Evaluation Report

Investigative Workshop: Optimal Control and Optimization for Individual-based and Agent-based Models

December 1-3, 2009

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Optimal Control and Optimization for Individual-based and Agent-based Models Workshop Evaluation Executive Summary

Brief Synopsis of Event

This report is an evaluation of a NIMBioS Investigative Workshop entitled "Optimal Control and Optimization for Individual-based and Agent-based Models," which took place at NIMBioS December 1-3, 2009. NIMBioS Investigative Workshops are relatively large (30-40 participants), focus on a broader topic or a set of related topics than Working Groups, attempt to summarize/synthesize the state of the art and identify future directions, and have the potential of leading to one or more future Working Groups. Participants may include post-docs and graduate students with less experience in the particular topic than those participating in Working Groups.

The Optimal Control and Optimization for Individual-based and Agent-based Models Workshop comprised 45 participants, including co-organizers Filippo Castiglione (Institute for Computing Applications, Rome); Volker Grimm (UFZ Center for Environmental Research, Leipzig); Reinhard Laubenbacher (Virginia Bioinformatics Institute); and Suzanne Lenhart (University of Tennessee, Knoxville).

The focus of the Workshop was to bring together researchers working in agent-based models and optimal control/optimization to consider the possible development of control theoretic approaches for agent-based models. Alternative formulations of the approximation models and optimal control/optimization methods appropriate for each formulation were also discussed.

Evaluation Design

An electronic survey aligned to the following evaluation questions was designed by the NIMBioS Evaluation Coordinator with input from the NIMBioS Director and Deputy Director:

1. Were participants satisfied with the Workshop overall?
2. Did the meeting meet participant expectations?
3. Do participants feel the Workshop made adequate progress toward its stated goals?
4. Do participants feel they gained knowledge about the main issues related to the research problem?
5. What impact do participants feel the Workshop will have on their future research?
6. Were participants satisfied with the accommodations offered by NIMBioS?
7. What changes in accommodations, group format, and/or content would participants like to see at future similar meetings?

The final instrument was hosted online via the University of Tennessee's online survey host mrInterview. Links to the survey were sent to 40 Workshop participants on December 7, 2009 (the four Workshop co-organizers and NIMBioS director Lou Gross were not included in the evaluation). Reminder emails were

sent to non-responding participants on December 12 and 17, 2009. By December 24, 35 participants had given their feedback, for a response rate of 88%.

An electronic demographic survey aligned to the reporting requirements of the National Science Foundation was designed by the NIMBioS Evaluation Coordinator with input from the NIMBioS Director. The final instrument was hosted online via the University of Tennessee's online survey host mrInterview. Links to the survey were sent to the 39 conference participants who had not previously attended a NIMBioS event on November 19, 2009. Reminder emails were sent to non-responding participants on November 17 and 24, 2009. By December 1, 39 participants had filled out the survey for a response rate of 100%. Demographic questions regarding gender, race, and ethnicity, and disability status were optional (disability status is not reported in this evaluation report). All demographic information is confidential, and results are reported only in the aggregate. When feasible, the evaluator filled in missing demographic data from other sources (e.g. address, institution, field of study). The evaluator did not assume race, ethnicity, or disability status for any participant who did not report this information.

Highlights of Results

- Overall satisfaction with the Workshop was high among respondents, the majority of whom indicated they either agreed or strongly agreed that the Workshop was productive (91%) and met their expectations (94%).

- Almost all respondents thought the presentations were useful (95%), and that the presenters were very knowledgeable about their presentation topics (97%), while fewer felt the group discussions were useful (78%).

- Ninety-seven percent of respondents either agreed or strongly agreed that they would recommend participating in NIMBioS Workshops to their colleagues.

- Overall, respondents reported being satisfied with the travel, housing, and other amenities provided by NIMBioS.

- Respondents reported relatively high gains in knowledge about the Workshop's topic. Respondents reported gaining the greatest understanding about ways in which agent-based models (ABMs) could be used in research, followed by understanding of the advantages and disadvantages of using agent-based models for understanding biological phenomena.

- Ninety-four percent of respondents said they felt that participating in the Workshop helped them gain insight about using control-theoretic approaches for ABMs that could be applied to studying interventions.

- All respondents felt the Workshop format was effective for achieving it goals. The majority of respondents felt the most useful aspect of the Workshop was the ability network with a diverse group of researchers.

- Sixty percent of respondents said they felt that the exchange of ideas that took place during the Workshop would definitely influence their future research, while 37% said it possibly would have influence.

- Thirty-one percent of respondents said that they developed plans for collaborative research with other Workshop participants, while 63% said the potential for collaboration was present.

Conclusions and Recommendations

Overall, the Workshop was successful in making progress toward its goals. Survey respondents were satisfied with the meeting, indicating that it was a productive experience that met their expectations. Respondents were also satisfied with the travel, housing, and other amenities offered by NIMBioS.

Respondents reported relatively high levels of learning about optimal control and optimization approaches for individual and agent-based models (ABMs). Respondents reported gaining the greatest understanding about ways in which ABMs could be used in research, followed by understanding of the advantages and disadvantages of using ABMs for understanding biological phenomena.

All respondents felt the Workshop format was effective for achieving it goals. The majority of respondents felt the most useful aspect of the Workshop was the ability network with a diverse group of researchers. Other respondents said the actual material presented during the Workshop was its most useful aspect, while some felt the break-out group discussions were very useful.

The majority respondents indicated they planned to take the knowledge they gained during the Workshop and apply it to their own research. Eleven respondents reported they had developed solid plans for collaborative research with other Workshop participants, while 22 indicated they saw potential for collaboration in the future.

Several suggestions for future Workshops were made by participants, including ideas for improving the Workshop format and miscellaneous suggestions about content. Suggestions regarding Workshop format included having more time for breakout discussion groups, and having more structure when breakout groups are organized. Another common suggestion from respondents was to have more preparatory information before the Workshop, including access to presentation materials, online discussion forums, or a short course on the Workshop topics preceding the actual event. Other suggestions included adding a social event to the program, shortening the presentations for 45 minutes, and having a more formal conclusion to the Workshop.

