

Simulated Worlds: Doing Science with Computers

K.A.Hawick

Computer Science, Institute of Information and Mathematical Sciences, Massey University, Albany, North Shore, Auckland, New Zealand



Introduction

Computer simulation is a powerful tool for exploring hard problems in many areas of science. Simulation modeling coupled with advanced graphics has enabled important new industries such as animation for computer games and computer-generated scenes and characters in movies.

Simulation models play important roles in 21st century science and simulation is a vital tool in computational science that helps form a bridge between theory and experiment. Often a simulated model forms the basis for numerical experiments that allow us to precisely control the parameter range of a system that corresponds to a particular theoretical prediction which we can then test.

Simulated Worlds

One of the best known applications of computer simulation is numerical weather prediction and climate modelling. The equations for describing the atmosphere are solved numerically on a mesh of discrete points superposed on the Earth's surface. Live data from satellites and weather stations is used to correct a numerical model[1] and many national weather centres use these models, running on supercomputers, to produce 1-day, 2-day and even 5-day forecasts. Recent work focuses on climate models that predict how the weather system will change over many years.

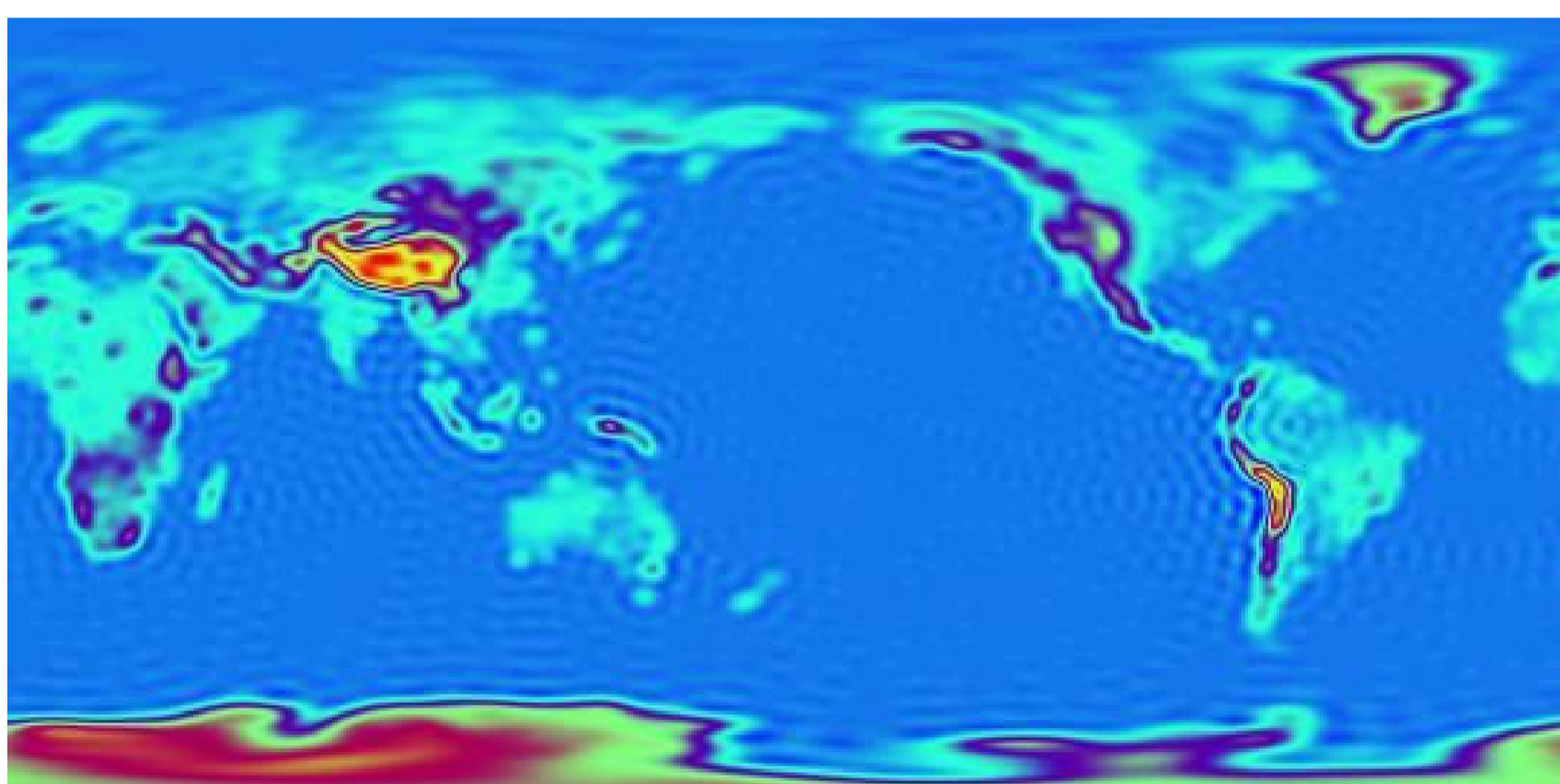


Figure 1: Weather Simulation - Geostrophic potential

Simulations can turn imagined structures and systems into definite images for real engineering models but also for designs that may be some years away from reality - such as space stations. Learn how to program simulations and 3-D graphical renderings like this in Massey's Computer Science courses.

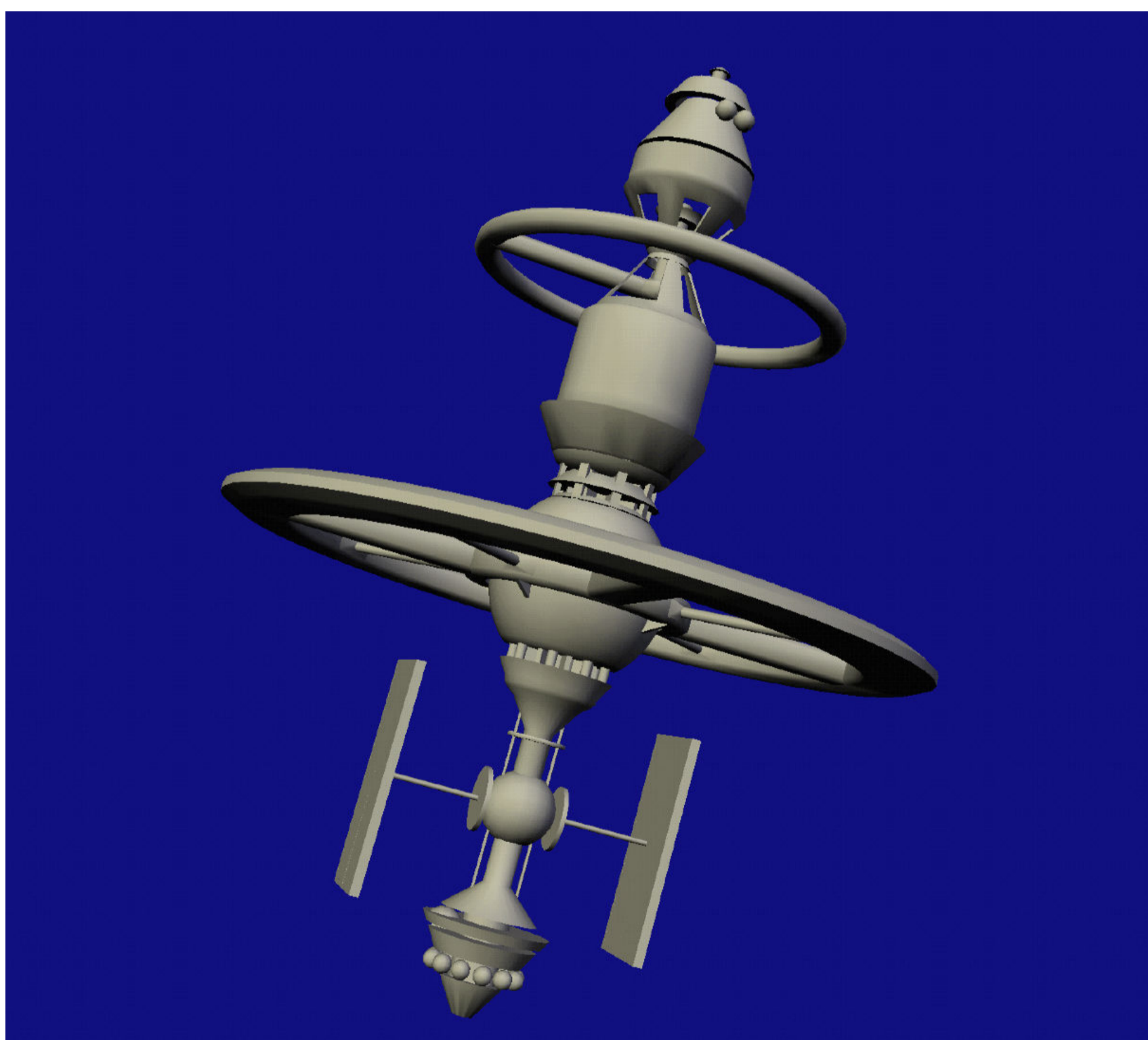


Figure 2: Simulated Space Station

Theoretical models such as cellular automata have been used as tools to explore a number of complex systems[2]. Simulating the time evolution of an automaton in 2-dimensions gives rise to a Sierpinski gasket-like structure in time, as shown below.

