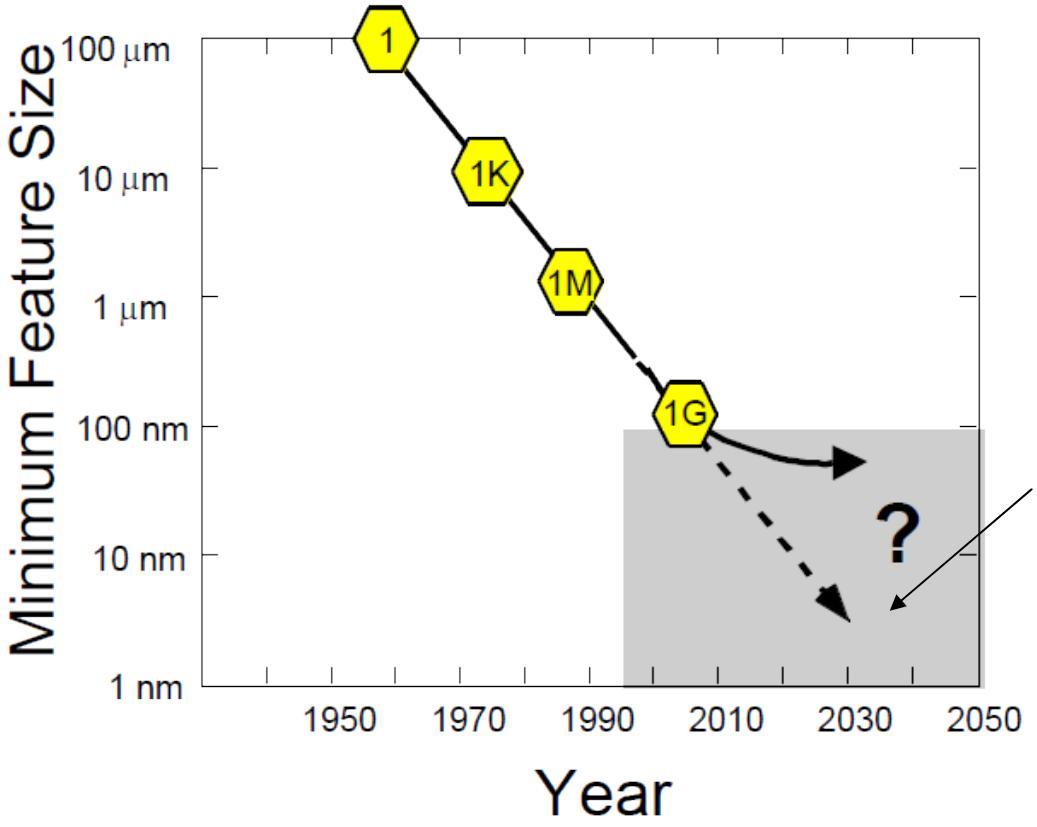
The MacDiarmid Institute
for Advanced Materials and Nanotechnology

IRL

Virtual Nanotechnology

The end of Moore's law?

