



Evaluation Report
**High Performance
Computing Tutorial**

March 16-18, 2009

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April 15, 2009

Table of Contents

Summary of Results	3
Brief Synopsis	3
Highlights of Results.....	3
Conclusion and Recommendations	4
High Performance Computing Tutorial Evaluation	1
Background	1
Introduction	1
Respondent Demographics.....	1
Evaluation Design.....	3
Evaluation Questions	3
Evaluation Procedures	3
Data analysis	3
Findings	4
Overall Satisfaction	4
Tutorial Content and Format	4
Accommodations	7
Suggestions for Future Tutorials.....	7
Conclusion and Recommendations	9
Appendix A.....	A-i
Appendix B	B-i
Appendix C.....	C-i

Summary of Results

Brief Synopsis

The High Performance Computing (HPC) Tutorial was conducted on the University of Tennessee (UT) campus March 16-18, 2009. The purpose of the tutorial was to disseminate the information necessary for organizations and individuals to leverage HPC resources for research at the interface of biological/computational/mathematical research. The tutorial consisted of a series of short (30 -90 minute) presentations by invited speakers, with hands-on sessions as well.

The majority of the HPC Tutorial participants found the information presented useful and relevant, but indicated they would like a more hands-on format for future tutorials. While the workshop appeared to meet its main goal of enhancing participant capabilities to leverage HPC resources for biological/computational/mathematical research, participant responses indicated a need for more tutorial offerings on a variety of HPC subjects.

Highlights of Results

- The HPC Tutorial participants comprised a diverse array of backgrounds, including graduate students, postdoctoral researchers, university faculty and staff, and those from the non-profit sector.
- Participants came from a diverse array of business/education/research backgrounds, including ecology, biology, engineering, mathematics, and biophysics.
- Most participants (95%) indicated they were either "very satisfied" or "satisfied" with the tutorial overall.
- Ninety percent of participants indicated they would recommend this tutorial to others.
- Most participants (75%) indicated they felt the amount of content offered during the tutorial was just right, 15% thought there was too much content for the allotted time, and 10% thought there was too little content offered.
- On the whole, most participants (90%) indicated that participating in the tutorial enhanced their capabilities to leverage HPC resources for research at the interface of math and biology.
- While most participants (85%) indicated the format of the tutorial was effective, the most common suggestion for improvement was to include more hands-on activities.
- Overall, participants were satisfied with the housing, travel, and tutorial facilities.

- Participants expressed interest in learning about a variety of HPC topics at possible future tutorials.

Conclusion and Recommendations

The majority of the HPC Tutorial participants found the information presented useful and relevant, but indicated they would like a more hands-on format for future tutorials. While the workshop appeared to meet its main goal of enhancing participant capabilities to leverage HPC resources for biological/computational/mathematical research, participant responses indicated a need for more tutorial offerings on a variety of HPC subjects. The recommendations from analysis of participant survey data are as follows:

- Offer more HPC tutorials on topics specified by participants Appendix B
- Consider offering a “networking” workshop where participants can present on their current HPC research/interests and discuss collaboration opportunities with other researchers
- Consider offering an online HPC tutorial
- Change the tutorial format to include more hands-on activities and demonstrations
- To better understand and meet participant needs, include a question on the tutorial application where applicants can indicate the top three topics they are interested in learning about during the tutorial

High Performance Computing Tutorial Evaluation

Background

Introduction

The High Performance Computing (HPC) Tutorial was conducted on the University of Tennessee (UT) campus March 16-18, 2009. The leadership team for the tutorial included staff from NIMBioS, UT's department of Electrical Engineering and Computer Science, and UT's National Institute for Computational Sciences. The purpose of the tutorial was to disseminate the information necessary for organizations and individuals to leverage HPC resources for research at the interface of biological/computational/mathematical research. The tutorial consisted of a series of short (30 -90 minute) presentations by invited speakers, with hands-on sessions included at the end of the first two days. The third day concluded at noon and had no hands-on session scheduled. Speakers at the tutorial presented on topics in the following areas:

