CHiMaD

Building an Interoperable Materials Data Infrastructure

CHiMaD Headquarters
2205 Tech Drive, Hogan 1160
Northwestern University
Evanston, IL
May 2, 2016

Hotel shuttle will leave at 7:00

7:15AM - 7:45AM	Registration & breakfast buffet
7:45AM - 7:55AM	*Peter Voorhees*, Northwestern U, Welcome & CHiMaD
7:55AM - 8:10AM	*James Warren,* NIST, Data in MGI

Brief presentations (~10 min Overview/Update Presentations with time for 1 question)

8:10AM - 8:30AM	*Ian Foster*, U of Chicago/ANL, Workshop Overview, Materials Data Facility
8:30AM - 8:45AM	*Gerhard Klimick*, Purdue, nanoHUB
8:45AM - 9:00AM	*Michael Zentner*, Purdue, HUBzero
9:00AM - 9:15AM	*Qimin Yan*, LBNL, Materials Project
9:15AM - 9:30AM	*Sharief Youssef*, NIST, Materials Data Curator System
9:30AM - 9:45AM	*Brian Puchala*, U of Michigan, Materials Commons
9:45AM - 10:00AM	*Kenton McHenry*, NCSA, National Data Service
10:00AM - 10:15AM	*Matt Jacobsen*, AFRL, ICE system
10:15AM - 10:30AM	*Bryce Meredig,* Citrine
10:30AM - 10:45AM	*Tam Mayeshiba*, U of Wisconsin, MAterials Simulation Toolkit (MAST)
10:45AM - 11:00AM	*V. Hegde/L. Ward,* Northwestern U, Open Quantum Materials Database (OQMD*)*
11:00AM - 11:15AM	BREAK
11:15AM - 11:30AM	*Alan Aspuru-Guzik*, Harvard, Harvard Clean Energy Project (remote presentation)
11:30AM - 11:45AM	*Cormac Toher*, Duke, AFLOWLIB
11:45AM - 12:00AM	*Steve Konstanty*, U of Illinois, Timely and Trusted Curation/Coordination (T2C2)
12:00AM - 12:10AM	*Vin Crespi*, Pennsylvania State, Two-Dimensional Crystal Consortium (2DCC-MIP)
12:10AM - 12:20AM	*Lynn Rathbun*, Cornell, Analysis, Discovery of Interface Materials (PARADIM-MIP)
12:20AM - 12:35PM	*Marco Giovoni*, ANL, Midwest Integrated Center Computational Mat'ls (MICCoM)
12:35PM - 12:50PM	*Ray Plante*, NIST, Materials Resource Registry
12:50PM - 1:50PM	Lunch & Informal Discussions
1:50PM - 3:10PM	Small Group Break-out Discussions - 4 small groups (~10 participants/group)
3:10PM - 3:55PM	Small Group Presentations, Discussions & Plans (~10 min/group)
3:55PM - 4:30PM	Questions, Discussion & Wrap up (Ian Foster)

For those who can stay beyond 4:30, informal demonstrations can be given in the CHiMaD HQ

Groups; Members; Readings; Question(s); Presentations

Presentations by each group: 10-minute presentation to be given by one member of each group (other than a workshop co-organizers). Template slides will be available on the workshop laptop provided to each group.

Group 1) Materials research & design
Group Members: B. Blaiszek (U of Chicago); C. Campbell (NIST); V. Cespi (Penn St U); P. Collins (Iowa St U); D. Belsito Cote; B. Gulsoy (Northwestern U); D. Hess (NSF); T. Mayeshiba (U of WI); K. Munch (NREL); L. Rathbun (Cornell U); J. Skone (U of Chicago)
Reading: Xiong, Wei, and Gregory B. Olson. "Integrated computational materials design for high-performance alloys." MRS Bulletin 40.12 (2015): 1035-1044. http://dx.doi.org/10.1557/mrs.2015.273
Question: What data and tools are needed for materials research and design?
Presentation: Describe in as much detail as possible one concrete, actionable, low-barrier activity your group would propose to address needed data &/or tools for materials design.