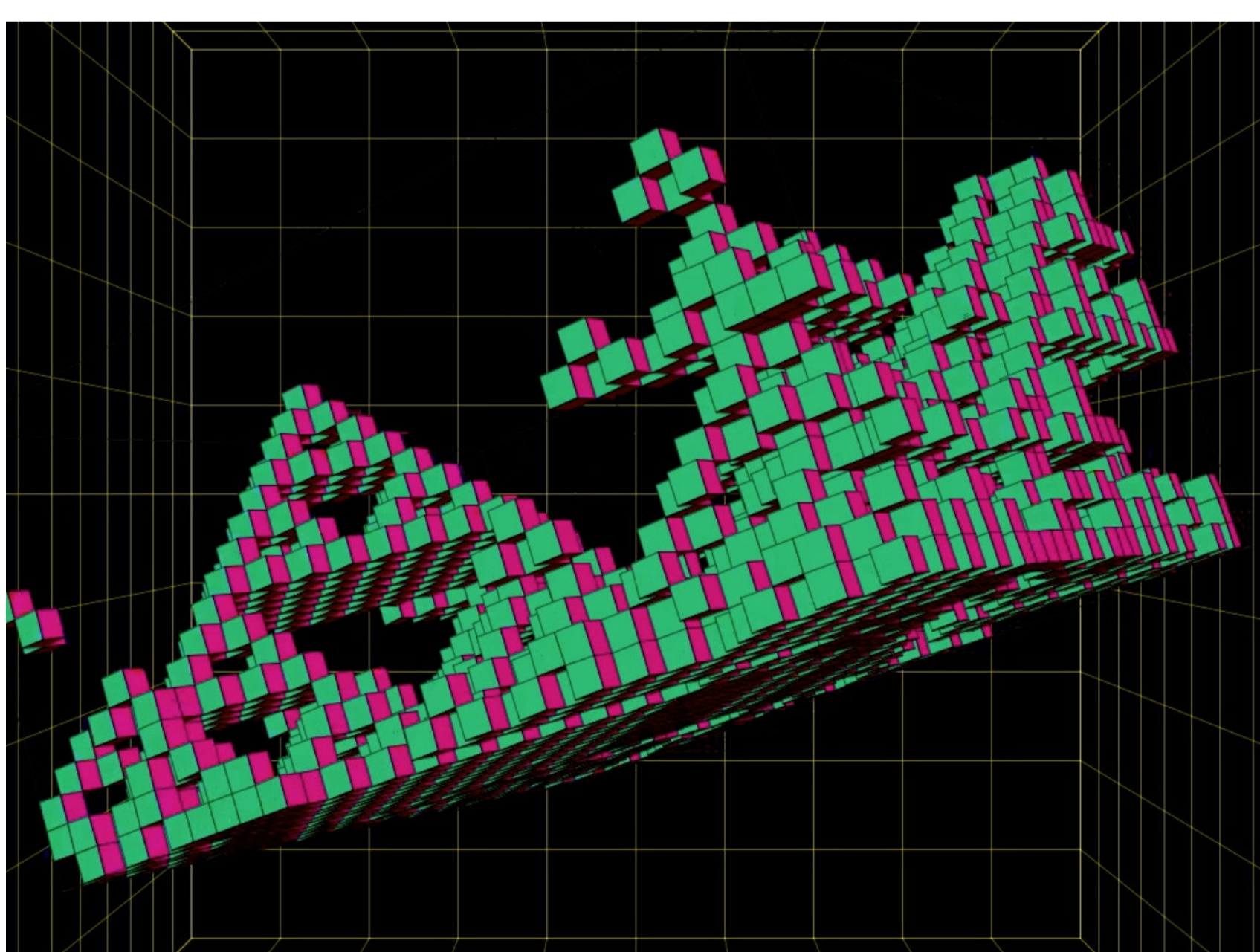


Figure 3: 2-D Cellular Automata - with time as the 3rd dimension

Other simulations approaches include field equations; discrete event models; particle methods; and systems using complex data structures such as graphs and queues.

