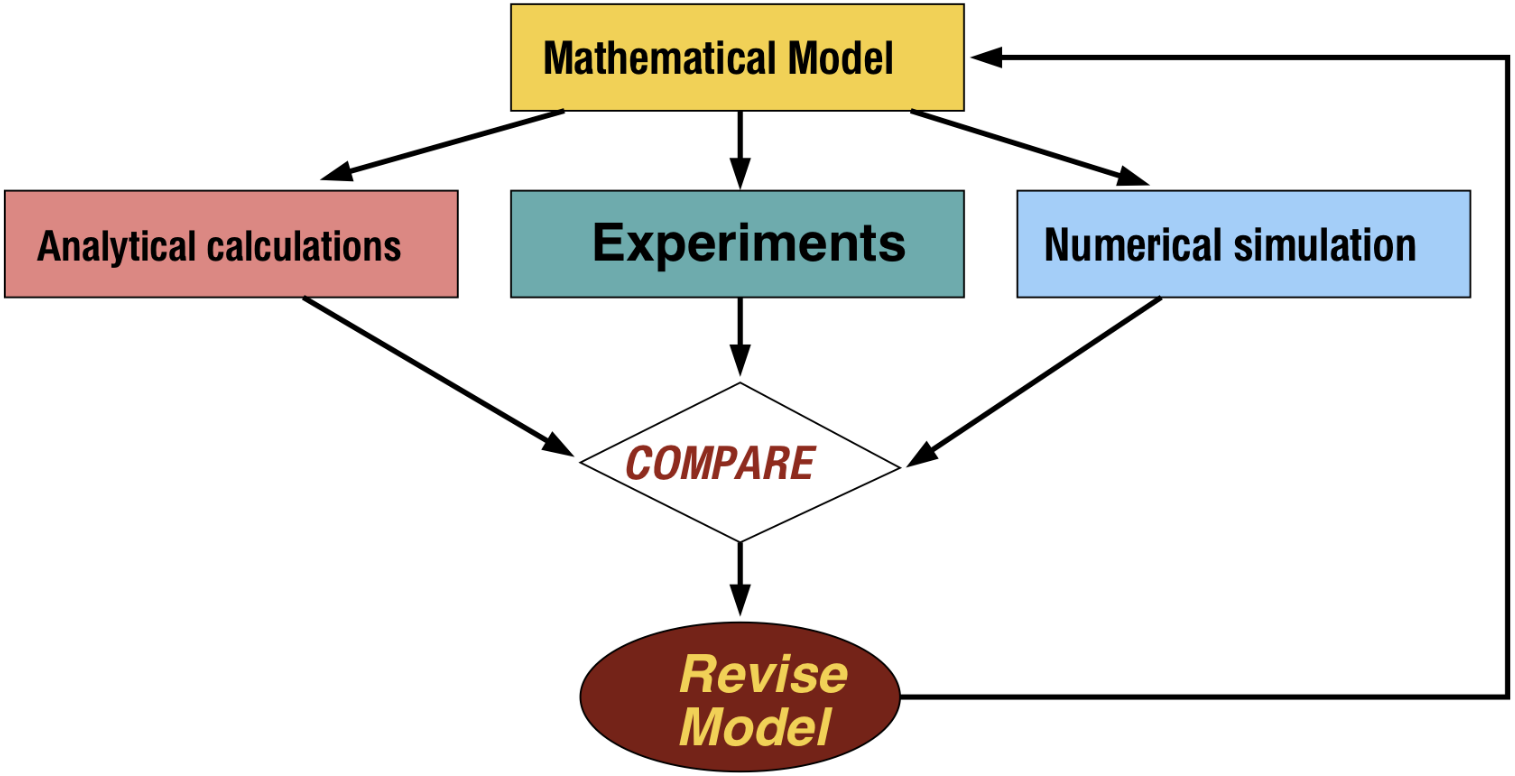


We do numerical simulation to

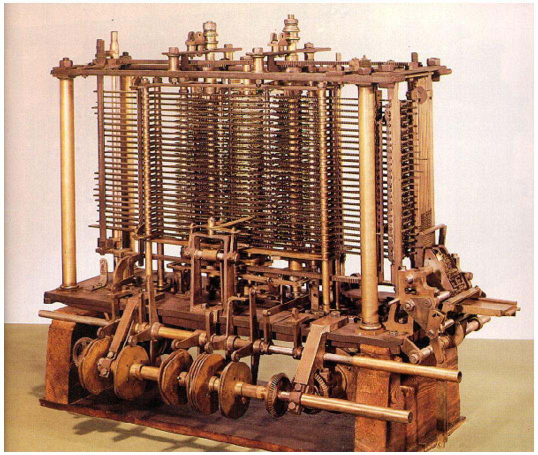
test our models

picks up where analytics gives out...





Computation...

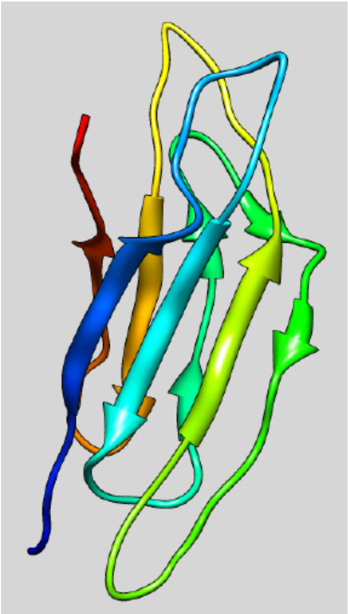


that it works is highly non trivial,
part of the
"unreasonable effectiveness of mathematics"
[Wigner 1960]

simple models work for highly complex things
-- gravity: planets and space probe trajectories
-- simulation time much shorter than real time

not so simple models
-- fluid flow and aeroplane wing design
