The 2017 Whole-Cell Modeling Summer School

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Abstract
Whole-cell models that predict phenotype from genotype are needed to advance biology, bioengineering, and medicine. Achieving whole-cell models will require extensive collaboration among modelers, experimentalists, mathematicians, computer scientists, and software engineers. In September 2017, we organized the second Whole-Cell Modeling Summer School to continue to build a whole-cell community by training new researchers. The school created new whole-cell training materials; trained 18 students, postdoctoral scholars, and faculty; and generated ideas about how to better teach whole-cell modeling. To build a whole-cell modeling community, we plan to continue to organize schools, continue to improve these schools based on the lessons that we learned this year, and initiate an annual workshop and/or online seminar series to facilitate sustained discussion about whole-cell modeling.

Introduction

Whole-cell (WC) models that predict phenotype from genotype are needed to advance biology, bioengineering, and medicine [1–3]. Despite recent progress, significant work remains to build WC models [4–7]. Achieving WC models will require extensive collaboration among modelers, experimentalists, mathematicians, computer scientists, and software engineers.

To begin to organize an interdisciplinary WC community, we and others have begun to organize annual WC modeling summer schools [8] and workshops [9] to train researchers in WC modeling. In September 2017, we organized the second school [10]. 28 scientists from ten countries participated in the school.

Here, we summarize the school, the lessons we learned from the school about how to teach WC modeling and build a WC community, and describe our plans to continue to build a WC community.

School content and logistics

Organizers and coordinators

The school was organized by Jonathan Karr from the Icahn School of Medicine at Mount Sinai and Maria Lluch-Senar and Luis Serrano from the Center for Genomic Regulation (CRG). The lectures and tutorials were presented by Jonathan Karr, Saahith Pochiraju, Yosef Roth, and Balázs Szigeti from Sinai and Verónica Llorens-Ríco, Maria Lluch-Senar, Samuel Miravet-Verde, Marie Trussart, and Marc Weber from the CRG. The school was coordinated by Damjana Kastelic, Gabriel Gonzalez Cano, Anna Sole Amat, and Ruben Ventura from the CRG.

Funding

The school was supported by EraSynBio, the Horizon 2010 Programme of the EU, the Ministry of Economy and Competitiveness of Spain, and the National Science Foundation of the USA.

Date and location
We held the school September 4-7 in a classroom at the CRG in Barcelona, Spain. The CRG was an excellent venue due to their experienced course staff, modern facilities, easy accessibility and desirable location for traveling participants, and proximity to affordable accommodations.

We arranged the classroom into rows of desks. Unfortunately, we found that this layout limits interaction among the participants and instructors. Going forward, we plan to arrange the classroom into clusters of desks to facilitate more interaction among the participants and instructors.

Advertising
We advertised the school through several online conference calendars, scientific communities, social media websites, and our personal networks (Table S1).

Participant selection
31 graduate students, postdoctoral fellows, staff, and faculty applied to the school. We invited 23 of these scientists to participate in the school based on their CVs and descriptions of their background and interest in participating in the school. We chose participants by reviewing the applications, ranking the applicants, giving preference to women and underrepresented minorities, and balancing the geographic distribution of the invitees. We believe that we received fewer applicants than previous WC schools because we held the school immediately after many scientists take vacation in August. However, the applicants were far more qualified than those for our previous schools.

Participants
18 scientists accepted our invitations. The participants were from nine countries and included nine graduate students, eight postdoctoral scholars, and one faculty and five women and 13 men.

Registration fee and travel scholarships
The registration fee was €400. On a competitive basis, we awarded travel scholarships totaling $5,000 to five non-European participants to help them travel to the school.

Schedule
The four-day school consisted of two motivational lectures, ten tutorials on the fundamentals of WC modeling, four group discussions about the future of WC modeling, and two networking activities (Table S2). Going forward, we plan to schedule more time for WC schools to provide participants more time to work on hands-on exercises and participate in group discussions.

Lectures
The goal of the lectures was to introduce WC modeling and inspire the participants to engage in WC modeling. The first lecture introduced the methods used in WC modeling and the latest WC models. The second lecture introduced the data types and data sources used in WC modeling.

Tutorials
The tutorials taught the fundamental concepts of WC modeling including aggregating and organizing data for modeling; building large models by merging smaller models; rule-based formats for describing cell models; the fundamental simulation algorithm algorithms used in cell modeling; emerging algorithms for co-simulating composite models; selecting, testing, verifying, and validating models; and Python programming. Each tutorial was three hours and consisted of a brief lecture, one or more hands-on exercises, and brief group discussions about how the participants completed the exercises. Going forward, to facilitate more interaction among the participants and instructors, we plan to allocate more time for the tutorials, arrange the participants into small groups, and assign one instructor to work with each group throughout the school.