Based on analysis of participant response data, the recommendations for future Workshops are as follows:

- Consider making more background research and reading materials available to participants before the Workshop. If feasible, consider offering a pre-Workshop webinar to Workshop participants to get everyone up to date on the latest research about the Workshop research problems.
- When possible, provide electronic copies of presentations to participants.
- Consider providing more time for breakout group discussions. Clearly define and communicate the goals of each of the breakout group discussion sessions each day.
- Before the conclusion of the Workshop, consider designating a specific time slot to synthesize the information provided, address the next steps that should be taken, and assign specific tasks to individuals or groups with tentative timelines for completion, if applicable.

Optimal Control and Optimization for Individual-based and Agent-based Models Workshop Evaluation Report

Background

Introduction

This report is an evaluation of a NIMBioS Investigative Workshop entitled "Optimal Control and Optimization for Individual-based and Agent-based Models," which took place at NIMBioS December 1-3, 2009. NIMBioS Investigative Workshops are relatively large (30-40 participants), focus on a broader topic or a set of related topics than Working Groups, attempt to summarize/synthesize the state of the art and identify future directions, and have potential for leading to one or more future Working Groups. Participants may include post-docs and graduate students with less experience in the particular topic than those participating in Working Groups.

The Optimal Control and Optimization for Individual-based and Agent-based Models Workshop comprised 45 participants, including co-organizers Filippo Castiglione (Institute for Computing Applications, Rome); Volker Grimm (UFZ Center for Environmental Research, Leipzig); Reinhard Laubenbacher (Virginia Bioinformatics Institute); Suzanne Lenhart (University of Tennessee, Knoxville). The focus of the Workshop was to bring together researchers working in agent-based models and optimal control/optimization to consider the possible development of control theoretic approaches for agent-based models. Alternative formulations of the approximation models and optimal control/optimization methods appropriate for each formulation were also discussed.

Workshop Background

Agent-based models (ABMs) are used increasingly to understand a broad range of biological phenomena, including tumor growth, the immune system, and the spread of infectious diseases across social networks. In all these cases it would be very useful to have analytic methods available to study in general how possible interventions would affect system dynamics. The advantage of agent-based models is that they integrate local relationships to capture global emergent dynamics, without needing global parameters as input. The disadvantage of this type of model is that very few mathematical analysis methods are available to produce general descriptions of model response particularly in terms of spatio-temporal patterns arising from even fairly simple ABMs. In particular, the absence of a state space description of ABMs makes it very difficult to apply available control theory methods to study effective interventions. Applications of ABMs in situations with possible interventions by human actions (e.g. vaccination and quarantine schemes) have usually been limited to scenario analyses. In this case the models are simulated numerous times to compare alternative scenarios for intervention.

One possible approach to this problem is to construct state space models that approximate the agent-based model, similar to approaches proposed for discrete event simulations. This uses system identification methods developed for the state space model framework for agent-based simulations. Control-theoretic approaches for this modeling framework have been explored in a few cases. A first

exploratory project in this direction resulted in a control method for in vitro competition of viruses. Such methods from approximate models may not work when there is spatial heterogeneity in the agent-based model. Various techniques from optimal control and discrete optimization should be considered to investigate alternative formulations of control in relation to a state-space approximation and then compared to a similar formulation applied to the ABM.

Participant Demographics

Program participants were college/university faculty (53%), graduate students (18%), business/industry (7%), government (7%), or non-profit employees (4%), and postdoctoral researchers (11%). Primary fields of study for the 45 participants included agricultural sciences/natural resources, biological/biomedical sciences, computer & information sciences, engineering, mathematics, physics, social sciences, and business (Table 1).

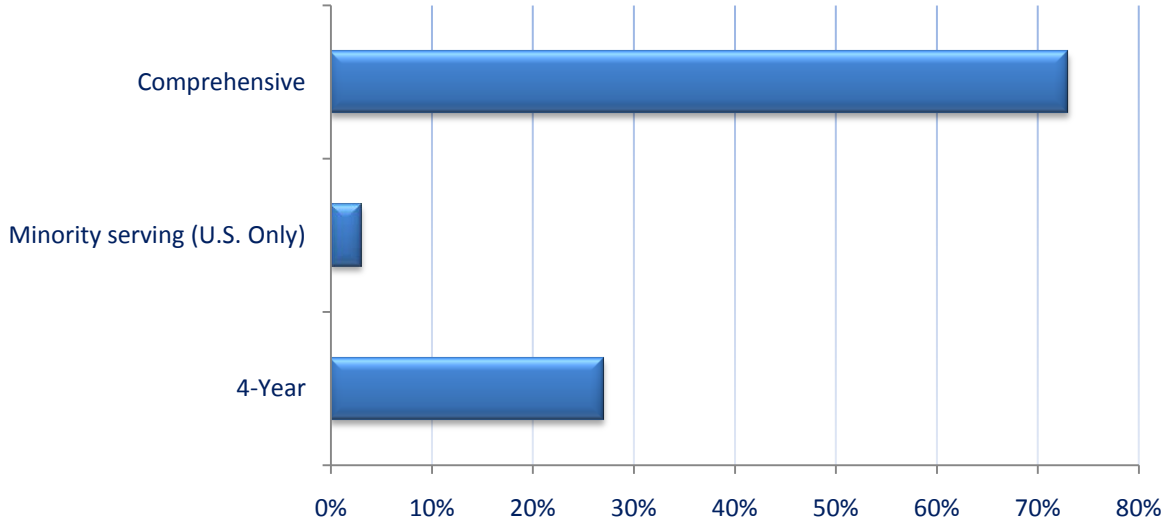
Table 1. Participant fields of study and areas of concentration

Field of Study	Concentration	# Participants
Agricultural Sciences/Natural Resources	Agricultural Economics	1
	Environmental Science	1
Biological/Biomedical Sciences	Biology/Biomedical Sciences	1
	Ecology	2
	Mathematical Biology	1
	Mathematical Ecology	1
	No Concentration given	1
Computer & Information Sciences	Computer & Information Science	3
	Computer Science	3
Engineering	Mechanical	1
	Mechanical Engineering	1
	Bioengineering & Biomedical	1

Mathematics	Algebra	1
	Applied Mathematics	7
	Math/Statistics, General	1
	Mathematical Biology	12
	Mathematical Ecology	2
	Operations Research	1
Other Professional Field	Business Management/Administrative	1
Physics	Condensed	1
Social Science	Geography	1
	Social Sciences, General	1

Participants represented 32 different institutions across 10 countries, including Canada, France, Germany, Ireland, Italy, South Korea, Nigeria, Russian Federation, United Arab Emirates, and the United States. Within the U.S., 11 different states were represented. Of the colleges/universities, most (71%) were classified as comprehensive (having undergraduate and graduate programs), while 26% were classified as 4-year institutes, and 3% as minority-serving (Figure 1).

