2015 Model Challenge Workshop
June 20/21, 2015 @
MIT Biology Building (#68) Room 121

Workshop Overview

The EMDataBank (www.emdatabank.org) is a research consortium among the leaders in RCSB, PDBe and NCMI under the support of NIGMS to establish a robust infrastructure and standard to archive cryoEM maps and models. One of the major goals is to work with the 3DEM community to establish data-validation methods that can be used in the process of structure determination, define key indicators of a well-determined structure that should accompany every 3DEM structure deposition, and implement appropriate validation procedures into a validation pipeline. Activities have thus far included hosting the EM Validation Task Force (EM VTF), which led to publication of initial recommendations to guide development of 3DEM validation criteria (Henderson et al 2012), and the CryoEM Modeling Challenge (Ludtke et al 2012).

EMDataBank, in collaboration with members of the community, are organizing an assessment of current approaches to interpretation of cryoEM maps with atomic models, to be held in 2015 to critically evaluate the map interpretation, model fitting, model refinement, and validation methods that are now coming into use. This cryoEM model validation challenge, along with a parallel map validation challenge, will be hosted at challenges.emdatabank.org.

In order to develop the structure for the model validation challenge, we have organized this weekend workshop focused on interpretation, refinement and validation of high resolution (3-5Å) 3DEM maps, and formulation of the 2015 model validation challenge, including selection of target maps (those maps currently under consideration are listed in this spreadsheet). We invite you to join in these activities and hope that you will be able to participate, provide valuable feedback and take part in discussions.

The meeting will be held at MIT (Biology Building) in Cambridge, MA, and will take place on June 20/21. We expect to start the meeting at about 1 pm on June 20 and finish about noon on June 21. We will have a workshop dinner on June 20th, and lunch will be provided on the 21st.

Agenda

Saturday June 20: Session I (13:00-18:30)

Introduction: Wah Chiu and Paul Adams	13:00	13:30
Practical experiences with high resolution cryoEM of membrane proteins : Sjors Scheres (via teleconference)	13:30	14:00
GTPase activation mechanism in ribosome translocation studied by cryo-EM : Joachim Frank	14:00	14:30
Practical experiences with large asymmetric complexes/flexible fitting: Klaus Schulten	14:30	15:00
Practical experiences: Cory Hryc	15:00	15:30
Break	15:30	16:00
Ab initio model building and refinement: Frank Dimaio	16:00	16:30
Model optimization: Paul Adams	16:30	17:00
Model validation: Jamie Fraser	17:00	17:30
Discussion	17:30	18:15
About EMDataBank/Charge for Session II: Cathy Lawson	18:15	18:30

Modeller Questions:
- How did you prepare your map for model building? (B-factors, segmentation, define molecular boundaries)
- How did you build your initial model? (de novo, homolog)
- How did you optimize your model? (refinement procedures)
- Did you check the complete biological assembly for clashes/model integrity?
- How did you validate your model (how do you know it is correct)?

Modelling Software Developer Questions:
- What kind of input is needed? (whole map, segmented map)
- Describe the algorithm in lay language
- How long does it take to run the method?
- What is the output of the modeling/optimization?
- What is the protocol for validation?
- Examples of application.

Saturday June 20: Workshop Dinner

Legal Seafoods Kendall Square 5 Cambridge Center	19:00	22:00

Sunday June 21: Session II (8:30-12:00)

Challenge Aims Discussion		
Aim 1: What should the scope of the challenge be?	8:30	9:15
Aim 2: Define map data sets: candidate maps for challenge	9:15	10:00
Aim 3: What should the evaluation criteria be?	10:00	10:45
Aim 4: Challenge logistics	10:45	11:30
Wrap up + Lunch (Sandwiches provided)	11:30	noon

