

# WORKSHOP: A SCIENCE GATEWAY FOR ATOMIC AND MOLECULAR PHYSICS

DEC 11-13, 2019



## Organizing Committee

Samantha Fonseca dos Santos – Rollins College  
Jimena Gorfinkiel – Open University, Milton Keynes UK  
Alicia Palacios – University of Madrid  
Marianna Safronova – University of Delaware  
Barry Schneider - NIST

## The AMP Gateway Group

Klaus Bartschat and Oleg Zatsarinny – Drake U  
Igor Bray – Curtin U, AU  
Armin Scrinzi – Ludwig-Maximilians U, DE  
Fernando Martin and Jesus Jesús González-Vázquez – U of Madrid, SP  
Jimena D. Gorfinkiel – Open University, Milton Keynes, UK  
Jonathan Tennyson – UCL, UK  
Sudhakar Pamidighantam - IU  
Barry Schneider – NIST

The organizing committee would like to take this opportunity to invite you to attend a workshop entitled, “A Science Gateway for Atomic and Molecular Physics”.

This project grew out of an NSF supported workshop held at ITAMP, May 14-16, 2018 entitled, “Developing Flexible and Robust Software in Computational Atomic and Molecular (A&M) Physics” organized by Barry Schneider (chair), Robert Forrey (Penn State), and Naduvalath Balakrishnan (UNLV).

Following the workshop six of the groups interested in atomic and molecular collisions and the interaction of those systems with electromagnetic radiation submitted an NSF proposal to the

eXtreme Science and Engineering Discovery Environment ( XSEDE ) to build and maintain a Science Gateway devoted to the codes developed in these groups. The purpose of the project is to explore mechanisms to collectively make codes available and easier to use by the partners as well as others in the community. With the proposal granted, the group was joined by Sudhakar Pamidighantam of the XSEDE project for development of the gateway.

With some of the codes being ported to various XSEDE platforms, we are now taking the next step by describing the science and the computational details of our codes to a larger community with the goal of making them available and useful to others and to also invite people who have similar interests to consider more direct participation in the project.

While we are still engaged in organizing the details of the workshop, the tentative agenda is;

- Day 1, Wednesday, Dec 11:
  - An introduction and some background to set the stage.
  - One-hour overview talks on the science and computational techniques used in each code and an additional 15 minutes for discussion. These talks will be designed to give the attendees enough background on the science problems that can be tackled with the code and the methods employed by the developers.
- Day 2, Thursday, Dec 12:
  - One-hour demonstrations of using the codes on the gateway with 30 minutes for questions, discussion, comments, etc.
- Day 3, Friday, Dec 13:
  - Short presentations from attendees, open discussions, suggestions, etc. This is currently planned to be a half day, but it could be extended to a full day if there is sufficient interest,

We considered a more hands-on process with breakouts into separate rooms, where participants would actually work with their own laptops on the gateway. That was eventually rejected as being too time consuming for a workshop of this length, and it has the additional downside of not allowing a participant to attend more than a single session. The use of the Science Gateway does not require users to download and install the code on their own platform, a process that many of us know can be filled with difficulties. The codes are already installed and running on various NSF supercomputers. Note that there will also be a presentation on the gateway itself and other aspects that are relevant to people interested in using the gateway for their science.

Practical details.

- The workshop will be held on the NIST campus.
- It is being supported by the Molecular Sciences Software Institute (MOLSSI), the NSF, and NIST but funds are extremely limited.

- All participants will be staying at the Hilton in Gaithersburg, as it will provide shuttle service to the NIST campus free of charge. There will be a dinner at the hotel on Day 2 of the workshop.
- There will be a small registration fee of \$100 USD to cover incidental expenses.

Please respond to Barry Schneider ( [bis@nist.gov](mailto:bis@nist.gov) ) by October 7 as attendance is limited and we need to make the necessary arrangements quickly. We are looking forward to an exciting few days.