Figure 1. Characteristics of participants' colleges/universities



The 14 females and 31 males (two of whom self-identified as being of Hispanic/Latino ethnicity) mostly self-identified racially as white (Figures 2 & 3).

Figure 2. Racial composition of program participants (n=45)

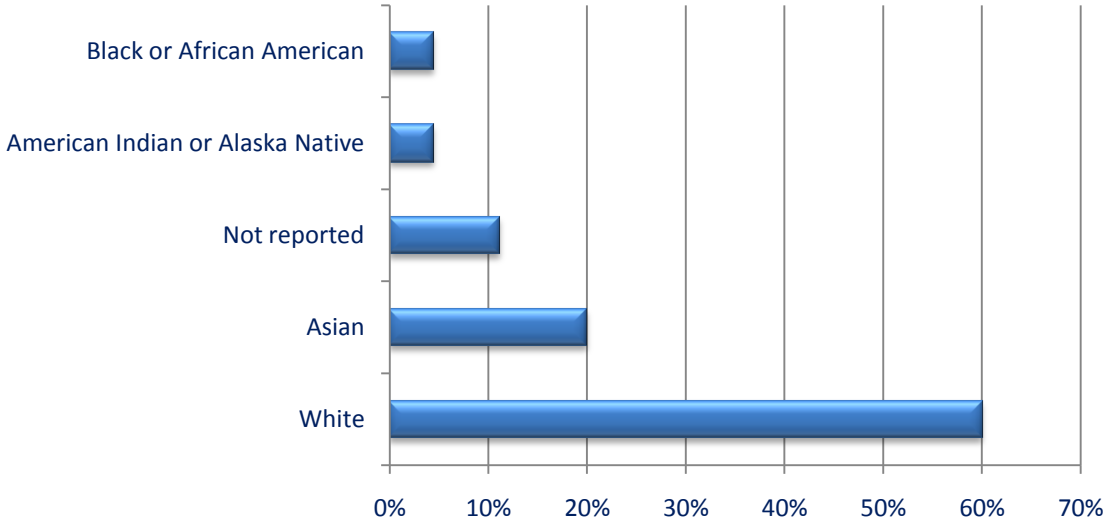
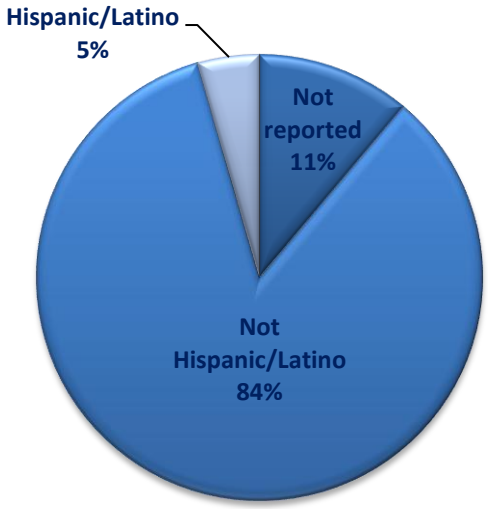


Figure 3. Ethnic composition of program participants (n=45)



Three respondents indicated their work is currently supported by a total of four National Science Foundation grants (Table 2).

Table 2. NSF grants supporting participant research

Name of grant	Institution(s) at which grant is held
Emerging Models and Technologies for Computation	Argonne National Lab, University of Pittsburgh, Yale University
Hierarchical Representation and Simulation of Modular Cellular Systems	Northwestern University at Chicago
Modeling Interaction Between Individual Behavior, Social Networks And Public Policy To Support Public Health Epidemiology	Virginia Polytechnic Institute and State University
Optimal control of Forward-Backward Stochastic Differential Equations and Related Topics	University of Central Florida

Evaluation Design

Evaluation Questions

The evaluation of the Workshop was both formative and summative in nature, in that the data collected from participants was intended to both gain feedback from participants about the quality of the current

Workshop and also to inform future meetings. The evaluation framework was guided by Kirkpatrick's Four Levels of Evaluation model for training and learning programs (Kirkpatrick, 1994[1]). The evaluation questions were developed according to level one of the model, participants' reactions, in order to gather information about how participants felt about the content and format of the Workshop, as well as the accommodations provided by NIMBioS. Several questions constituted the foundation for the evaluation:

1. Were participants satisfied with the Workshop overall?
2. Did the meeting meet participant expectations?
3. Do participants feel the Workshop made adequate progress toward its stated goals?
4. Do participants feel they gained knowledge about the main issues related to the research problem?
5. What impact do participants feel the Workshop will have on their future research?
6. Were participants satisfied with the accommodations offered by NIMBioS?
7. What changes in accommodations, group format, and/or content would participants like to see at future meetings?

Evaluation Procedures

An electronic survey aligned to the evaluation questions was designed by the NIMBioS Evaluation Coordinator with input from the NIMBioS Director and Deputy Director. The final instrument was hosted online via the University of Tennessee's online survey host mrInterview. Links to the survey were sent to 40 Workshop participants on December 7, 2009 (the four Workshop co-organizers and NIMBioS director Lou Gross were not included in the evaluation). Reminder emails were sent to non-responding participants on December 10 and 17, 2009. By December 24, 2009, 35 participants had given their feedback, for a response rate of 88%.

