

# Workshop Agenda: A Science Gateway for Atomic and Molecular Physics

**Location:** Hilton Hotel - NIST Building 101, Lecture Room D

**Date:** 12/11/2019-12/13/2019

**Time:** 12/11/2019-12/12/2019: 8:30am - 5:30pm

12/13/2019 : 8:30am -12:00pm

## Agenda 12/11/2019

To be negotiated with hotel

**Shuttles depart from Hilton to NIST  
Please set time details at check  
in for all days.**

8:30am - 9:00am	Welcome and Introduction	Barry Schneider
9:00am - 10:00am	<a href="#">Introduction to the B-Spline R-Matrix Method: Methodology and Implementation</a>	Kathryn Hamilton and Klaus Bartschat – Drake University, Des Moines, Iowa
10:00am - 10:30am	Coffee Break	NIST Cafeteria
10:30am - 11:30am	<a href="#">Introduction to the Convergent Close Coupling Method: Methodology and implementation</a>	Igor Bray – Curtin University, Perth, Australia
11:30am - 12:30pm	<a href="#">Introduction to the UK Molecular R-Matrix Method: Methodology and implementation</a>	Jimena Gorfinkiel – The Open University, Milton Keynes, UK
12:30pm - 1:30pm	Lunch	NIST Cafeteria
1:30pm - 2:30pm	Introduction to tRecX- Methodology and implementation	Armin Scrinzi -Ludwig Maximilians University, Munich, Germany
2:30pm - 3:30pm	Introduction to Xchem - Methodology and implementation	Jesus Gonzales Vasquez – UAM, Madrid, Spain
3:30pm - 4:00pm	Coffee Break	NIST Cafeteria
4:00pm - 5:00pm	<a href="#">Introduction to the AMP Gateway: How do we use the gateway</a>	Sudhakar Pamidighantam, Indiana University, Bloomington, Indiana
5:00pm - 5:30pm	Questions and Comments	All
5:45pm	Shuttle to return to hotel	
7:00pm	Dinner	Possible ad hoc groups to nearby restaurants if cars available

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8:30am - 9:00am	<a href="#">The AMP Gateway: More hands-on details</a>	Sudhakar Pamidighantam
9:00am - 9:30am	<a href="#">Using the B-Spline R-Matrix Codes: Setting up input for cases and running codes</a>	Kathryn Hamilton and Klaus Bartschat
9:30am - 10:00am	Coffee Break	NIST Cafeteria
10:00am - 10:30am	Using the Convergent Close Coupling Codes: Setting up input for cases and running codes on the gateway – Using GPGPU's on XSEDE	Igor Bray
10:30am - 11:00am	<a href="#">Using the UKRmol + suite: Setting up input for cases and running codes on gateway</a>	Jimena Gorfinkiel
11:00am - 11:30am	Using the tRecx Codes: Setting up input for cases and running codes on gateway	Armin Scrinzi
11:30am - 12:30pm	Lunch	NIST Cafeteria
12:30pm - 1:00pm	Using the Xchem Codes: Setting up input for cases and running codes on gateway	Jesus Gonzales Vasquez
1:00pm - 1:30pm	Coffee Break	NIST Cafeteria
1:30pm - 2:00pm	The Belfast R-Matrix Codes	Connor Ballance
2:00pm - 2:30pm	An Online portal for high-precision atomic physics data and Computation	Marianna Safronova
2:30pm - 3:00pm	LUCIA – A versatile quantum chemistry code.	Jeppe Olsen
3:00pm - 3:30pm	<a href="#">MOLSSI &amp; SEAMM</a>	Paul Saxe MOLSSI
3:30pm - 4:45pm	<p>Panel plus questions and comments</p> <ol style="list-style-type: none"> <li>1. What do you want out of gateway</li> <li>2. Can you contribute and if so how</li> <li>3. Is this just a production environment or more</li> <li>4. How to transparently interact with home machines</li> <li>5. Dealing with version control, and documentation</li> <li>6. Dealing with files, especially large files</li> </ol>	<ul style="list-style-type: none"> <li>• Panel Chair: Rudi Eigenmann</li> <li>• Panelists: Armin Scrinzi, Alicia Palacios, Bob Lucchese, Lars Madsen, Frank Yip, Loren Greenman.</li> <li>• 5 min for each then open discussion</li> </ul>

	This should be freewheeling and open. Audience participation is necessary.	
5:00pm	Shuttle to return to hotel	
7:00pm	Banquet	Hilton

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8:30am - 9:30am	Codes for attosecond Physics	Luca Argenti and Nicholas Douquet
9:30am - 11:00am	Breakout Sessions	LR C, LR D, B-111, B113
11:00am - 11:30am	Wrap up discussion	
12:00pm	Depart	

## BlueJeans Participants

- Zdenek Masin
- Bogdan Mihaila