-- sometimes use wind tunnel experiments as well

Bio systems:



in general simple models not adequate

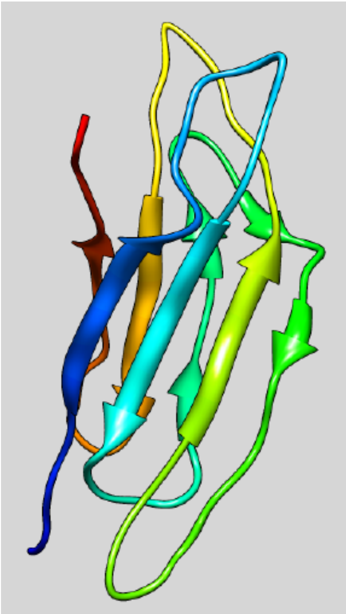
complex behaviour the norm

phenomenological models make

severe approximations

work only for restricted cases, with exceptions...

Biology is a BIG field:

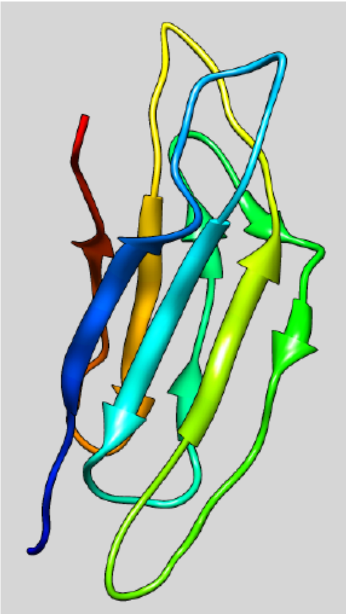


highest cited papers:
journal impact factors order of magnitude greater than physics

cut throat competition:
don't do preprints, little trust...

very reliant on experiments:
descriptive science dominates, understanding and prediction limited