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[1] From Kirkpatrick, D.L. (1994). *Evaluating Training Programs: The Four Levels.* San Francisco, CA: Berrett-Koehler.

Data Analysis

Data from the electronic survey included both forced-response and supply-item questions. All data were downloaded from the online survey host into the statistical software package SPSS for analysis. Quantitative data were analyzed using SPSS, while qualitative data were analyzed in SPSS Text Analysis for Surveys. Qualitative responses were categorized by question and analyzed for trends.

Findings

Overall Satisfaction

Overall satisfaction with the Workshop was high among respondents, the majority of whom indicated they either agreed or strongly agreed that the Workshop was very productive (91%) and met their expectations (94%). Some general participant comments:

> *"Overall I thought the Workshop was excellent. The range of expertise was very impressive, but it was still possible to have useful discussions."*
>
> *"I really had a productive experience during the Optimal Control for Agent-based Models Workshop. I hope NIMBioS continues to hold intensive/focused Workshop like this one. Thank you!"*
>
> *"Overall I thought it was an excellent Workshop with a great, diverse collection of high-quality participants."*

Almost all respondents thought the presentations were useful (95%), and that the presenters were very knowledgeable about their presentation topics (97%), while fewer felt the group discussions were useful (78%). Additionally, 97% of respondents either agreed or strongly agreed that they would recommend participating in NIMBioS Workshops to their colleagues (Table 2).

Table 3. Participant satisfaction with various aspects of the Workshop

	n	Strongly agree	Agree	Neutral	Disagree	Strongly disagree
I feel the Workshop was very productive.	35	54%	37%	6%	3%	0%
The Workshop met my expectations.	34	47%	47%	6%	0%	0%
The presenters were very knowledgeable about their topics.	34	76%	21%	3%	0%	0%
The presentations were useful.	35	49%	46%	6%	0%	0%
The group discussions were useful.	35	29%	49%	23%	0%	0%
I would recommend participating in NIMBioS Workshops to my colleagues.	35	83%	14%	3%	0%	0%

Satisfaction with Accommodations

Overall, respondents reported being satisfied with the travel, housing, and other accommodations provided by NIMBioS during the Workshop. Of the 28 and 30 respondents who answered questions about their travel and housing accommodations, respectively, all indicated they were satisfied. All participants reported being satisfied with the comfort and resources of the NIMBioS facility, as well (Table 3). Some participant comments:

> *"The institute facilities are very nice."*
>
> *"Everything was great!"*

Table 4. Participant satisfaction with Workshop accommodations

Please indicate your level of satisfaction with the Workshop accommodations:	n	Very satisfied	Satisfied	Neutral	Dissatisfied	Strongly dissatisfied	Not applicable
Travel arranged by NIMBioS	35	66%	14%	0%	0%	0%	20%
Housing arranged by NIMBioS	35	80%	6%	0%	0%	0%	14%
Resources of the facility in which the Workshop took place	33	85%	15%	0%	0%	0%	0%

Workshop Content and Format

Participant Learning

Ninety-four percent of respondents said they felt that participating in the Workshop helped them gain insight about using control-theoretic approaches for ABMs that could be applied to studying interventions. One respondent's comment:

> *"This Workshop was the only way to put control-theoretic approaches for ABMs in the right direction."*

Other respondents felt the Workshop was informative about ABMs, but would have liked to have explored other issues further:

> *"I would qualify my yes answer for the following reasons. The Workshop was very helpful in framing the questions, but not as helpful in providing the answers. I learned that there may be*

certain contexts and certain problem classes for which control theoretic approaches could be useful, but it is unclear to me as to what those contexts and classes actually are at this point. This is understandable given that this Workshop is merely an introductory gathering involving a meeting of minds from many disciplines. In that regard, the Workshop was successful as it could be. However, I do have concerns as to whether there are extensible meaning connections between control theory and ABM from the standpoints of what is logical and desirable."

"It would be more useful to communicate in more detail the different ideas of control-theoretic approaches available, so we start comparing which one is more appropriate."

"It was very informative for me to find out about issues of control, and while I do think that 'optimal control' has a very limited application to ABM, I think that some of the principles of 'some control' would be useful. It is also very useful to find out what is not applicable, so that in further discussions attention can be directed at more fruitful approaches."

Respondents were also asked several questions to gauge their levels of learning about specific issues related to the Workshop's research area. Respondents reported relatively high levels of gains in all areas. The topic on which respondents reported the greatest gains in understanding was ways in which ABMs could be used in research, followed by understanding of the advantages and disadvantages of using agent-based models for understanding biological phenomena (Table 3).

Table 5. Participant learning about the Workshop's research topic

As a result of participating in this Workshop, I have a better understanding of:	n	Strongly agree	Agree	Neutral	Disagree	Strongly disagree
advantages and disadvantages of using agent-based models (ABMs) for understanding biological phenomena	35	46%	37%	17%	0%	0%
ways to develop mathematical control theory methods for ABMs	35	26%	54%	20%	0%	0%
ways in which ABMs could be used in research	35	49%	34%	17%	0%	0%

Workshop Format

All respondents felt the Workshop format was effective for achieving it goals. A majority of respondents felt the most useful aspect of the Workshop was the ability network with a diverse group of researchers:

"There were people from different backgrounds with different expertise and approaches, and each one of them has an application in mind. These applications are very valuable as they could provide guidelines and help develop useful theories for control of ABM."

"Learning about the different groups/individuals who are working on agent-based models."

"Bringing together a diverse group of researchers that approach the Workshop topic from different points of view."

Many respondents said the actual material presented during the Workshop was its most useful aspect:

"I think the discussion/presentation of how to apply optimal control theory for ABMs is most useful in my opinion."

"The opportunity to hear about a wide variety for applications of agent based models in many contexts."

"[The most useful aspect was d]eveloping a better understanding of agent-based modeling and optimal control."

Other respondents felt the break-out group discussions were the most useful aspect of the Workshop:

"…the good solid talks that provided a good common basis for discussion, as well as the discussion sessions themselves, were both really useful."