Group discussions
During the first two discussions, we facilitated dialogues about scientific, engineering, and medical problems that WC models could help address. The third discussion focused on how to build a WC community. For this discussion, we divided the participants into breakout groups, gave each group a whiteboard, asked each group to brainstorm how to build a WC community, and then asked the groups to share their ideas. In the fourth discussion, we asked the participants how to improve the school. Going forward, we plan to allocate more time for group discussions and begin each discussion with breakout groups.

Networking activities
We organized two social activities to encourage the participants to network with each other and the instructors. At the beginning of the school, we organized an icebreaker activity. At the end of the first day of the school, we organized a cooking party at a local teaching kitchen.

Accommodations
The participants stayed at several nearby hotels and vacation rentals. Going forward, to facilitate more interaction among the participants, we plan to arrange accommodations at a single venue.

Website
We created a website to distribute the materials for the school [10]. This included the schedule, slides, coding exercises, suggested reading list, and participant list.

Computers
To enable the participants to focus on the intellectual content of the tutorials, we provided the participants laptops with all of the software needed for the tutorials.

School evaluation
We solicited feedback from the participants in two ways. First, as described above, at the end of the school, we organized a discussion about how to improve the school. Second, we invited the participants to complete a web-based survey about the school. Below, we summarize the participants' feedback and describe our plans for future WC school which incorporate this feedback.

School outcomes
The school produced two major outcomes. First, the school produced additional WC training materials. To make these materials accessible to researchers who could not attend the school, we are reformatting these materials into a website [11]. Second, the school expanded the WC community by training 18 graduate students, postdoctoral scholars, and faculty.

Participant feedback
Below are the average ratings (on a 1.0 to 5.0 scale, with 5.0 indicating "excellent") reported by the participants on several aspects of the school:

- Overall satisfaction: 4.4
- Content: 4.6
- Tutorials: 4.3
- Instructor expertise: 4.8
- Instructor communication skills: 4.6
- Format: 4.6
- Venue: 4.7
- Organization: 4.7
- Would you recommend the school?: 4.6

In addition, the participants we summarize the feedback that we received on the school.

- Several participants suggested increasing the length of the school to provide more time for each tutorial and discussion.
- The participants had conflicting feedback on the balance of conceptual and practical tutorials. Some participants suggested focusing on conceptual tutorials and others suggested focusing on concrete coding exercises.
- Several participants gave several suggestions for focusing the school on more advanced concepts. Some participants suggested increasing the prerequisite knowledge required to participate in the school. Other participants suggested providing participants with materials to read, lectures to watch, and/or exercises to complete before the school. Yet other participants suggested creating separate tracks within the school for experienced modelers, novice modelers, and experimentalists.

Plans for future WC community building activities

Based on this feedback and our own observations, we plan to make several improvements to our efforts to build a WC community.

- **Increase the length of the school.** We plan to increase the length of the school to allow more time for tutorials and discussions. This will provide participants more time to assimilate concepts, work through exercises, and ask questions. This will also allow us to incorporate breakout groups into each group discussion.
- **Organize the participants into tutorial groups.** To help the participants learn from each other and the instructors, we plan to divide the participants into small groups, provide each group a cluster of desks, and assign one instructor to work with each group. We plan to try to balance the groups so they have similar amounts of experience.
- **Host the meeting at a more inclusive venue.** We plan to hold future schools at more inclusive venues that could also facilitate interaction over breakfast and dinner.
- **Apply for additional funding.** We plan to apply for additional funding from EMBO [12] to increase the length of the school, decrease the registration fee, and support more scholarships.
- **Organize workshops and online seminars to support sustained discussion about WC modeling.** To help more experienced researchers engage in WC modeling and to help researchers continuously engage in WC modeling, we plan to organize an annual WC workshop and organize an online WC seminar. We plan to hold the annual workshops immediately after the annual schools.

Conclusion

We organized the 2017 Whole-Cell Modeling Summer School to continue to build a WC community. The school created new WC training materials, trained 18 young scientists in WC modeling, and gathered valuable feedback about how to better teach WC modeling. To continue to build a WC community, we plan to continue to organize WC schools, continue to develop an online WC primer, and initiate an annual WC workshop and/or online seminar series.

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