Biomolecular simulation



- can model with less approximations
- necessary to interpret experiments

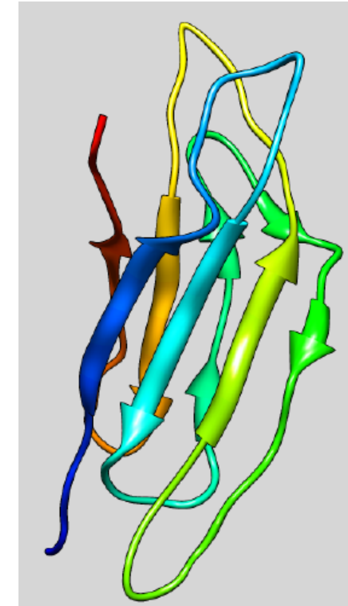
BUT simulation takes much longer than time evolution of real system!

small protein (162 amino acids, $3x10^4$ atoms) model for 10 μs took 100 days (Freddolino et al 2008)

100 ns takes one day to simulate on 32 CPUs

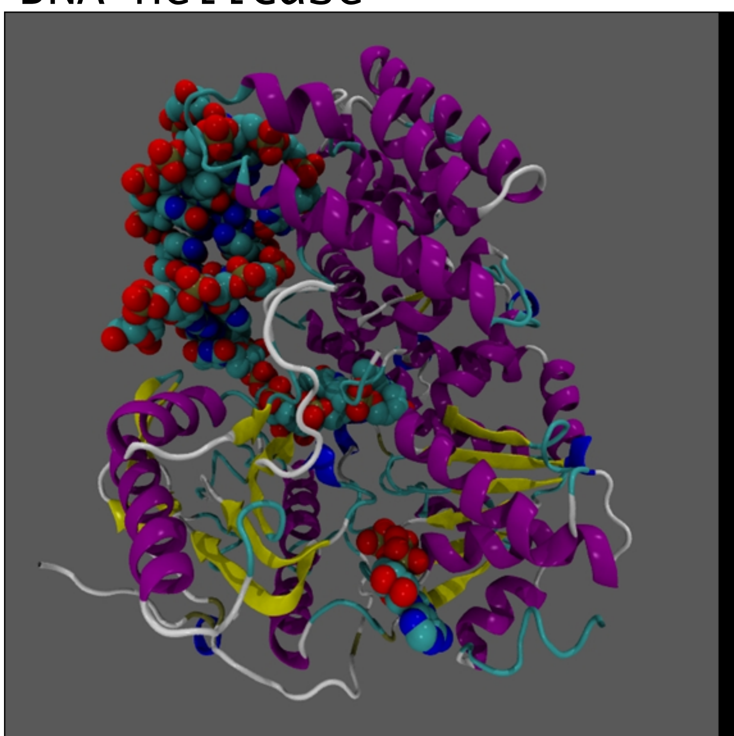
important conformational changes for biomolecular function occur over far longer timescales (μs–ms) and many proteins far larger