- Transistors are getting smaller and smaller …



Techniques exist but they are slow and expensive

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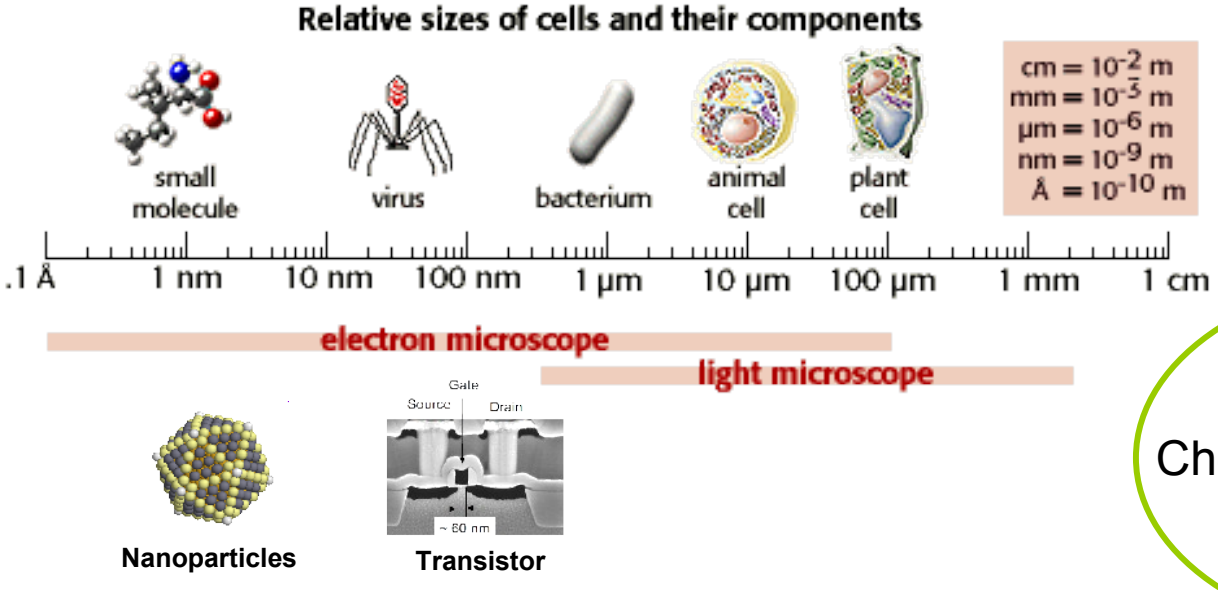
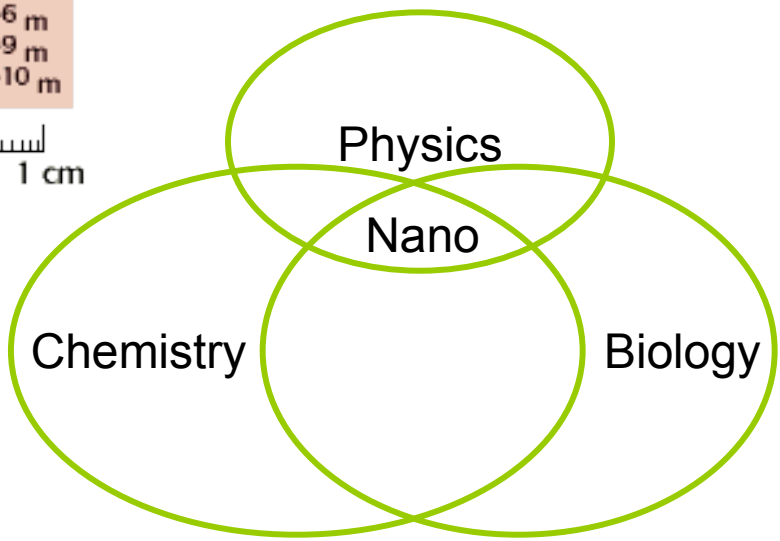
What is nanotechnology?

Manipulating materials and devices on lengths scales < 100 nm = 10^{-7} m



Nanoparticles

Transistor



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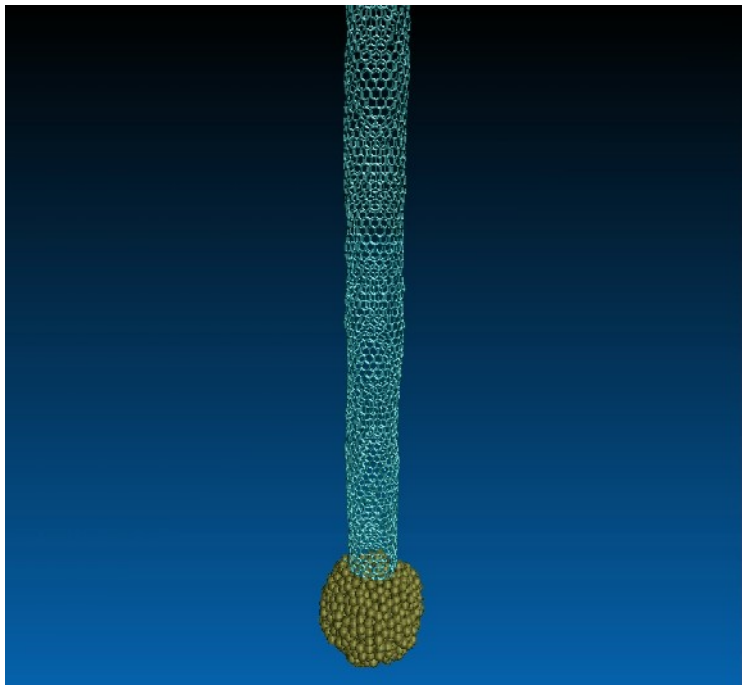
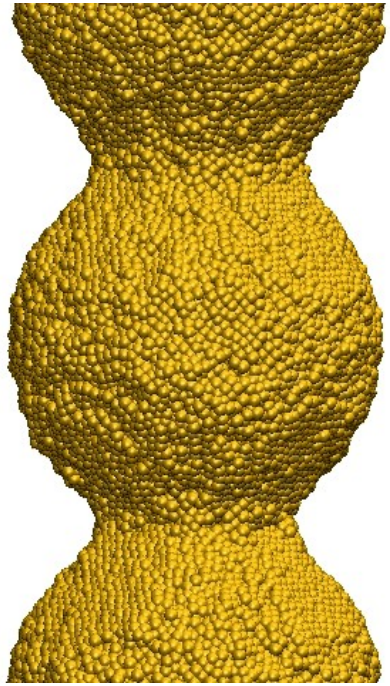
Virtual nanotechnology

