doi:10.1017/S1431927620017183
Microsc. Microanal. 26 (Suppl 2), 2020

cloudEMAPS: A Cloud Computing Environment for Electron Microscopy Application Simulations

Jian-Min Zuo[1], Xiurong Zhu[2], Elaine Ang[1] and Rahul Shah[1]

[1]University of Illinois at Urbana-Champaign, Urbana, Illinois, United States, [2]EMLab Solutions, Champaign, Illinois, United States

Cloud computing (CC) is a computational paradigm that delivers on-demand computing resources, everything from customized applications to data centers, over the internet. This paradigm has several advantages over the traditional on-premise approach, including dynamically scalable, virtualized computing resources and the economics of scale. Remarkable advances have been made over the past decade, with competing cloud services emerging from major technological companies as well as research institutions. However, scientists in general, including microscopists, are slow to embrace and adopt the CC environment. There are examples of shared computing resources, but the technologies enabling such services are varied. The NSF supported NANO-HUB[1] runs via a distributed computing network at Purdue University, as well as the TeraGrid and Open Science Grid, while the popular, but now decommissioned, *WebEMAPS* was hosted on a single server by the University of Illinois[2]. In electron microscopy, methods such as STEM or dynamical diffraction simulations are widely used in quantifying images and diffraction patterns, producing applications that require a great amount of computational resources. Cloud platforms could provide the infrastructure support for allocating the resources needed as well as system support to implement high-performance computing algorithms used in electron microscopy simulations. Here, we explore the CC based computing for electron microscopy using ***cloudEMAPS,*** which is designed and developed to demonstrate the feasibility of CC for both microscopy research and teaching. The objective is to develop a CC platform to further CC-based applications for microscopy-related, and materials science in general, simulations, as well utilities serving the microscopy community.

Fig. 1 illustrates how electron microscopy simulation in *cloudEMAPS* works [3]. The electron microscopy computations hosted on the cloud are electron diffraction pattern and image simulations using a defined crystal model. Such applications require a few input data and computational steps that range from being relatively simple as in the case of kinematical diffraction simulation to relatively complex in the case of dynamical convergent beam electron diffraction simulations. The output data that comes back from the simulations is also relatively small in the form of an image or descriptive data about diffracted beam positions and intensity. These simulations are backed by the command-line software hosted on Amazon Web Service (AWS). On the client side, users run a browser-based front-end GUI on their local device. When a user “operates on the microscope” by loading sample materials and adjusting microscope control settings, the front-end browser sends an HTTP request to the cloud server which contains the user’s control settings as payload. In addition to the microscope control settings, the payload data can also include other control parameters such as zone axis. Once the client request is received, the server parses and validates the request, allocates necessary computing resources, and executes the corresponding computation on the allocated resources. When computation finishes, the server parses, elicits a response with the results in a payload formatted in JSON for the front-end client to render in a graphical canvas. This way, the end-user could observe in real-time the result of their operation on the simulated microscope. The key underlying program design is the web services that conforms to the REST (Representational State Transfer) architectural style.

The cloudEMAPS currently includes most of the *WebEMAPS*[2] features such as crystal structure and rendering, kinematic diffraction including Kikuchi and HOLZ lines, convergent beam electron diffraction by the Bloch wave method. To host computationally expensive applications, such as Bloch wave simulation of large unit cell crystals, future development will include optimization in computation with parallelization and load balancing the computation to more efficiently utilize the cloud computing resources.

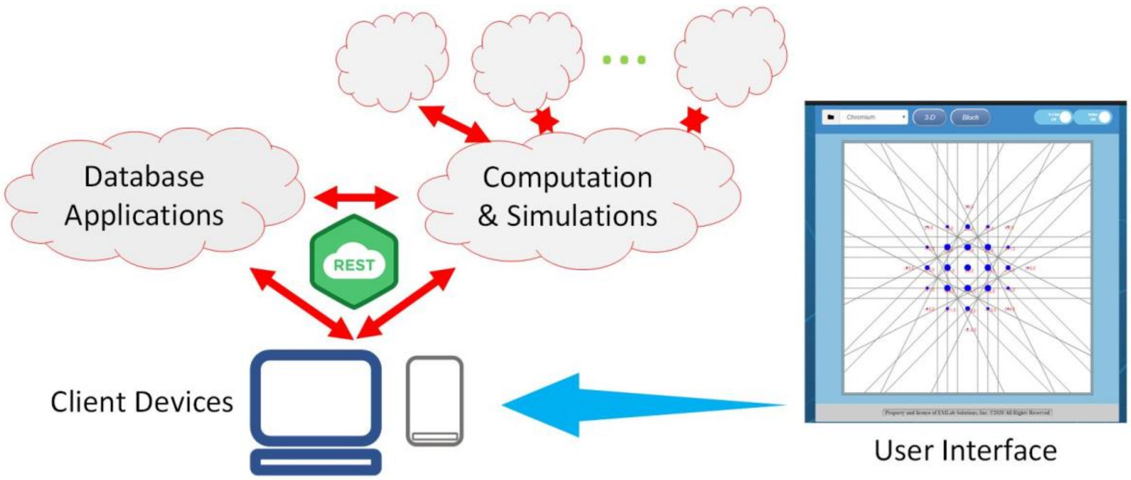

Figure 1. Cloud-based computing and implementation for cloudEMAPS, where users interactions occur on a client device through a user interface while data and applications and computation are on cloud.

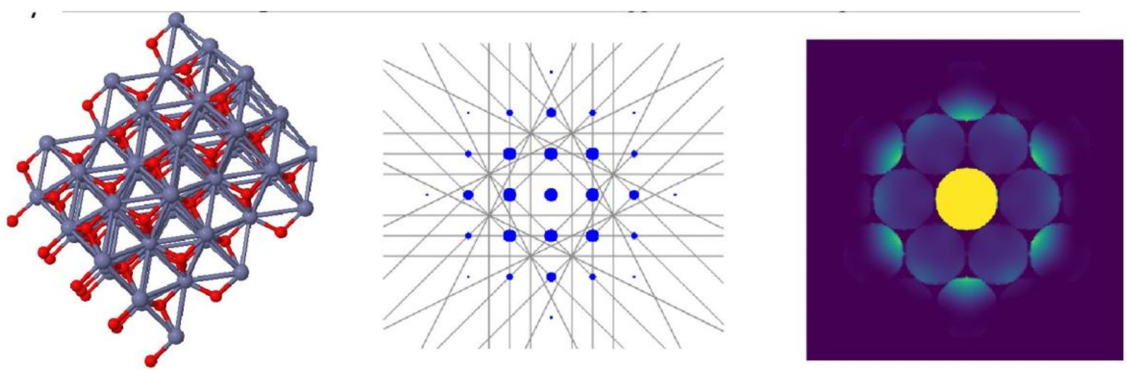

Figure 2. Example of microscopy applications through cloud computing.

References

[1] G. Klimeck et al., Computing in Science & Engineering, vol. 10, pp. 17-23, 2008.
[2] Zuo, J., & Mabon, J. (2004). *Microscopy and Microanalysis, 10*(S02), 1000-1001.
[3] https://emaps.emlabsolutions.com/