Biomolecular simulation

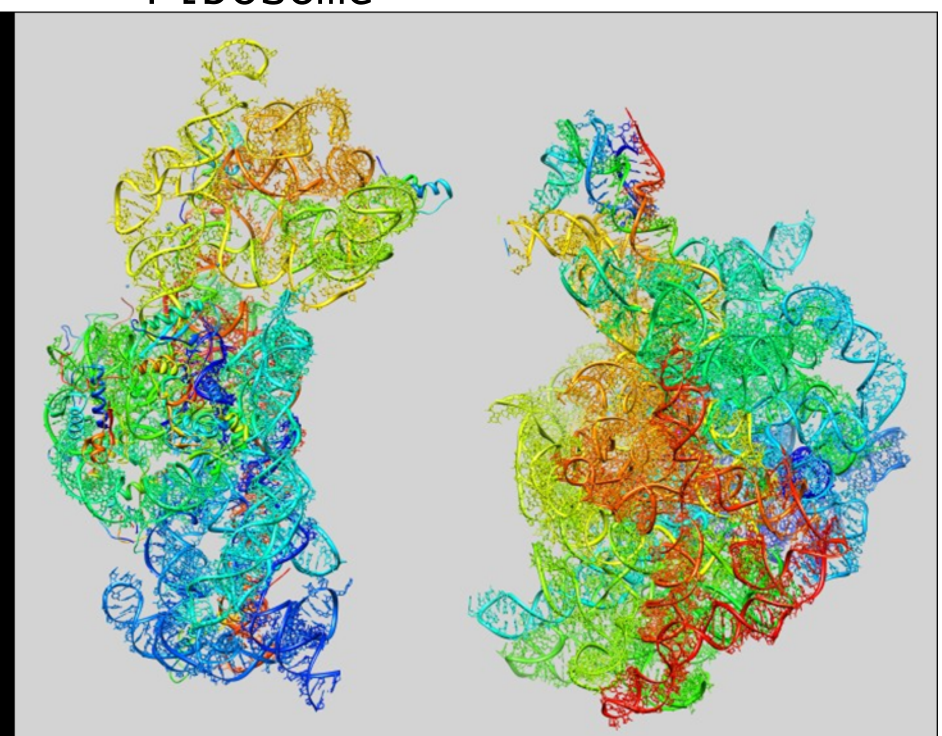


20 ns simulation of ribosome
2.6 million atoms (inc. water)
10^6 CPU hours on 768 CPUs (55 days)
(Sanbonmatsu & Tong 2006)

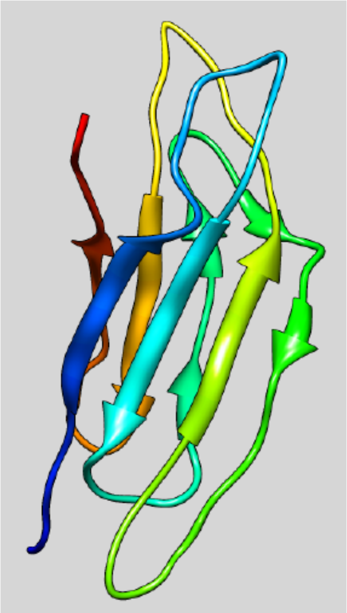
DNA helicase



ribosome



Biomolecular simulation



20 ns simulation of ribosome
2.6 million atoms
10^6 CPU hours on 768 CPUs (55 days)
(Sanbonmatsu & Tong 2006)

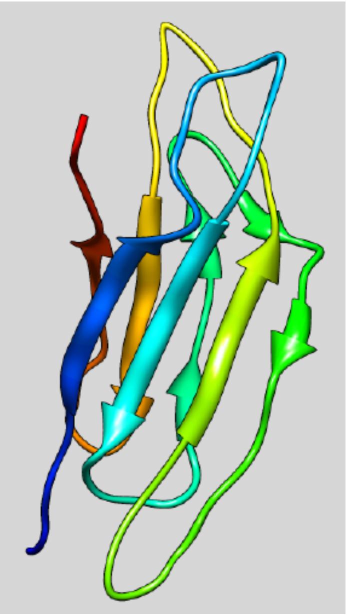
ribosome synthesises new proteins at rate of one per 0.1 s (Wen 2008)

would need simulation a million times longer:
1.5 million CPU years

-- role for quantum computation?

(Sarah Harris & VK, Phil Trans Roy Soc **368** 3581-3592 2010)

Biomolecular simulation



-- role for quantum computation?

Sarah would like to do atomistic simulation of a whole ecoli bacterium!

not realistic?

streamline model to use detail only where needed
(Moritsugu et al 2009)

to make progress over today's capabilities need 10^3 to 10^4 in time and 10^2 size

Quantum bio...

electrons pretty much always quantum

when do quantum correlations survive decoherence
at bio temperatures? (Seth Lloyd's talk)

bio timescales usually much longer
so average quantities good approximation

quantum chemistry required to get good estimates
of these values is not so easy -- source of error
in current biomolecular simulation

quantum computers could improve calculations
(Aspuru-Guzik group, Kassel et al Proc NAS 105 18681-18686 2008)

Quantum bio - summary

not about entanglement...