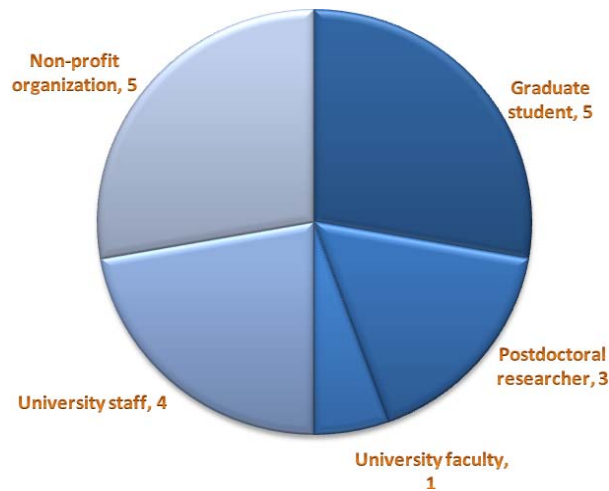
- TeraGrid resources,
- visualization and storage,
- queue and submission management,
- storage and data management,
- constraints and benefits of different parallelization approaches,
- computational biology resources,
- MATLAB distributed computing toolbox; and
- case studies in use of HPC in computational/integrative biology.

Respondent Demographics

A survey, which included optional demographic questions, was disseminated to all participants to gather information about their perception of the tutorial. Eighteen of the twenty tutorial participants responded to optional demographic survey questions about themselves. Of the 17 males and one female responding to these questions, 11 self-identified as white, 5 as Asian, and 1 as black or African American. One respondent did not indicate a racial identification.

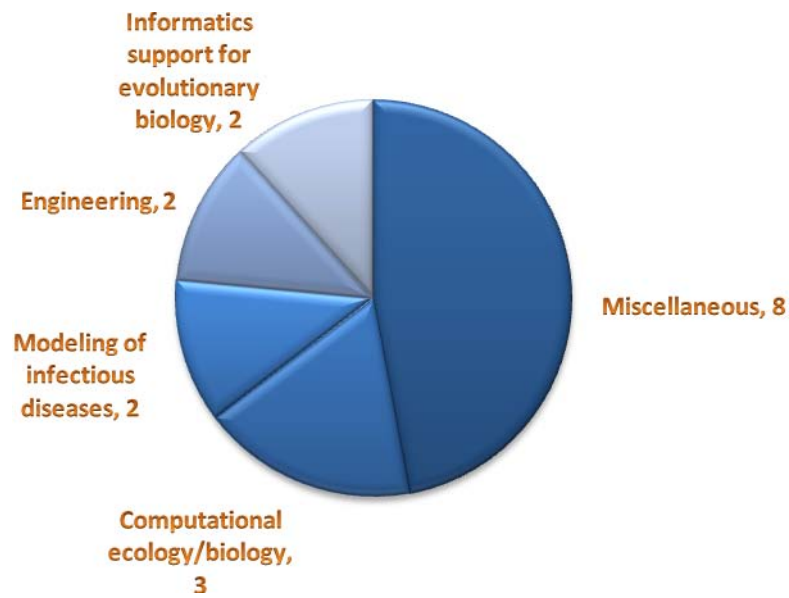
Respondents indicated they came from a variety of backgrounds, including graduate students, postdoctoral researchers, university faculty and staff, and non-profit organizations (Figure 1). Of the 13 respondents from institutes for higher education, 11 indicated they were from 4-year colleges/universities, two of which were classified as minority-serving.

Figure 1. Status of tutorial survey respondents



Respondents indicated came from diverse areas of business/education/research as well (See Appendix B for a full listing). The majority of business/education/research areas listed in response to this question did not fit into a particular theme; however, some themes did emerge during analysis of these responses, including computational ecology/biology, modeling of infectious diseases, engineering, and informatics support for evolutionary biology (Figure 2).

