- A MolSSI Workshop -
Distributed Workflows for Biomolecular Simulation

September 12-13, 2017
Autodesk Gallery (2nd Floor), One Market Street, Landmark Building, San Francisco

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SEPTEMBER 12, 2017

8:00am - 8:30am	**Participants arrive and Breakfast**
8:30am - 8:40am	**Welcome** (Details and Logistics) - *Merry Wang (Autodesk Life Sciences)*
8:40am - 9:00am	**Workshop Introduction and Bootcamp Kickoff** - *Aaron Virshup (Autodesk Life Sciences), John Chodera (MSKCC)*
	---WORKFLOW BOOTCAMP---
9:00am -9:05am	<u>Introduction to Session 1: "Workflow Success Stories"</u> Moderator: *Daniel Smith (MolSSI)*
9:05am - 9:25am	**The Materials Project: Experiences from running a million computational materials science simulations and sharing the results with tens of thousands of researchers through the Materials Project -** *Anubhav Jain (LBNL)*
9:25am - 9:45am	**Seven Bridges: Enabling Standardized, Reproducible Analysis at Production Scale -** *Anurag Sethi (Seven Bridges)*
9:50am - 9:55am	<u>Introduction to Session 2: "Industry Needs"</u> Moderator: *John Chodera (MSKCC)*
9:55am - 10:15am	**How Workflows can Enable Industry/Academic Collaboration** - *Brad Sherborne (Merck)*
10:15am - 10:35am	**What Pharma Needs from Workflows** - *Jeff Blaney (Genentech)*
10:35am - 10:50am	**--- REFRESHMENTS AND BREAK ---**
10:50am - 10:55am	<u>Introduction to Session 3: "Existing Systems"</u> Moderator: *John Chodera (MSKCC)*
10:55am - 11: 10am	**Orion – CADD Re-imagined on the Cloud** - *Bob Tolbert (Open Eye)*
11:10am - 11:25am	**Open Source Infrastructure for Computational Chemistry** - *Aaron Virshup (Autodesk Life Sciences)*
11:25am - 11:40am	**Collaborative Drug Discovery with LIveDesign: Cloud-based platform for *in sillico* Modeling, Cheminformatics, and Data Warehouse -** *Cecilia Cheng (Schrodinger)*
11:40am - 11:45am	<u>Introduction to Session 4: "Cloud Computing"</u> Moderator: *Aaron Virshup (Autodesk Life Sciences)*
11:45am - 12:00pm	**Google Cloud Life Sciences Efforts** - *Joe Corkery (Google), Matt Bookman (Verily)*
12:00pm - 12:15pm	**Scientific Computing on Amazon Web Services** - *Jamie Kinney (Amazon Life Sciences)*

12:15pm - 1:15pm	**--- LUNCH ---**
1:15pm -1:30	**Introduction to MolSSI** *- Daniel Crawford (Virginia Tech/MolSSI)*
	--- HANDS ON WORKSHOP ---

1:30pm - 1:50pm	**Workflow Objectives and Opportunities for Coordination** *John Chodera*
	
	Lightning Talk: 1-2 minute introduction by workflow group leaders
	
	    ● **Free energy calculations** *Michael Shirts*
	    ● **Molecular dynamics simulation** *Pek Leong & Paul Saxe*
	    ● **Biomolecular complex setup pipeline** *David Mobley*
	    ● **Docking and scoring** *Ajay Jain*
	    ● **Quantitative affinity prediction blind assessment** *Jeffrey Wagner*

1:50pm - 2:00pm	**Ground Rules for Design Thinking -** *Edward de Guzman, Autodesk*
2:00pm - 3:35pm	**Session A: Identify Workflow Components** Goal: In individual groups, this session uses guided discussion techniques to identify objectives and components for your target workflow.
3:35pm - 3:50pm	**--- REFRESHMENTS AND BREAK ---**
3:50pm - 4:50pm	**Session B: Create Workflow Posters** Goal: In individual groups, this session uses guided discussion techniques to iterate on workflow diagramming and formulate ideas into a concept poster.
4:50pm - 5:00pm	**Day One Wrap Up** *John Chodera and Brad Sherborne*
5:30pm - 8:00pm	**--- RECEPTION AND DINNER (Le Colonial)---** (20 Cosmo Pl., San Francisco)

SEPTEMBER 13, 2017

8:30am - 9:00am	**Participants arrive and Breakfast**
9:00am - 9:10am	**Day Two Welcome** *John Chodera and Daniel Smith*
9:10am - 9:40am	**Building Blocks for Domain Specific Workflows** *Shantenu Jha (Rutgers/MolSSI)*
9:40am - 10:50am	**Session C: Workflow system requirements**

	Goal: Present workflow concept posters and refine requirements
10:50am - 11:05am	**--- REFRESHMENTS AND BREAK ---**
11:05am - 12:10pm	**Session D: Prioritization and Community Action Items**
12:10pm - 1:10pm	**--- LUNCH ---**
1:10am - 2:45pm	**Working Session I** Facilitator: Aaron Virshup
2:45pm - 3:15pm	**--- REFRESHMENTS AND BREAK ---**
3:15pm - 4:15pm	**Working Session II** Facilitator: Aaron Virshup
4:15pm - 4:45pm	**Wrap up discussion** *Facilitator: John Chodera and Daniel Smith*
4:45pm - 5:00pm	**Closing Remarks** *John Chodera, Aaron Virshup, and Daniel Smith*