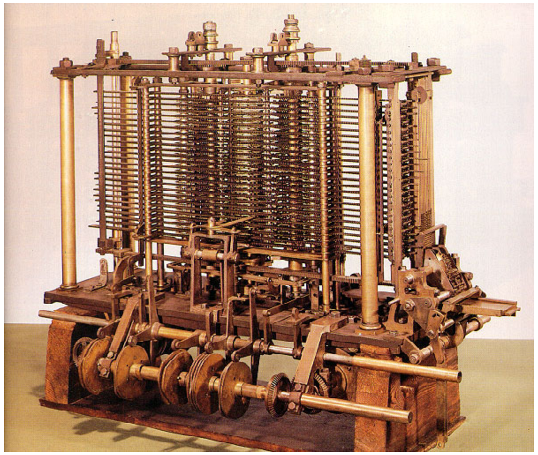
interplay between quantum correlations and decoherence at bio temperatures...(Seth Lloyd's talk)

needs quantum chemistry: quantum computers could improve calculations... (Aspuru-Guzik group)

could quantum computers do larger biomolecular simulations? (Devitt, Munro, Nemoto, 2008. High performance quantum computing. ArXiv:0810.2444v1)

(Sarah Harris & VK, Phil Trans Roy Soc A **368** 3581-3592 2010)

When does numerical simulation work?



- very well for gravitation...
- not so well for bio systems...
- quantum systems are even harder...

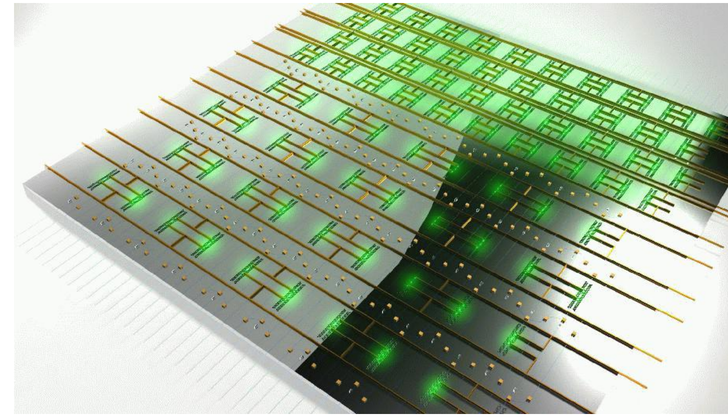
absolute limit on size of Hilbert space for classical computer simulation:

2^{36} is record (de Raedt et al Comp Phys Comm 176 127-136 2007)
2^{20} more realistic with non-unitary evolution

this is tiny: we are within an order of magnitude of useful quantum simulations of quantum systems

(KL Brown Munro VK Review of quantum simulation ArXiv:1004:5528v2)

When will quantum simulation of quantum systems work??



- it does now, for small systems (Chris Monroe's talk)

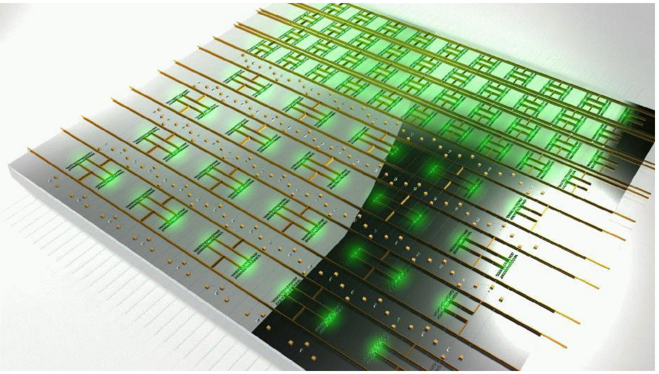
a possible problem is error correction:

quantum simulation works by directly mapping Hilbert space from system to simulator
– consequence is errors scale as $1/\epsilon$
rather than $\log(1/\epsilon)$ for binary computations

hence need more error correction for imperfect gates, etc. (Brown et al PRL 97 050504 2006)

...and hence CV quantum computing might do as well
(VK,Munro,Nemoto Phil Trans Roy Soc A **368** 3609-3620 2010)

Computing something we can't classically...



