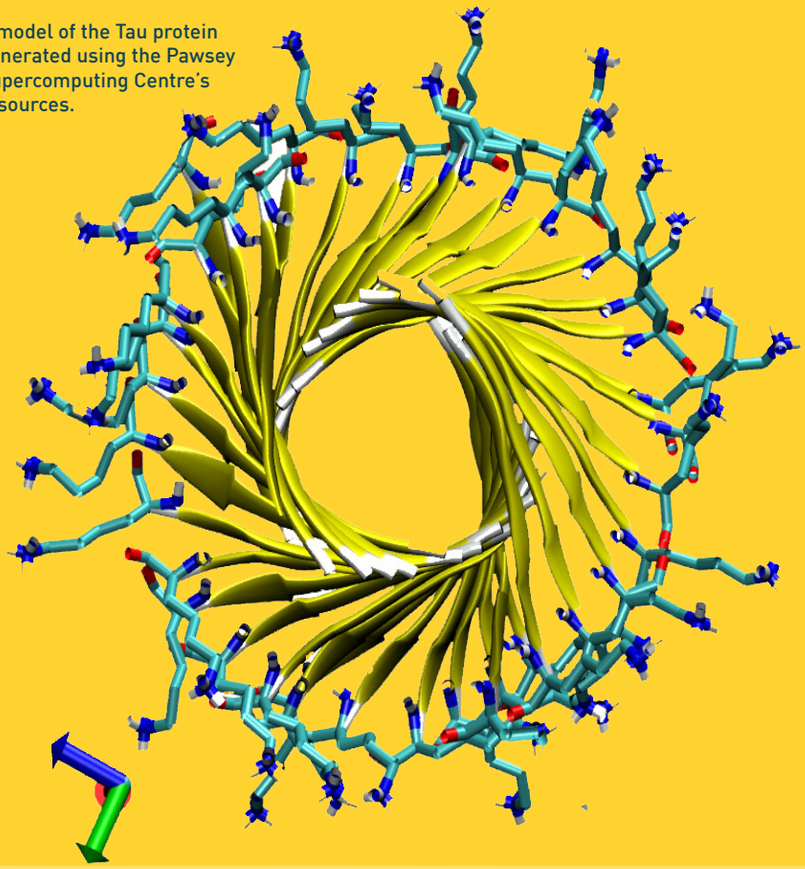
PAWSEY supercomputing centre

PARTNER INSTITUTION

Curtin University



A model of the Tau protein generated using the Pawsey Supercomputing Centre's resources.

PROJECT LEADER
DR NEHA S. GANDHI

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Main collaborators
Albert Lyons
Yu Jie Kan

SYSTEM
EPIC

TIME ALLOCATED
2,000,000 hours

AREA OF SCIENCE
MEDICINE

APPLICATION USED
AMBER 11 AND 12
GROMACS 4.5.5
FFTW
AUTODOCK 4.2
CONCOORD

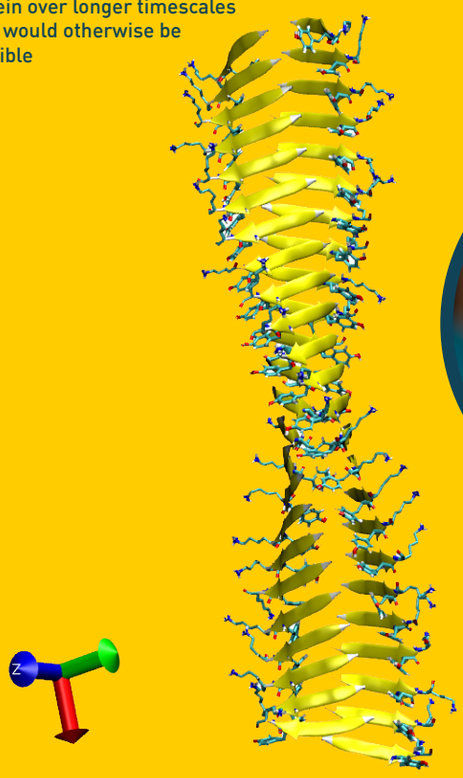
COMBATING ALZHEIMER'S AND DEMENTIA

Thanks to advances in medical science, life expectancy has greatly increased in developed nations like Australia. However, an unwanted side effect of this is a rise in neurodegenerative diseases like dementia and Alzheimer's, with the number of Australians with dementia predicted to rise almost 500% by 2050. Tau protein aggregation is a common pathological process in many of these diseases. Researchers from Curtin University are using the power of the Pawsey Supercomputing Centre to simulate and model protein aggregation to help better understand these debilitating diseases, and develop new management strategies.

2014

MOLECULAR MODELLING OF TAU PROTEIN

Supercomputing enables researchers to model the Tau protein over longer timescales than would otherwise be possible



THE CHALLENGE

Dr Gandhi's project is focused on increasing the fundamental understanding of the molecular mechanisms that lead to the abnormal formation of Tau protein in neurodegenerative diseases like Alzheimer's. These diseases, which are progressive and can affect all areas of the brain, are thought to be responsible for up to 70% of all cases of dementia.

Advanced molecular simulation methods can be used to help researchers develop a better understanding of the ways in which these proteins form in neurodegenerative disease cases.

However, this simulation work is extremely computationally intensive. Dr Gandhi's project worked with representative systems, containing 100,000 atoms.

Using traditional computing methods, simulating the formation of these proteins over just a one microsecond timescale could take an entire year. This makes supercomputing necessary to perform these simulations in a practical timeframe.

Similarly, visualising the data produced by these simulations is very memory intensive, and can only be done using the type of cutting-edge visualisation tools provided by the Pawsey Supercomputing Centre.

THE SOLUTION

Advanced molecular dynamics simulations were performed using AMBER14, the world's fastest molecular dynamics program, as well as other applications. These applications scaled extremely well on the Pawsey Supercomputing Centre's advanced systems.

"I was able to simulate up to 50 nanoseconds per day," says Dr Gandhi.

This means Dr Gandhi and her team of researchers were able to simulate in 20 days what would take an entire year using normal methods.

OUTCOME

The world-class resources provided by the Pawsey Supercomputing Centre were able to process the immense amounts of data produced by this project efficiently and in a practical timeframe.

This gives researchers more time to interpret their data and deliver practical results.

Dr Gandhi says this project will help to further the understanding of how the Tau protein is formed, and how it contributes to diseases like Alzheimer's.

"The outcomes of this project will create opportunities for the development of new therapeutic interventions that can inhibit protein aggregation and halt the progression of these diseases," says Dr Gandhi.

Dr Gandhi plans to continue her research into Tau protein aggregation in 2015 using the Pawsey Supercomputing Centre's new petascale 'Magnus' supercomputer.