Meeting Registration

http://ncmi.bcm.edu/ncmi/events/workshops/workshops_144/workshop_home_html

Accommodations

The meeting hotel is the Residence Inn Boston Cambridge. (Rutgers Room Block # M-3HHONB2"). The hotel address is 120 Broadway, Six Cambridge Center, Cambridge, MA 02142. Phone # is +1-617-349-0700.Check-in is at 4 pm and check-out is at noon. Parking is available for a fee. The contact phone number for the hotel is 1-800-331-3131 or +1 617 349 0700. We will pay for two nights of your stay (one representative per laboratory, June 19-21).
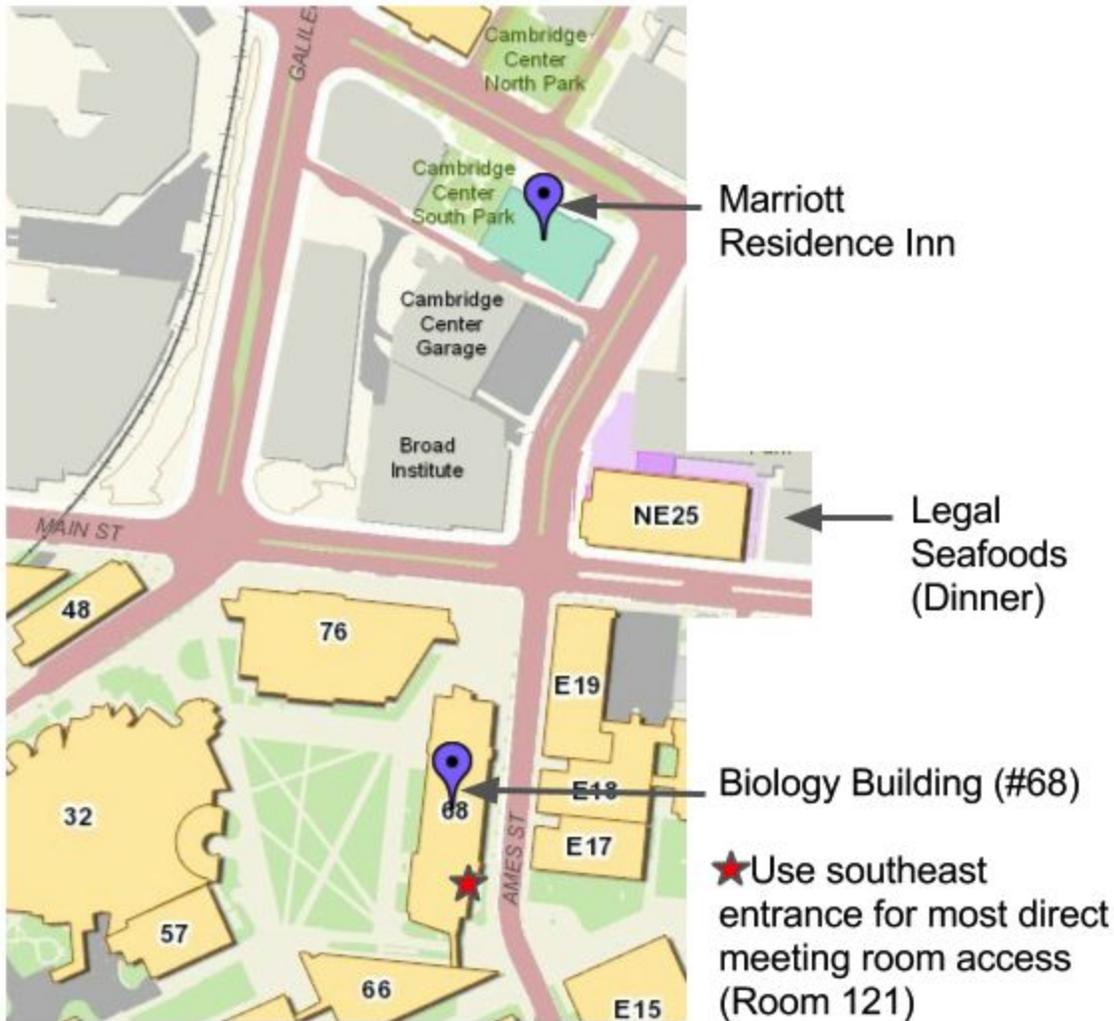
Getting to the Residence Inn from the Airport

Estimated taxi fare is $35, and estimated subway fare is $3. The hotel is a short walk (0.2 miles) from the Red Line MIT/Kendall Square subway stop. From the airport (BOS) take the Silver line to South Station (20 min), and then transfer to the Red Line to MIT/Kendall Square (10 min).

Workshop Meeting Site and Logistics

The meeting site is a short walking distance from the Hotel. The meeting will be held in the MIT Biology Building (#68), 31 Ames Street, conference room 121.

Building Access: The building will be locked over the weekend but we will have several key-cards. Call Wah or Cathy's cell (see next page) if you need access.

Computer: Choose "MIT" (free, no registration) or "MIT Guest" (free, with registration) for wireless access. more info at this link. Multiple outlet strips will be available to plug in your laptop. A projector will be available at the meeting for presentations.

Speakers please remember to bring any special adaptors required for your laptop.

Attendee Email Addresses / Contact Info
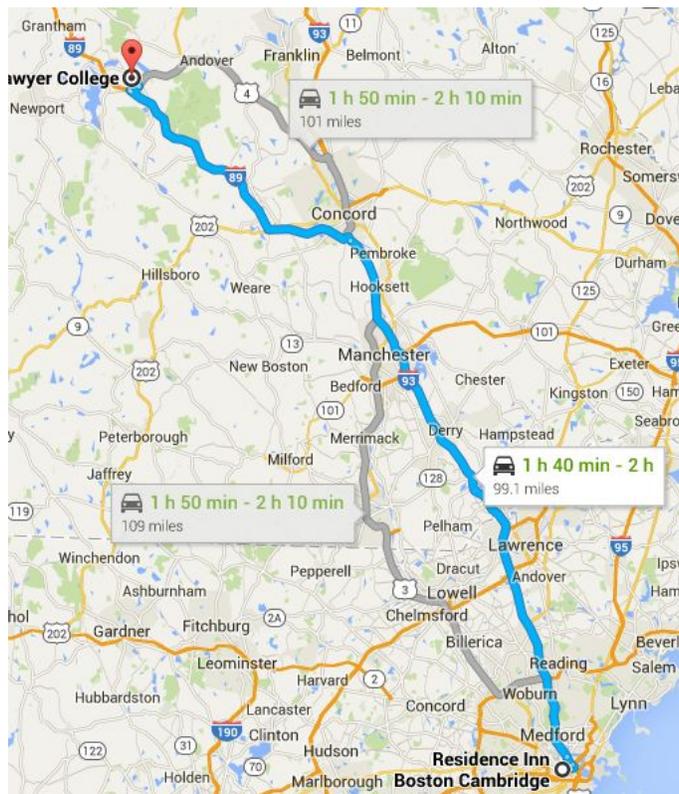
Cathy cell: 732 277 0034
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Registration website
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MIT local contact
Cindy Woolley <cwoolley@mit.edu>

as of June 10: 22 on-site meeting attendees

Post Meeting Transportation to 3DEM GRC

For those of going to the 2015 3DEM GRC at Colby-Sawyer College on Sunday.

Check-in at the GRC is 2-6 pm.

The GRC bus departs @ noon, 2 pm, and 4 pm on Sunday from the Embassy Suites Boston at Logan Airport. (bus reservations can be made/changed from the GRC registration email receipt).

people who are driving:
Cathy, Joachim, Paul

people who need rides:
Ardan, Frank DiMaio