- We simulate nanotechnology on computers



Dmitri Schebarchov (MSc)



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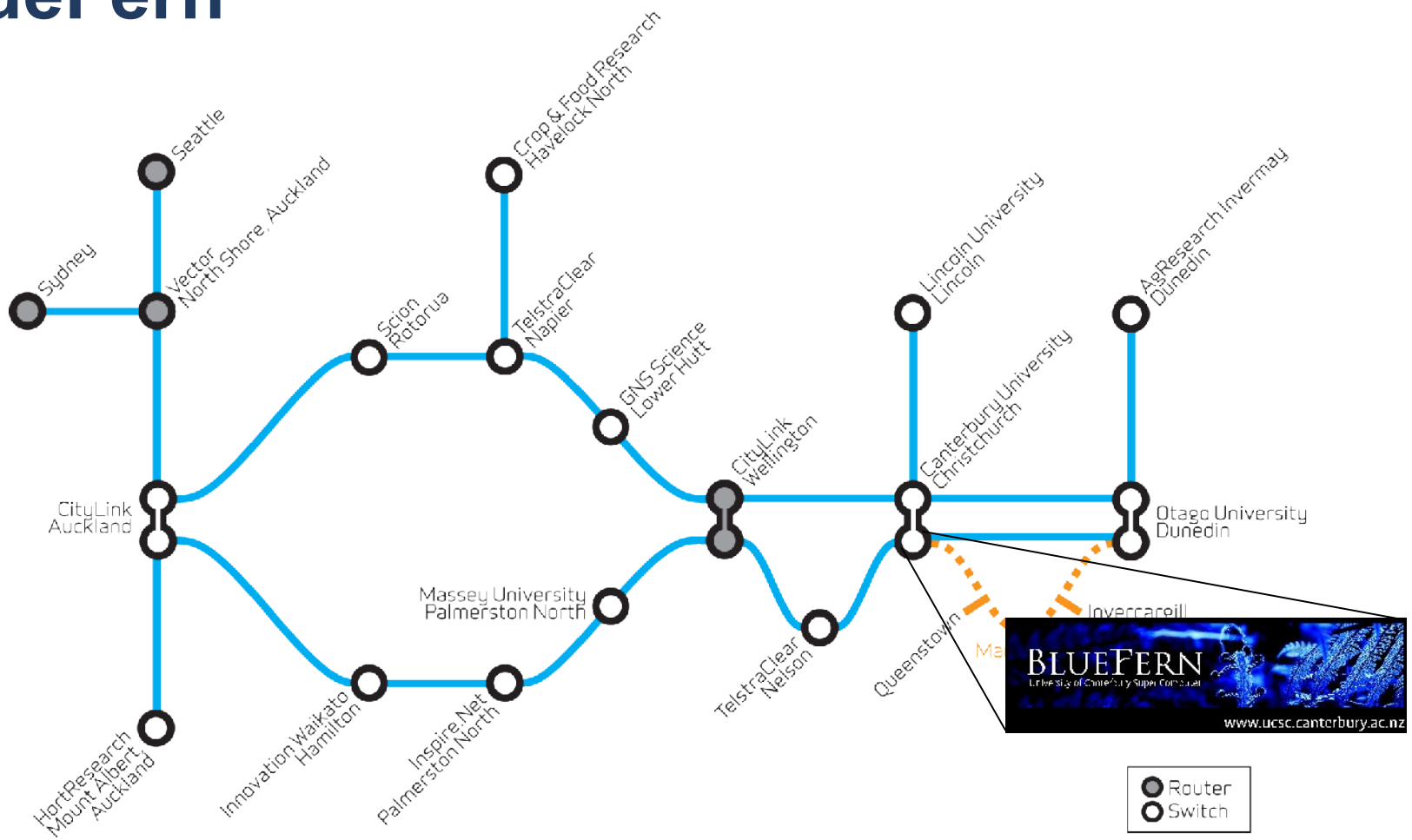
BlueFern



