

## What is the National Grid Service?

The National Grid Service (NGS) aims to provide coherent electronic access for UK researchers to all computational and data based resources and facilities required to carry out their research, independent of resource or researcher location.

You can find further information about the NGS on its website at [www.ngs.ac.uk](http://www.ngs.ac.uk). The website contains a wide range of documentation including technical details, software listings, user case studies and online tutorials for self-guided learning.

## Keep in touch with the NGS

If you would like to be kept up to date with news from the NGS then join our mailing list to receive fortnightly news updates including events and training opportunities.

[www.jiscmail.ac.uk/lists/NGS-NEWS.html](http://www.jiscmail.ac.uk/lists/NGS-NEWS.html)

If you are a user of NGS resources then join our status mailing list to be kept up to date with service news and updates.

<http://www.jiscmail.ac.uk/lists/NGS-STATUS.html>

The NGS produces a quarterly newsletter containing a large variety of news about the NGS

including user case studies, NGS site news, application updates and conference reports. The latest edition of NGS News can be found on our website in the Outreach section or join our mailing list to receive an announcement when the latest edition is released.

## Contact the NGS

If you have any queries regarding the NGS or if you would like more information, then contact our helpdesk:

NGS Support Centre  
Email: [support@grid-support.ac.uk](mailto:support@grid-support.ac.uk)  
Tel: +44 (0) 1235 446 822

NGS  
e-Science Centre  
STFC Rutherford Appleton  
Laboratory  
Harwell Science and Innovation  
Campus  
Didcot  
Oxfordshire  
OX11 0QX

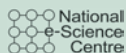
Dr Philip Fowler

University of Oxford, Department of Biochemistry

# Ion channel simulations and free energy calculations



[www.ngs.ac.uk](http://www.ngs.ac.uk)



Name: **Dr Philip Fowler**  
Institution: University of Oxford, Department of Biochemistry  
Research: **Ion channel simulations and free energy calculations**



Dr Philip Fowler uses classical molecular dynamics to study membrane proteins, in particular the proteins that allow ions such as potassium to diffuse in and out of cells, otherwise known as ion channels. Ion channel research is extremely important, not only for its scientific interest, but also because ion channels are intimately involved in, for example, the functioning of the brain and heart.

Well-established molecular dynamics packages such as NAMD and GROMACS are used to produce simulations that can be used in either a quantitative or qualitative way.

Qualitative simulations are run by taking the structure of a protein and putting it in a more realistic environment, such as in a membrane surrounded by water and with ions added to simulate a salt solution. The results are then visualised so the structure can be looked at and sampled, providing understanding of how particular parts of the function work.

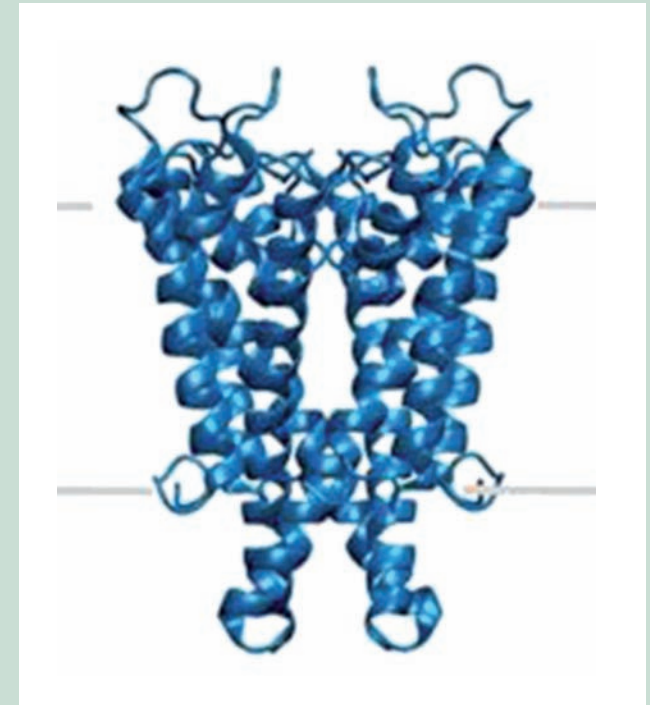
Quantitative simulations on the other hand usually produce a number that can then be compared to experimental results. How the free energy of binding changes when a potassium ion is changed to a sodium ion is one example of such a number. This can be determined experimentally and compared to the value yielded by the simulation. This free energy tells us how selective a certain ion channel is for potassium over sodium—vital for their function.

The techniques used to achieve such results are well-known and have been around for a long time but the time it takes to run them has put people off. With 34 parallel simulations taking 1-2 days each it's not surprising. Using the NGS, 34 parallel simulations can now be run in under two weeks. With such a drastic reduction in time, researchers can run more complicated simulation scenarios such as running two mutations, checking the results by repeating simulations and running simulations backwards.

Dr Philip Fowler was a user of the National Grid Service before he even went into production. He is now a veteran of the service, having used it for over three years, but would he recommend it to others? "No way," he laughs. "I want it all to myself!"

### Further Information

University of Oxford  
Department of Biochemistry:  
<http://sbc.bioch.ox.ac.uk>



*Visualisation of the KcsA ion channel.*