Figure 2. Survey respondents' main area of business/education/research



Six respondents indicated their education/research activities were currently supported through NSF awards, including the iPlant Collaborative and the National Center for Ecological Analysis and Synthesis (See Appendix B for a full listing of NSF award titles).

Evaluation Design

Evaluation Questions

Because this was the first tutorial hosted by NIMBioS, the focus of the evaluation was formative for the purpose of improving the content and format of future tutorials. The evaluation framework was guided by Kirkpatrick's Four Levels of Evaluation model for training and learning programs (Kirkpatrick, 1994¹). 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 tutorial. Several questions constituted the foundation for the evaluation:

1. Did participants find the tutorial useful?
2. Were participants satisfied with the tutorial content?
3. Was the format of the tutorial appropriate?
4. Was the tutorial appropriate to participants' level of expertise?
5. What would participants change about the tutorial to make it better?
6. What topics would participants like to cover at future tutorials?
7. Will participants be able to use the information and resources presented in order to leverage HPC resources?
8. Were participants satisfied with the tutorial facilities?
9. Were participants satisfied with the housing and travel accommodations?

Evaluation Procedures

An electronic survey covering the evaluation questions was designed by the Evaluation Coordinator and sent to the Director and Deputy Director of NIMBioS for review and approval. The final instrument was hosted online via UT's secure survey web host mrInterview. Links to the survey were sent to all 20 participants in the tutorial on the morning of the last day of the tutorial, March 18, 2009. The Evaluation Coordinator spoke briefly during the concluding remarks presentation to let the participants know that they should have received the survey link, and also to convey the importance of getting their feedback about the tutorial for the purpose of improving future offerings. Reminder emails were sent to non-responding participants on March 23 and 25, 2009. By April 1, 20 participants had given their feedback, for a response rate of 100%.

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 analysis software SPSS for analysis. Quantitative data were summarized descriptively using SPSS, while qualitative data were transferred to SPSS Text Analysis for Surveys. Qualitative responses were categorized by question and analyzed for trends.

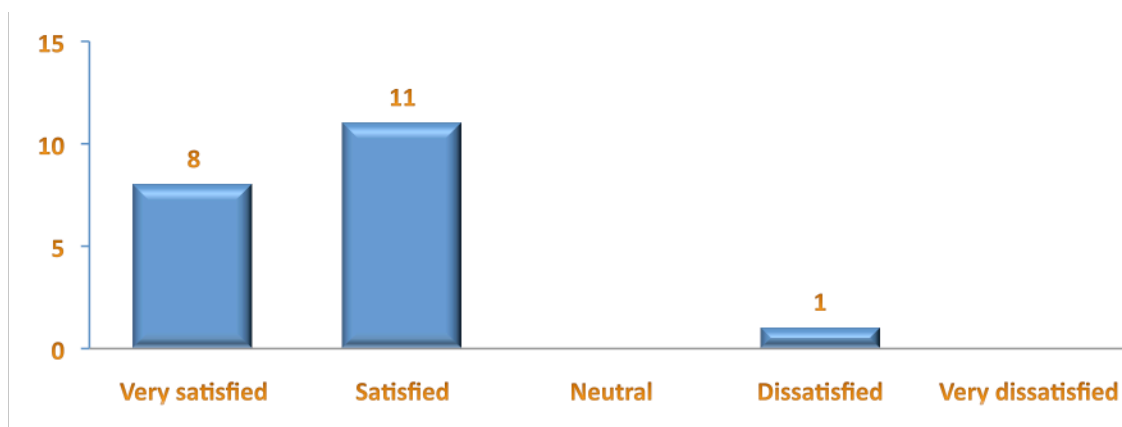
From Kirkpatrick, D.L. (1994). *Evaluating Training Programs: The Four Levels*. San Francisco, CA: Berrett-Koehler¹

Findings

Overall Satisfaction

Most respondents responded favorably to a question about overall satisfaction with the tutorial (Figure 3). The single respondent who indicated dissatisfaction with the tutorial overall was unhappy with the format of the tutorial, indicating that more hands-on time would have been more appropriate. The dissatisfied respondent also indicated he/she felt the tutorial offered too much content for the allotted time.