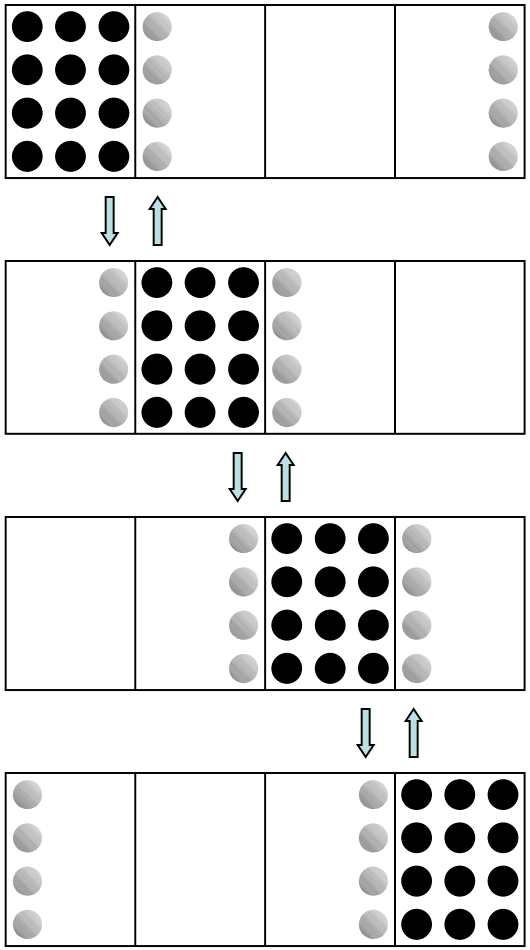
What is Blue Fern?

- A Blue Gene/L massively parallel supercomputer capable of > 12 TFlops
- The ***Blue Fern*** in Canterbury has 2048 nodes (4096 CPUs)
- Each node has two CPUs – one handles communication and one handles computation
- To take advantage of the many CPUs, code needs to work in parallel (uses MPI)