"Being able to talk to peers in a relaxed environment."

"Having a lot time for discussions, those organized into working groups as well as those during the coffee and lunch breaks (it maybe sounds funny, but having the lunches on site actually helps to approach all other participants)."

Impact on Future Research Plans

Sixty percent of respondents said they felt that the exchange of ideas that took place during the Workshop would definitely influence their future research, while 37% said it possibly would. Some participant comments:

"My interest in applying optimization methods in general to ABM was renewed and invigorated. I now see that as an important area for further research. However, within the general rubric of optimization, the specific approach of applying optimal control to ABM remains is much more narrow and its value remains to be seen in my view."

"I intend to use optimal control in an aggregated IBM. I am now more aware of the pros and cons of this approach. I am now more aware of what can go wrong and how to assess whether or not the solution is a true optimum."

"I might use optimization techniques in ABMs. Now I know that the math of control theory for ABMs is not around the corner yet and heuristics are needed instead."

"The discussions gave me insight into how I can tie Agent-Based Models into my current fields of interest. I thought that the talks were focused enough to be coherent, but diverse enough to appeal to researchers in a wide variety of fields."

"I have been working on ODE/PDE models and I am very interested in ABM models now."

In addition to new ideas for research, 31% of respondents said that they developed plans for collaborative research with other Workshop participants, while 63% said the potential for collaboration was present:

"Beyond the usual networking, I made arrangements to further discuss some of my work with another participant and also attend an upcoming Workshop."

"I have made a few research contacts that resulted in the following collaborative projects that (hopefully) will be completed in the near future: 1) initiation of a small working group focused on using control theory for tumor-immune interactions; 2) initiation of a small working group focused on review paper on IMBs in medical problems; 3) joining a local researcher in organizing future Workshops on cancer modeling."

"We (at Virginia Tech) are planning to start a working group using the Discrete Event Systems approach."

"I exchanged contact information with a few like-minded individuals, and we have communicated since the conference about potential collaboration. The conference definitely opened avenues I would not have otherwise found."

"[I] Strengthened ties to existing relationships with some of the participants, and also raised the possibility of specific projects with a few other participants."

Suggestions for Future Workshops

Respondents were asked several questions soliciting suggestions for future Workshops. Two themes emerged from analysis of participant data: suggestions about content and suggestions about format. Suggestions for content were miscellaneous in that no two respondents made the same suggestion. For instance, one participant would have liked the scope of the material to be broader; while another felt it should have been more narrowly focused:

"I think that the scope was really broad and I think having a sample problem and everything moving around that would have helped scope a bit."

"I would have not had such a narrow topic for the Workshop. Rather the topic would have been broader, such as optimization (in general, and by whatever means, analytical or computational). Also, I also would have made sure to identify a good set of problems in biology that were good

candidates for applying control theoretic techniques to ABM. As it were, I do not recall seeing a single example of a problem in which control theoretic approaches would be beneficial to ABM."

Another respondent would have liked to have seen more presentations that integrated mathematics and biology:

"I think the Workshop should have more presentations between mathematical methods (optimal control theory) and interesting biological problems. ABMs that are not related to any interesting biological issues might be avoided if possible."

Suggestions regarding Workshop format included having more time for breakout discussion groups, and having more structure when breakout groups are organized:

"…Organize breakout group sessions in more detail beforehand, and be less 'democratic'."

"More constructive discussion sessions. The discussion sections needed topics that were more focused and moderators who were prepared to facilitate the discussions."

"I would like to have had a bit more structure in the discussion groups."

"I would have liked more time for just discussion…"

Another suggestion from respondents was to have more preparatory information before the Workshop, including access to presentation materials, online discussion forums, or a short course on the Workshop topics:

"It would be nice to have a short course about the topics involved in the Workshop before the main Workshop takes place. I am very familiar with OPT but not with the ABM. It would have been so helpful if I had learned about ABM."

"It would help to have earlier access to Workshop preparatory material and documentation so that we know more about the presenters, participants and specific goals of the Workshop."

"I know that all the participants are very busy, but it would have been nice to have some kind more coordinated discussion/background on the Wiggio. I did read the papers that were posted, but it would have been nice to have a bit more structure of what to expect."

Additionally, one presenter indicated he/she would have liked to have seen more guidance from organizers regarding presentation topics:

"I think it would have been helpful for the Workshop organizers to provide guidance on and even coordinate the topics of the Workshop presenters. There was a general uncertainty among many of the speakers about what they should talk about even after they arrived at the Workshop and what the goals of the Workshop actually were. More advanced communication of this on the part of the Workshop organizers would be very helpful. Essentially speakers just talked about

what they were able to talk about that seemed like it might be applicable. No one actually presented work involving optimal control as applied to agent-based modeling."

A final suggestion from respondents was to have a more clearly defined conclusion to the Workshop:

"Have the organizers summarize the Workshop at the end."

"I would also outline more definitive conclusions at the end of the Workshop."

Other suggestions included adding a social event to the program and shortening the presentations for 45 minutes.

Conclusions and Recommendations

Overall, the Workshop was successful in making progress toward its goals. Survey respondents were satisfied with the meeting, indicating that it was a productive experience that met their expectations. Respondents were also satisfied with the travel, housing, and other amenities offered by NIMBioS.

Respondents reported relatively high levels of learning about optimal control and optimization approaches for individual and agent-based models (ABMs). Respondents reported gaining the greatest understanding about ways in which ABMs could be used in research, followed by understanding of the advantages and disadvantages of using ABMs for understanding biological phenomena.

All respondents felt the Workshop format was effective for achieving it goals. The majority of respondents felt the most useful aspect of the Workshop was the ability network with a diverse group of researchers. Other respondents said the actual material presented during the Workshop was its most useful aspect, while some felt the break-out group discussions were very useful.