Figure 3. Overall respondent satisfaction with the tutorial



The majority of respondents responded favorably to overall questions about the tutorial, including level at which content was presented, usefulness of the hands-on exercises, and knowledge of the instructors. All but one of the respondents agreed they would recommend the seminar to others (Table 1).

Table 1. Number of responses to general tutorial rating questions, by response category

	Strongly agree	Agree	Neutral	Disagree	Strongly disagree
The tutorial was appropriate to my level of expertise.	6	12	2		
The tutorial met my expectations.	8	9	1	2	
The hands-on exercises were useful.	9	6	5		
The presentations were useful.	9	9		2	
The instructors were very knowledgeable about their topics.	14	5	1		
I would recommend this tutorial to others.	10	8	1	1	

Tutorial Content and Format

Respondents answered several questions about the tutorial content and format. Most respondents (75%) felt the amount of content offered was just right, and the majority of respondents (85%) felt the format was effective (Figures 4 & 5).

Figure 4. Amount of content offered during tutorial

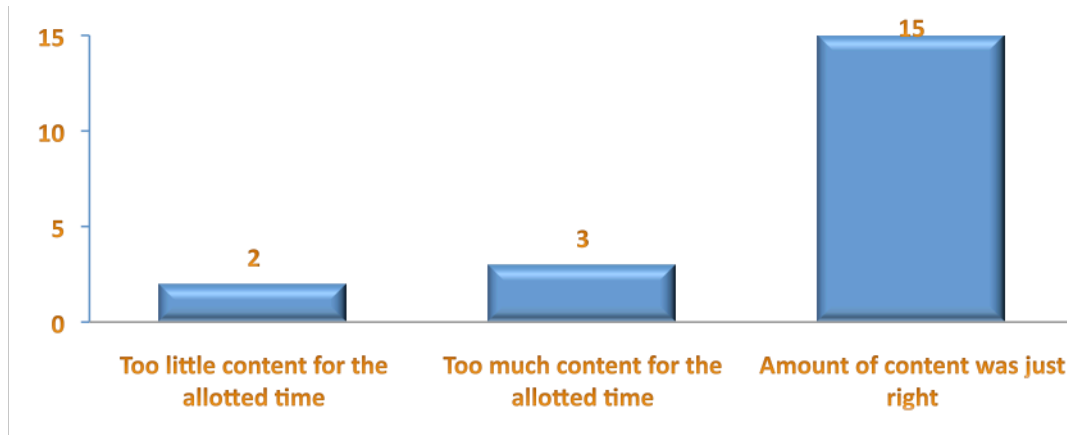
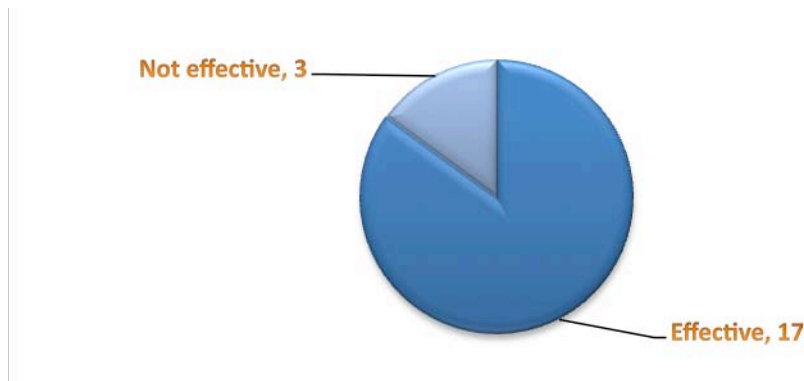


Figure 5. Effectiveness of tutorial format



Two of the respondents indicating they felt the format was not effective said they would have liked to have seen more hands-on activities and less time devoted to lecture (See Appendix B for a full listing of responses to all open-ended questions):

