Contribution ID: **47** Type: **Oral**

Moorhen: a web molecular graphics program

Here we present Moorhen, a next-generation client-side web-based application for the visualisation and manipulation of molecules in structure determination and analysis.
Recent developments in the field of cloud-based computing have enabled a rapid increase in the range of crystallographic tools available on the web, which crystallographers can use without the need for installing software locally. This provides great opportunities in making scientific software more available in teaching contexts and to previously underrepresented communities. However, several challenges remain untackled, in particular those in the field of molecular graphics. There is the need to provide users with web-based tools for the visualisation and manipulation of complex molecular structures together with their associated experimental data.
Moorhen is a new web-based application which provides access to a large number of functionalities developed as part of the Coot model building software and exposed in the libcoot API via an interactive user-friendly graphical interface built with React. Thus, Moorhen is the first generally available tool of its kind offering tools for interactive model editing and model refinement on the web. All of Moorhen's refinement and visualisation calculations are performed "in browser", which means users have the ability to access these model editing tools with near-native performance without the drawback of installing any additional software in their machines. Moorhen has been made available as a stand-alone web-app at moorhen.org, and also through the CCP4 Cloud graphical user interface (GUI). Additionally, there are plans in place to extend its availability through the CCP4i2 and CCPEM GUIs.

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