Shor's factoring algorithm:
need to beat best classical to date (Kleinjung et al. 2010):
(RSA challenge list) 232 digits = approx 768 bits
Shor's quantum algorithm needs: 2n qubits in QFT register plus 5n qubits for modular exponentiation = 7n logical qubits – 768 bit number needs 5376 logical qubits

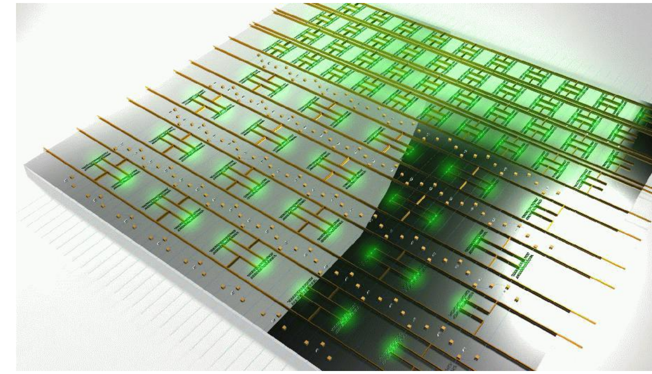
now add error correction: depends on error rates...
if error rate close to threshold of 10^{-3} to 10^{-4}, need more
(note: threshold error rate smaller than any experiment has achieved)

for low error rates, maybe 20–200 physical qubits per logical qubit
for high error rates, blows up quickly, maybe 10^5 per logical qubit

suggests we may need Teraqubit quantum computers to break factoring

– scaling favours quantum, but the crossover point is high

Computing something we can't classically...



Quantum simulation: 36 qubits is record so 40+ qubits...

CVQC (continuous variable quantum computation):

amount of squeezing → estimate how large classical simulation would be Suzuki et al. (2006) achieved 7dB of squeezing in optical expts

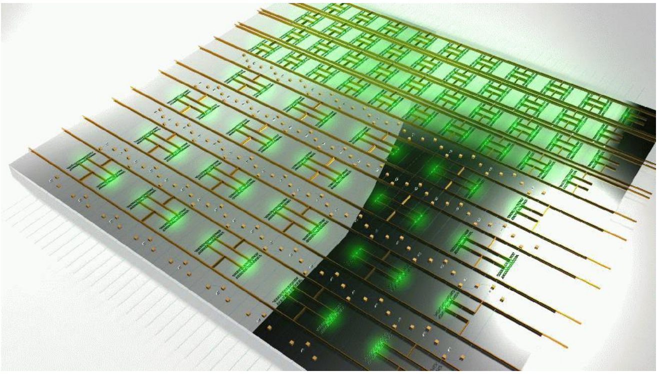
one mode with 7dB of squeezing = 2 to 3 bits of precision
i.e., ~ 5 distinguishable outcomes when state is measured

→ more than 17 modes coupled together ≡ more than 40 (qu)bits
– with arbitrary perfect coupling = beyond classical simulation

Aoki et al, 2009 achieved 9 modes combined in CV error correction - only Gaussian states thus still efficiently classically simulatable

(VK,Munro,Nemoto Phil Trans Roy Soc A **368** 3609-3620 2010)

Quantum speed limit?