Supercomputers for Simulations

There have been great developments in the power of supercomputer platforms over the last 30 years. These have been largely driven by the need for faster simulation engines.



Figure 4: ICL's Distributed Array Processor (DAP) occupying a whole machine room.

Computer systems like the Distributed Array Processor (DAP) occupied a whole machine room but represented the state-of-the-art in the early 1980s.

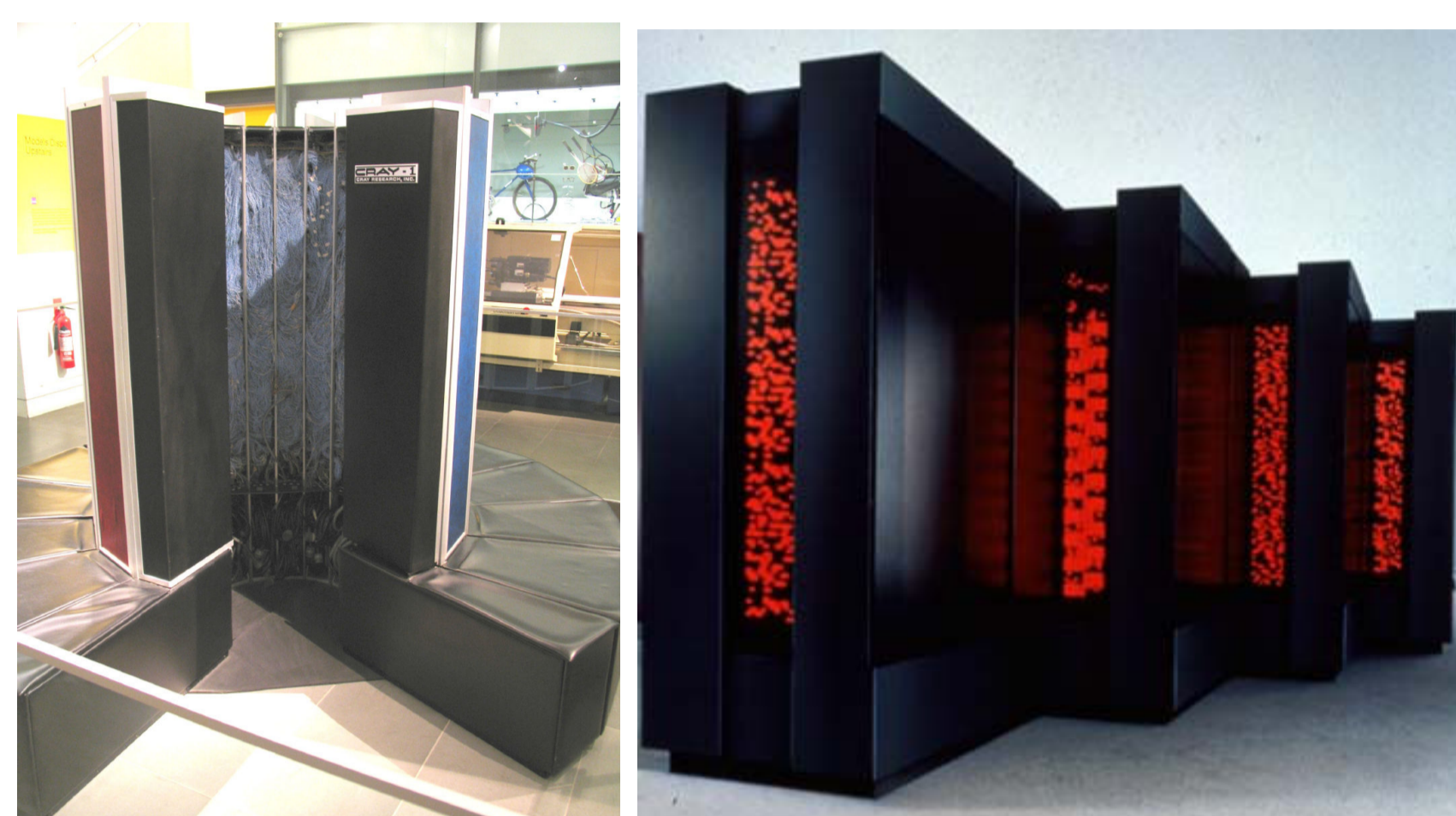


Figure 5: Cray-1 Vector Computer - now in London Science Museum (left) and Thinking Machines Connection Machine CM5 (right.)