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Several suggestions for future Workshops were made by participants, including ideas for improving the Workshop format and miscellaneous suggestions about content. Suggestions regarding Workshop format included having more time for breakout discussion groups, and having more structure when breakout groups are organized. Another common suggestion from respondents was to have more preparatory information before the Workshop, including access to presentation materials, online discussion forums, or a short course on the Workshop topics preceding the actual event. Other suggestions included adding a social event to the program, shortening the presentations for 45 minutes, and having a more formal conclusion to the Workshop.

Based on analysis of participant response data, the recommendations for future Workshops are as follows:

- Consider making more background research and reading materials available to participants before the Workshop. If feasible, consider offering a pre-Workshop webinar to Workshop participants to get everyone up to date on the latest research about the Workshop research problems.
- When possible, provide electronic copies of presentations to participants.
- Consider providing more time for breakout group discussions. Clearly define and communicate the goals of each of the breakout group discussion sessions each day.
- Before the conclusion of the Workshop, consider designating a specific time slot to synthesize the information provided, address the next steps that should be taken, and assign specific tasks to individuals or groups with tentative timelines for completion, if applicable.

Appendix A: List of Participants

Last name	First name	Institution
Agusto	Folashade	NIMBioS
An	Gary	Northwestern University
Bewick	Sharon	NIMBioS
Bhattacharya	Sudin	The Hamner Institute for Health Sciences
*Castiglione	Filippo	Consiglio Nazionale delle Ricerche
Eubank	Stephen	Virginia Polytechnic Institute and State University
Fenichel	Eli	Arizona State University
Fitzpatrick	Ben	Loyola Marymount University
Ge	Weihao	University of Tennessee Knoxville
Gillette	Shana	Colorado State University
*Grimm	Volker	Helmholtz Center for Environmental Research-UFZ
Gross	Louis	NIMBioS
Hinkelmann	Franziska	Virginia Polytechnic Institute and State University
Hughes	Joe	University of Tennessee Knoxville
Hyder	Ayaz	McGill University
Jarrah	Abdul	American University of Sharjah
Joo	Jaewook	University of Tennessee Knoxville
Kwon	Hee-Dae	Inha University
*Laubenbacher	Reinhard	Virginia Polytechnic Institute and State University
Leander	Rachel	University of Tennessee Knoxville
Lee	Dongjun	University of Tennessee Knoxville

Last name	First name	Institution
Lee	Jeehyun	Yonsei University
*Lenhart	Suzanne	NIMBioS
Lu	Zhao	Cornell University
Mac Namee	Brian	Dublin Institute of Technology
Macal	Charles	University of Chicago
Medina	Richard	Oak Ridge National Laboratory
Miller Neilan	Rachael	Louisiana State University Baton Rouge
Murrugarra Tomairo	David	Virginia Polytechnic Institute and State University
North	Michael	Argonne National Laboratory
Pasour	Virginia	Army Research Office
Penland	Andrew	Western Carolina University
Perminov	Valeriy	BioTeckFarm
Protopopescu	Vladimir	Oak Ridge National Laboratory
Radunskaya	Ami	Pomona College
Railsback	Steven	Lang, Railsback and Associates
Rejniak	Kasia	H. L. Moffitt Cancer Center and Research Institute
Salinas	Rene	Appalachian State University
Sethi	Suresh	University of Texas Dallas
Simoni	Diglio	RTI International
Tridane	Abdessamad	Arizona State University Polytechnic Campus
Veliz-Cuba	Alan	Virginia Polytechnic Institute and State University
Xiong	Jie	University of Tennessee Knoxville
Yong	Jiongmin	University of Central Florida

Zhao	Xiaopeng	University of Tennessee Knoxville

* Organizer of Workshop

Appendix B: Optimal Control and Optimization for Individual-based and Agent-based Models Workshop Survey

Optimal Control and Optimization for Individual-based and Agent-based Models Survey

Thank you for taking a moment to complete this survey. Your responses will be used to improve the Workshops hosted by the National Institute for Mathematical and Biological Synthesis. Information supplied on the survey will be confidential, and results will be reported only in the aggregate.

Workshop Evaluation

How did you hear about this Workshop?

Please check the appropriate box to indicate your level of agreement with the following statements about this Workshop: (Very satisfied, Satisfied, Neutral, Dissatisfied, Very dissatisfied)

I feel the Workshop was very productive.
The Workshop met my expectations.
The presenters were very knowledgeable about their topics.
The presentations were useful.
The group discussions were useful
I would recommend participating in NIMBioS Workshops to my colleagues.

Please check the appropriate box to indicate your level of agreement with the following statements. As a result of participating in this Workshop, I have a better understanding of:
(Strongly agree, Agree, Neutral, Disagree, Strongly disagree)

advantages and disadvantages of using agent-based models (ABMs) for understanding biological phenomena
ways to develop mathematical control theory methods for ABMs
ways in which ABMs could be used in research

Do you feel that participating in the Workshop helped you gain insight about using control-theoretic approaches for ABMs that could be applied to studying interventions?

Yes
No

Do you feel that the exchange of ideas that took place during the Workshop will influence your future research? Please explain:

Did you develop unanticipated plans for collaborative research with other Workshop participants? Please explain:

What do you feel was the most useful aspect of the Workshop?

What would you have changed about the Workshop?

How do you feel about the format of the Workshop?

This was a very effective format for achieving our goals
This was not a very effective format for achieving our goals ->
The Workshop format would have been more effective if:

Please indicate your level of satisfaction with the Workshop accommodations:
(Very satisfied, Satisfied, Neutral, Dissatisfied, Very dissatisfied, Not applicable)

Travel arranged by NIMBioS
Housing arranged by NIMBioS
Comfort of the facility in which the Workshop took place
Resources of the facility in which the Workshop took place
Quality of meals
Quality of drinks and snacks provided

Please indicate any changes NIMBioS can make to improve the resources and/or accommodations available to Workshop participants:

Communications Evaluation

NIMBioS is currently exploring innovative avenues for communication among its Workshop participants. Your responses to the following questions will allow us to better understand the communication needs of our scientific communities.

How satisfied were you with the opportunities provided during Workshop presentations and discussions to ask questions and/or make comments?