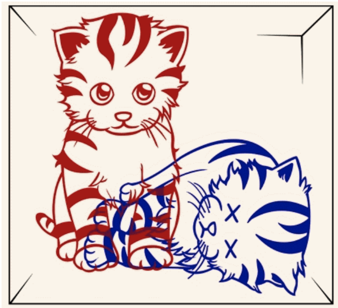
Theorem (Berry at al 2006)
proves cannot simulate quantum evolution faster than the real thing

but this is scaling result: no faster than O(t)

absolute limits on data processing?
Seth Lloyd has entertaining version: black holes

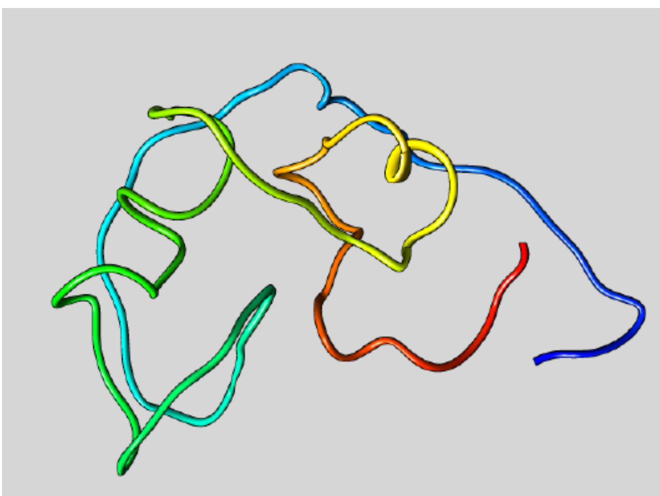
 - doesn't answer practical questions!

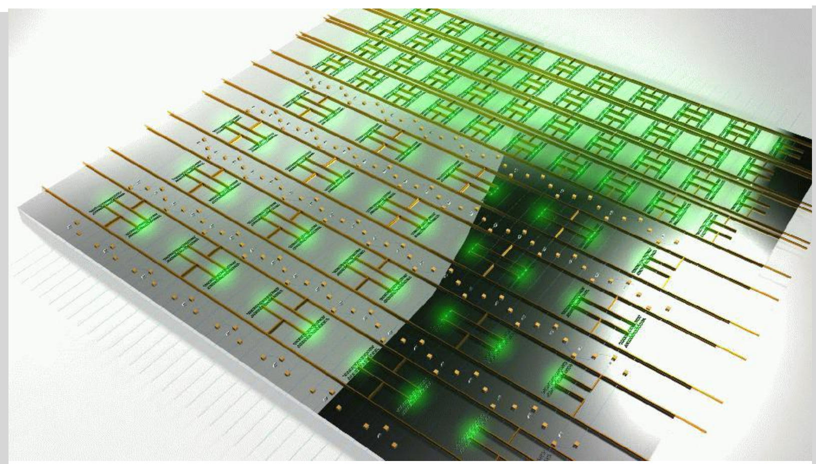
(compare communications...know limits and can actually operate quite close to them)



Biggest quantum contribution to biology could be through computation:

unfolded





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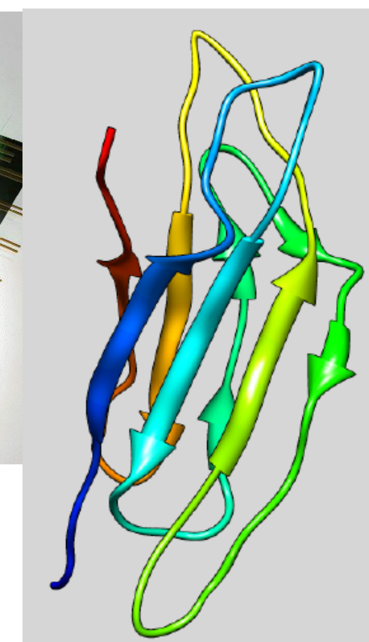

Given relative sizes of fields and funding this could be important for survival of physics...