Conventional supercomputers like the CRAY-1 used special cooling and an elaborate cable harness to interconnect a vector of processors that could work in tandem on a single calculation.

In the 1990s the Connection Machine not only looked fantastic, it was a powerful simulation engine with 65,536 separate processors.



Figure 6: Massey's Helix Cluster Supercomputer

Modern cluster computers such as Massey's Helix system and its derivatives consist of an array of relatively cheap commodity computers, wired together to work in parallel on a complex simulation problem.

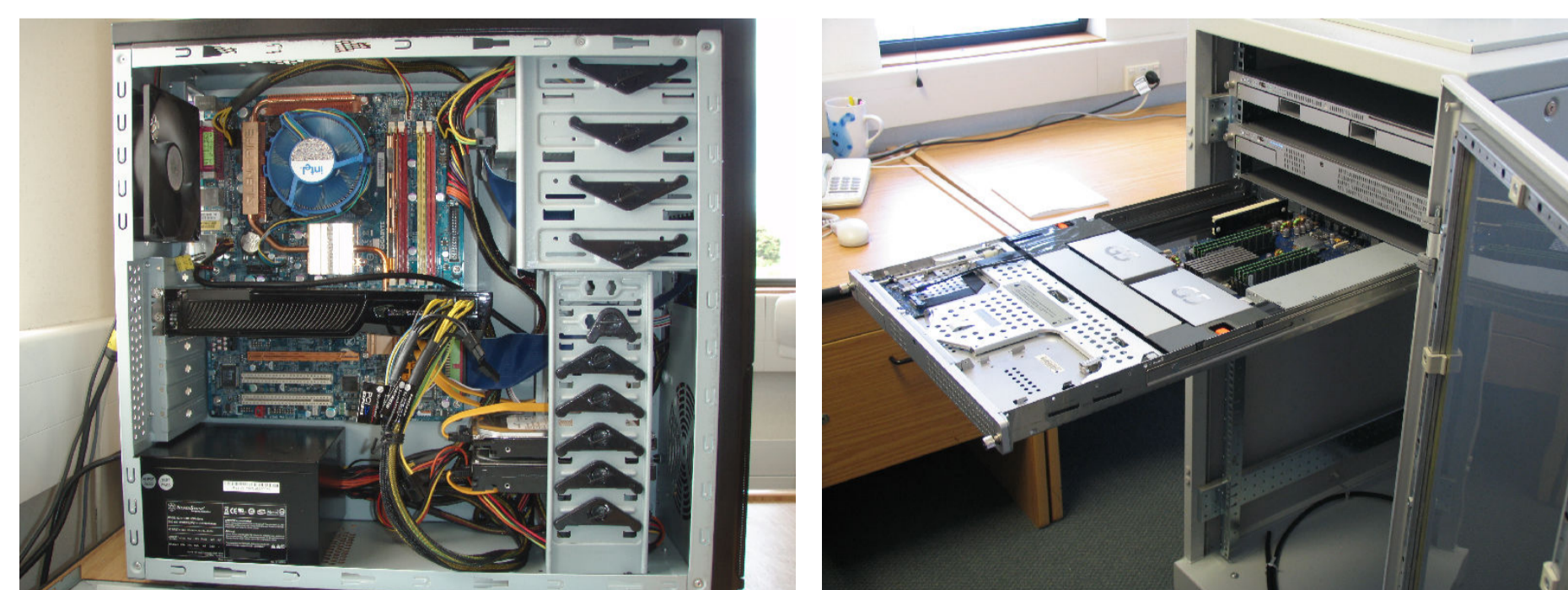


Figure 7: A Modern GPU supporting a quad-core processor (left) and a blade-based rack (right.)

Very modern computer systems make use of special purpose processors such as GPU - Graphical Processing Units - that can accelerate some simulations and calculations to much greater speeds than possible with ordinary processors.

Modern architectures also make use of "blade" cabinets, where each individual processor and its motherboard take up less physical space by being stacked.

Learn how to program parallel and distributed computers in Massey Computer Science courses.