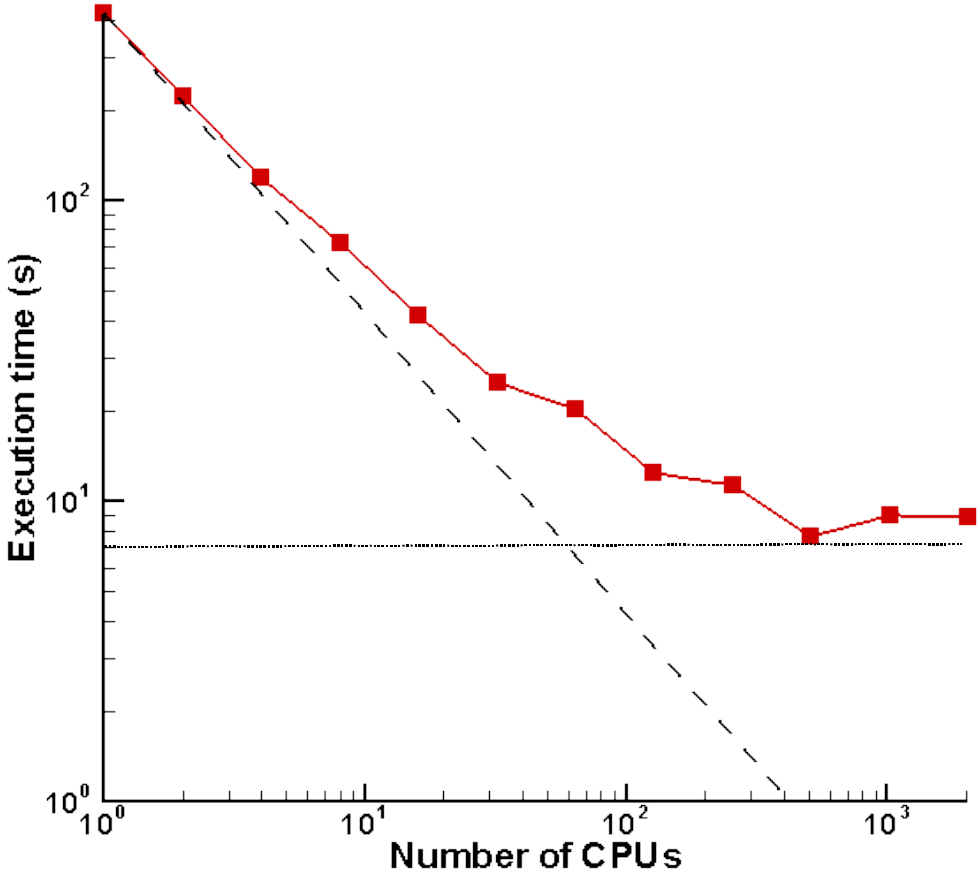
Parallel Computation

- The volume is divided between the processors.
- Each process tells other processes about atoms near the boundary.

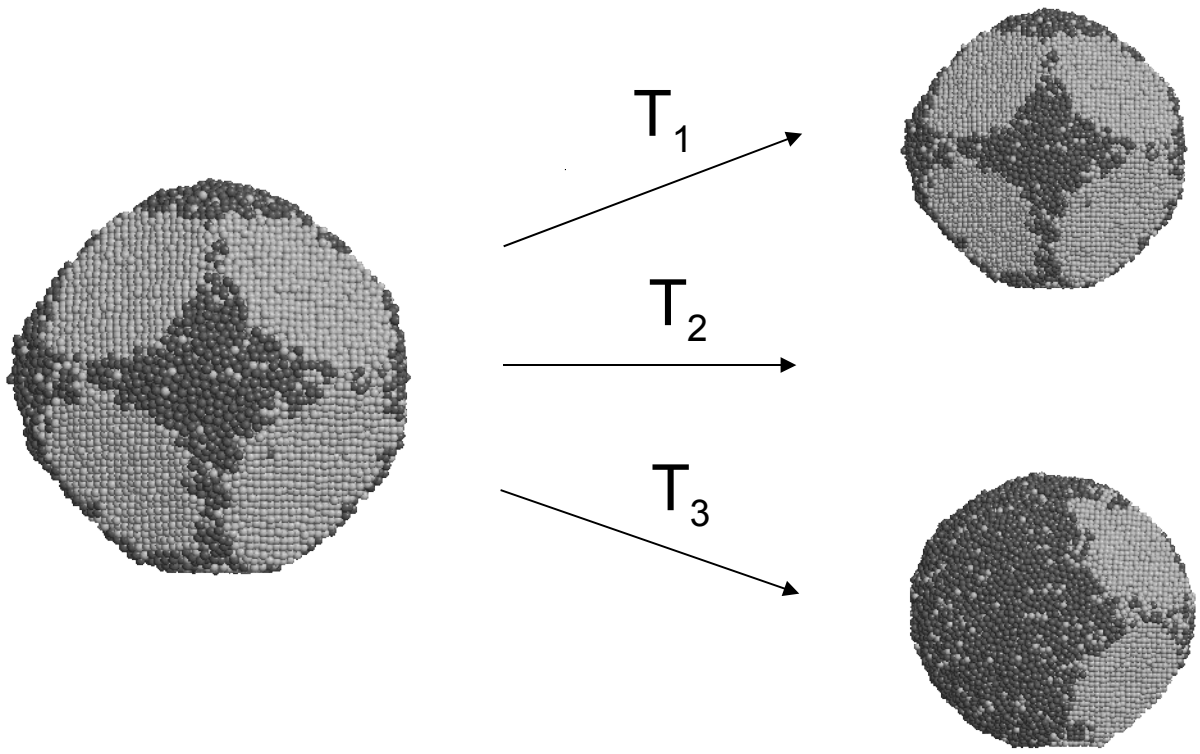
QuickTime™ and a
YUV420 codec decompressor
are needed to see this picture.



Parallel scaling



Ridiculously parallel computation



37766 atoms for 2 ns - 32 x 16 (=256) CPUs - 2 days

To use Blue Gene

- Sign up on the University of Canterbury Supercomputer website

http://www.bluefern.canterbury.ac.nz/

Conclusion

- Blue Gene has allowed us to simulate nanosystems atomistically on ~10 nm scales
- Available to all VUW staff and MacDiarmid PIs
- Users must consider how their application will take advantage of Blue Gene's massive parallelism
- Programs can be in Fortran or C/C++ with MPI