Group 2) Tools & services "Necessary for the completion of work...Allows access and manipulation... Is intended to be easily usable." [A]
Group Members: A. Agrawal (Northwestern U); N. Ferrier (Argonne NL); M. Giovani (U of Chicago); V. Hegde (Northwestern U); W. Joost (DOE); K. McHenry (NCSA); C. Toher (Duke U); J. Warren (NIST); H. Wu (U of WI); M. Zentner (Purdue U)
Reading: Curtarolo, Stefano, et al. "AFLOWLIB. ORG: A distributed materials properties repository from high-throughput ab initio calculations." Computational Materials Science 58 (2012): 227-235.
Available at http://dx.doi.org/10.1016/j.commatsci.2012.02.002
AND Jain, Anubhav, et al. "Commentary: The Materials Project: A materials genome approach to accelerating materials innovation." Apl Materials 1.1 (2013): 011002.
DOI: http://dx.doi.org/10.1063/1.4812323
Questions: What challenges/barriers do materials tools and services face in working with 1) the materials research community; 2) industry 3) other materials tools and services
Presentation: Describe in as much detail as possible one concrete, actionable, low-barrier activity your group would propose to address support of materials tools and services working with 1) the materials research community; 2) industry 3) other materials tools and services

Group 3) Infrastructure "Underlying foundation or basic framework" Data Infrastructure "a digital infrastructure promoting data sharing and consumption" [B]
Group Members: J. Allison (U of MI); I.Foster (U of Chicago); S. Jones (NSF); G. Klimick (Purdue U); T. Mayeshiba (U of WI); W. Mullins (ONR); X. Sun (PNNL); Z. Trautt (NIST); D. Trinkle (UI-UC); R. White (NREL); S. Youssef (NIST)
Reading: Blaiszek, B et al. " The Materials Data Facility: Data Services to Advance Materials Science Research." The Journal of The Minerals, Metals & Materials Society (TMS) under review (attached)[C]

[A] "Tool." "Services." Merriam-Webster.com. Merriam-Webster, n.d. Web. 18 Apr. 2016.
[B] "Data Infrastructure." Merriam-Webster.com. Merriam-Webster, n.d. Web. 18 Apr. 2016.
[C] Sections may change, as well as misspellings may be discovered and fixed before final acceptance.

AND Klimeck, Gerhard, et al. "nanohub. org: Advancing education and research in nanotechnology." Computing in Science & Engineering 10.5 (2008): 17-23. DOI http://dx.doi.org/10.1109/MCSE.2008.120
AND O'Mara, J, Meredig, B and Michel, K. "The Citrination Platform: A Comprehensive Materials Data Infrastructure" The Journal of The Minerals, Metals & Materials Society (TMS) under review (sent out)
Questions: What are the primary challenges that a federated materials infrastructure would present to different platforms and diverse stakeholders?
Presentation: Describe in as much detail as possible one concrete, actionable, low-barrier activity your group would propose to move toward a federated materials infrastructure.

Group 4) Interoperability "The ability of systems to exchange and use information from other systems."[D]
Group Members: L. Bartolo (Northwestern U); F. De Carlo (Argonne NL); O. Heinonen (Argonne NL); M. Jacobsen (AFRL); S. Konstanty (UI-UC); K. Munch (NREL); R. Plante (NIST); B. Puchala (U of MI); C. Ward (AFRL); L. Ward (Northwestern U); Q. Yan (LBNL)
Reading: Wilkinson, Mark D., et al. "The FAIR Guiding Principles for scientific data management and stewardship." Scientific data 3 (2016). DOI: http://dx.doi.org/10.1038/sdata.2016.18
Questions: What are key challenges do interoperability and reusability of data present to materials researchers as well as service providers?
Presentation: Describe in as much detail as possible one concrete, actionable, low-barrier activity your group would propose to improve interoperability and reusability of materials data.

[D] Institute of Electrical and Electronics Engineers, IEEE Standard Computer Dictionary: A Compilation of IEEE Standard Computer Glossaries, New York, NY: 1990. "Interoperabilty"

Workshop Observers(*) & Participants:

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