Computational Science

Many of the ideas used in simulations can be applied in computer generated characters and other special effects in movies and in computer gaming engines. Soem serious quantitative science can be done too however, and often the results of a series of numerical simulation experiments can be compared with a theoretical model to verify a law or a way of describing the behaviour of a model system. The background image shows simulated ferromagnetic domains in a simulation system known as the Ising model.

Conventional mathematical approaches cannot solve the Ising system problem, but simulations were able to locate the critical temperature of the 3-D Ising magnet. This temperature - known as the Curie temperature - is the critical point at which the system's inherent magnetism is destroyed. Computing this property took over 3 supercomputer-years of calculation and simulation[3].

Other complex systems that exhibit "phase transitions" include the Cahn-Hilliard model [4]; the Ginzburg-Landau system [5] and several graph and network model systems [6]. The Complex Systems and Simulations Group (CSSG) at Massey is researching problems like these for use in better understanding physical and social systems like: motorway and urban traffic; Internet congestion; artificially intelligent agent models [7]; and complex new materials.

Complex systems are made up of a large number of relatively simple or understandable components or "sub-systems" and exhibit an emergent or "unexpected" collective behaviour when the component parts are all put together. The study of complex systems will be an important mission in science over the next century [8] and computer science and simulations will be important tools to support this.

Further Information

See Computational Science Technical Note: CSTN-052 [9] for more information on computer simulations.

This poster is based on the Professorial Lecture given on 4th March 2009 [10]. Slides are available from:

<http://www.massey.ac.nz/~kahawick/cssg>

You can learn more about many of the technical ideas behind "simulated worlds" in the Computer Science Undergraduate and Postgraduate programmes at Massey University, Albany - for more details see:

<http://iims.massey.ac.nz/computerscience.html>.

and

<http://www.massey.ac.nz/~kahawick/postgraduate>

More information on Massey's Centre for Parallel Computing (CPC) at:

<http://iims.massey.ac.nz/research/cpc>.

Thanks and Acknowledgements

Special thanks to the Complex Systems & Simulations Research Group (CSSG) & Students:

Dr Chris Scogings; Daniel Playne; Arno Leist; Anton Gerdelan; Guy Kloss; Mitchell Johnson; Steven Hosking; Helen Durrant; Gligor Kotusevski; Brad Heap; Dr Heath James; Dr Paul Coddington.

and thanks also to members of the Computer Science and Information Technology groups at Massey:

Dr Martin Johnson; Dr Peter Kay; Dr Andre Barczak; Dr Napoleon Reyes; Dr Ian Bond; Ursula Scogings; Dr Elena Calude; Dr Rosemary Stockdale; Dr Brian Whitfield.

References

- [1] K. A. Hawick, R. S. Bell, A. Dickinson, P. D. Surry, and B. J. N. Wylie, "Parallelisation of the unified model data assimilation scheme," in *Proc. Fifth ECMWF Workshop on Use of Parallel Processors in Meteorology*, (Reading), European Centre for Medium Range Weather Forecasting (ECMWF), November 1992.
- [2] S. Wolfram, *Theory and Applications of Cellular Automata*. World Scientific, 1986.
- [3] K. A. Hawick, "Domain Growth in Alloys." Edinburgh University, Ph.D. Thesis, 1991.
- [4] K. Hawick and D. Playne, "Modelling, simulating and visualizing the cahn-hilliard-cook field equation," Tech. Rep. CSTN-075, Massey University, January 2009.
- [5] D. Playne and K. Hawick, "Visualising interfaces in scalar and vector field-model simulations," Tech. Rep. CSTN-074, Massey University, January 2009.
- [6] A. Leist and K. Hawick, "A small-world network model for distributed storage of semantic metadata," Tech. Rep. CSTN-064, Massey University, September 2008.
- [7] C. Scogings and K. Hawick, "Intelligent and adaptive animat resource trading," Tech. Rep. CSTN-076, Massey University, February 2009.
- [8] J. Gribbin, *Deep Simplicity - Chaos, Complexity and the Emergence of Life*. No. ISBN 0-141-00722-2, Penguin, 2004.
- [9] D. P. Playne, A. P. Gerdelan, A. Leist, C. J. Scogings, and K. A. Hawick, "Simulation modelling and visualisation: Toolkits for building artificial worlds," *Research Letters in the Information and Mathematical Sciences*, vol. 12, pp. 25-50, 2008.
- [10] K. A. Hawick, "Simulated worlds: Educating students in doing science with computers," Tech. Rep. CSTN-080, Massey University, 2009.