Very satisfied
Satisfied
Neutral
Dissatisfied
Very Dissatisfied

Please indicate any suggestions you have for facilitating communication among participants during the Workshop:

If you maintain a blog about your research and would like a link posted on the NIMBioS website, please provide the URL here, along with a brief description of the blog:

Please provide any additional comments about your overall experience with the Workshop:

Appendix C: Open-ended Survey Responses

Do you feel that participating in the Workshop helped you gain insight about using control-theoretic approaches for ABMs that could be applied to studying interventions? (n=11)

Overall I thought it was an excellent Workshop with a great, diverse collection of high-quality participants.

I really had a productive experience during the Optimal Control for Agent-based Models Workshop. I hope NIMBioS continues to hold intensive/focused Workshop like this one. Thank you!

This Workshop was the only way to put control-theoretic approaches for ABMs in the right direction.

I was completely ignorant of how such an approach might work before this Workshop.

This Workshop was very helpful for me to understand ABS.; I would like to express "my thanks" to the organizers.

I see how the two mess and do not mess now. It is clear, like always, getting the question right first is key. As opposed to trying to form a question to use a tool.

I would qualify my yes answer for the following reasons. The Workshop was very helpful in framing the questions, but not as helpful in providing the answers. I learned that there may be certain contexts and certain problem classes for which control theoretic approaches could be useful, but it is unclear to me as to what those contexts and classes actually are at this point. This is understandable given that this Workshop is merely an introductory gathering involving a meeting of minds from many disciplines. In that regard, the Workshop was successful as it could be. However, I do have concerns as to whether there are extensible meaning connections between control theory and ABM from the standpoints of what is logical and desirable.

It would be more useful to communicate in more detail the different ideas of control-theoretic approaches available, so we start comparing which one is more appropriate.

It was very informative for me to find out about issues of control, and while I do think that "optimal control" has a very limited application to ABM, I think that some of the principles of "some control" would be useful. It is also very useful to find out what is not applicable, so that in further discussions attention can be directed at more fruitful approaches.

I gained insight but not necessarily positive insight. The Workshop was focused on theoretical optimization approaches that seem quite clearly impossible to apply to ABMs (unless you simplify the ABMs to the point where they no longer serve their original purpose). On the other hand, it does appear that simpler, more approximate "optimization" methods could be applied to ABMs productively.

I was ill and therefore unable to attend the Workshop.

Do you feel that the exchange of ideas that took place during the Workshop will influence your future research? (n=15)

I am exploring these new ideas to see if I can use them.

I enjoyed being exposed to a broad array of ideas that will help me focus my research in the future.

The issue for me is not whether I will use ABMs, I have and certainly will continue to do so. Rather, this conference helped identify what means of analyzing and manipulating ABMs will be available in the future

It depends on arising new projects.

There are plans to establish several working groups that I want to participate in.

I will think more about potential uses of various kinds of control in modeling.

My interest in applying optimization methods in general to ABM was renewed and invigorated. I now see that as an important area for further research. However, within the general rubric of optimization, the specific approach of applying optimal control to ABM remains is much more narrow and its value remains to be seen in my view.

I intend to use optimal control in an aggregated IBM. I am now more aware of the pros and cons of this approach. I am now more aware of what can go wrong and how to assess whether or not the solution is a true optimum.

Better insight on areas where ABMs are used - i.e. epidemiology, organ modeling etc

I broaden my understanding on both topics: IBMs and control theory, and I will definitively pursue some (collaborative) paths to match these area in my research

I might use optimization techniques in ABMs. Now I know that the math of control theory for ABMs is not around the corner yet and heuristics are needed instead.

I have been working on ODE/PDE models and I am very interested in ABM model now.

I have to admit that this Workshop was the starting point for me discovers the realistic way to use OC in Modeling biology.

The discussions gave me insight into how I can tie Agent-Based Models into my current fields of interest. I thought that the talks were focused enough to be coherent, but diverse enough to appeal to researchers in a wide variety of fields.

Agent based models will be more ubiquitous in many applications as computing power increases, and as computing environments are developed. Optimization will be essential in answering many questions about these models (e.g. in medical applications, design questions, evolutionary modeling).

Did you develop plans for collaborative research with other Workshop participants? (n=17)

Beyond the usual networking, I made arrangements to further discuss some of my work with another participant and also attend an upcoming Workshop.

I plan to apply control strategies discussed during the Workshop to my model. After I check the feasibility, I would like to collaborate with proper person/group.

I have made a few research contacts that resulted in the following collaborative projects that (hopefully) will be completed in the near future: 1) initiation of a small working group focused on using control

theory for tumor-immune interactions; 2) initiation of a small working group focused on review paper on IMBs in medical problems; 3) joining a local researcher in organizing future Workshops on cancer modeling

We (at Virginia Tech) are planning to start a working group using the Discrete Event Systems approach.

I plan to participate in 2 of the working groups

1) Planning a working group focused on computational support for very large scale ABMs, 2) Planning a Workshop on multiscale ABMs focused on malaria

Three collaborative research are on the way... thank You NIMBioS.

Yes there is a working group that has been proposed on large-scale ABM applications to epidemic modeling.

(a) I am already too busy! (b) Potential collaboration between optimal control mathematicians and agent-based modelers seems too hypothetical for the work I do.

Not on control theory.

The group was very diverse - there perhaps wasn't quite enough time for prolonged interactions

There are a lot to be done in the area and I am interested in exploring the possible collaborations with other participants.

I exchanged contact information with a few like-minded individuals, and we have communicated since the conference about potential collaboration. The conference definitely opened avenues I would not have otherwise found.

A possibility of such collaboration has been discussed during the Workshop. Now we (both sides) are waiting for our administrators' approval. My possible collaborative research with NIMBioS has been discussed as well.

There are two groups that might take form in the close future each tackling a different problem (one related to this Workshop content, the other not)

I developed ideas for collaborations on journal articles and grant-funded projects.

Strengthened ties to existing relationships with some of the participants, and also raised the possibility of specific projects with a few other participants.

What do you think was the *most* useful aspect of the Workshop? (n=27)

hard to say - the good solid talks that provided a good common basis for discussion, as well as the discussion sessions themselves, were both really useful

Being able to talk to peers in a relaxed environment

Discussion sessions - although only the first one was useful.

having a lot time for discussions, those organized into working groups as well as those during the coffee and lunch breaks (it maybe sounds funny, but having the lunches on side actually helps to approach all other participants)

Discussion sessions.

I think it were discussions in the groups.

Interdisciplinary aspect.

There were people from different backgrounds with different expertise and approaches, and each one of them has an application in mind. These applications are very valuable as they could provide guidelines and help develop useful theories for control of ABM.

Having people from different areas got together.

Learning about the different groups/individuals who are working on agent-based models.

Bringing together a diverse group of researchers that approach the Workshop topic from different points of view.

The diversity and expertise of the presenters.

diversity of participants

Learning about optimal control and interfacing with other ABM researchers.

The presentations on ABMs

Build framework concepts, size the problem, define ABMs, and define the control.

Developing a better understanding of agent-based modeling and optimal control.

It was very intensive and focused to share the ideas about the topic.

I think the discussion/presentation of how to apply optimal control theory for ABMs is most useful in my opinion.

broad range of presentations

Understanding ABM and IBM

The opportunity to hear about a wide variety for applications of agent based models in many contexts.

Find out about the different approaches out there.

Making new contacts and potential collaborations.

networking

Meeting smart and open people

An opportunity to interact with a diverse collection of people.

What would you change about the Workshop? (n=24)

The group discussions should lead to concrete projects.

I think that the scope was really broad and I think having a sample problem and everything moving around that would have helped scope a bit.

I think the Workshop should have more presentations between mathematical methods (optimal control theory) and interesting biological problems. ABMs that are not related to any interesting biological issues might be avoided if possible.

To me it seemed clear from the start that classical optimal control has limited application to problems complex enough to require ABMs. I would have liked to think about other less rigid kinds of control and optimization.

a bit more focus on ABM rather than generic topics

I would have not had such a narrow topic for the Workshop. Rather the topic would have been broader, such as optimization (in general, and by whatever means, analytical or computational). , Also, I also would have made sure to identify a good set of problems in biology that were good candidates for applying control theoretic techniques to ABM. As it were, I do not recall seeing a single example of a problem in which control theoretic approaches would be beneficial to ABM.

Nothing.

nothing

Nothing in particular

Slightly smaller discussion groups would have worked out better.

However, most of the attendees were from the application side which had the drawback that they were not interested in developing control theory for ABM but rather were interested in whatever techniques or tricks that works for their applications. , Having a more focused group with people from different theoretical background such as control of Markov chains and control of discrete event systems would have been more productive from that point of view. However, as a starting point for discussion, I think the Workshop had the right balance.

Shorter presentations (45 minutes would be fine). Perhaps give non-presenters the chance to present posters? Organize, breakout group sessions in more detail beforehand, and less "democratic".

Perhaps a social event might be added to the programme?

I would only do one discussion session. Perhaps increased the length of time in the discussion. I would also outline more definitive conclusions at the end of the Workshop.

having non-speaker participants to present their areas of research would definitively help in starting new collaborations - maybe to encourage the non-speakers to present posters (if they want to) will help

to achieve that goal

It would be nice to have a short course about the topics involved in the Workshop before the main Workshop takes place. I am very familiar with OPT but not with the ABM. It would have been so helpful if I had learned about ABM.

More constructive discussion sessions. The discussion sections needed topics that were more focused and moderators who were prepared to facilitate the discussions.

I would like to have had a bit more structure in the discussion groups.

I would add discussions of key presentation(s) if participants have such a desire.

More informal discussion time.

It seems that there was too little time for informal discussions with other participants.

I know that all the participants are very busy, but it would have been nice to have some kind more coordinated discussion/background on the Wiggio. I did read the papers that were posted, but it would have been nice to have a bit more structure of what to expect.

I would have liked more time for just discussion (hard to fit in to the school semester).

Have the organizers summarize the Workshop at the end

The Workshop would have been more effective if: (n=0)

Please indicate any changes NIMBioS can make to improve the resources and/or accommodations available to Workshop participants: (n=6)

The institute facilities are very nice. Maybe a larger common breakfast and lunch area would be helpful, but this is minor.

none

Everything was great!

Jennifer did a great job!

I do not see the changes that would be necessary.

Nothing

Please indicate any suggestions you have for facilitating communication among participants during the Workshop: (n=6)

More informal discussion time would be good to have.

Make the discussions after each presentation longer!

As indicated before, more time for informal discussions would have been helpful.

It would help to have earlier access to Workshop preparatory material and documentation so that we know more about the presenters, participants and specific goals of the Workshop.

A bit longer breaks would facilitate ideas exchange

Not more than 25 participants. Have tables arranged in a circle so that participants can see each other.

Other social networking tools used: (n=12)

e-mail

email, telephone

Google groups

Linked-In

LinkedIn

LinkedIn

Linked In

wiggio,Skype

Skype

Skype, Yahoo

Most of my communication takes place on an individual basis. Now I hope to use Wiggio.

If you maintain a blog about your research and would like a link posted on the NIMBioS website, please provide the URL here, along with a brief description of the blog: (n=2)

No blog

I am thinking to do that!

Please use this space for any additional comments: (n=5)

I think it would have been helpful for the Workshop organizers to provide guidance on and even coordinate the topics of the Workshop presenters. There was a general uncertainty among many of the speakers about what they should talk about even after they arrived at the Workshop and what the goals of the Workshop actually were. More advanced communication of this on the part of the Workshop

organizers would be very helpful. Essentially speakers just talked about what they were able to talk about that seemed like it might be applicable. No one actually presented work involving optimal control as applied to agent=based modeling.

Overall I thought the Workshop was excellent. The range of expertise was very impressive, but it was still possible to have useful discussions.

Many thanks to NIMBioS for the financial support of my trip to the Workshop.

Thank You to the organizers. Thank You NIMBioS. Thank You NFS and rest of the funding agencies.

I was very grateful for the opportunity to participate in this Workshop.