*“There needs to be *much* more time for hands-on sessions. Programming knowledge and know-how is best learned and most effectively retained by doing it, not by hearing about it. My suggestions would be to give the hands-on sessions in fact the majority of the time - lectures in between can introduce the learning goals, give an overview and hints, and then respondents can work through the material in a hands-on way through exercises.”*

“MPI and other parallel programming lectures (should be) allotted less time and concentrated on explaining concepts (with minimal, if at all, use of code examples), while hands-on sessions (should be) given more time and (be) more structured (interspersed with 5min mini-lectures based on the code examples).”

Participants were asked to comment on the most useful aspect of the tutorial. Analysis of responses to this question revealed the most commonly mentioned aspect was the hands-on exercises (n=8). Specifically, the MPI hands-on exercises were mentioned by several respondents. Other aspects mentioned by more than one respondent were the HUB and profiling presentations. Some respondent comments about the most useful aspects of the tutorial:

“The MPI programming exercise AND the 'from the trenches' perspectives, of Christian Halloy and others on how to port existing applications, into the MPI environment”.

“For me it was the presentation on Science Gateways, and Nano Hub in particular. The Rapture toolkit.”

“I found the analysis and profiling session very interesting.”

In addition to the most useful aspect of the tutorial, respondents were asked their opinions of the least useful aspect. Only six participants responded to this question, and no particular themes emerged during analysis of these responses. One of these participants responded that the whole tutorial was useful:

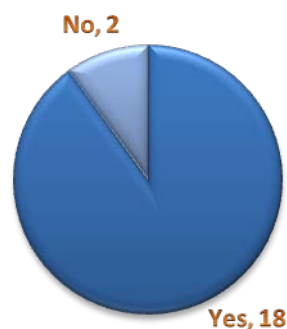
“I could not pick one: all presented material was appropriate for this tutorial.”

Responses from the remaining five respondents indicated they felt the MATLAB programming, science portal, and graduate student presentations were the least useful aspects of the presentation. One respondent’s comment:

“CS grad student presentations on clique/graph processing. The topics appeared disjointed and very narrowly focused. While interesting theoretically, perhaps using "real world" problems to illustrate these concepts would have been more helpful.”

When asked if they felt the tutorial would enhance their capabilities to leverage HPC resources for research at the interface of math and biology, the majority of respondents (90%) answered “yes” (Figure 6).

Figure 6. Enhanced participant capabilities to leverage HPC resources



One of the two respondents who answered “no” to this question indicated that they did not have sufficient background knowledge to understand all of the information presented:

“Well... I think this tutorial was above my level and therefore I think it would be nicer if it was longer and about more basic topics. However, I am delighted about the possibilities that I was exposed during this tutorial.”

Accommodations

Housing and Travel

Of the six respondents indicating their housing arrangements during the tutorial were handled by NIMBioS, four reported being “very satisfied” with the housing, while two reported feeling “neutral” about it. One respondent indicated that the hotel was nice, but the “wireless Internet did not work all the time.”

Of the four respondents indicating their travel arrangements were handled by NIMBioS, all reported being either “satisfied” or “very satisfied” with this aspect.

Tutorial Accommodations

The six participants who answered questions about the tutorial accommodations all responded favorably about facility comfort and resources, as well as food and drinks supplied by NIMBioS (Table 2).

Table 2. Number of responses to general tutorial accommodations questions, by response category

	Very satisfied	Satisfied	Neutral	Dissatisfied	Very Dissatisfied
Comfort of the facility in which the tutorial took place	5	1			
Resources of the facility in which the tutorial took place	5	1			
Quality of meals	4	2			
Quality of drinks and snacks provided	4	2			

Suggestions for Future Tutorials

Participants were asked several questions about what they would like to see at future NIMBioS tutorials. Analysis of open-ended responses indicated that a common request was to make future tutorials more hands-on in nature. One respondent indicated he/she felt that programming knowledge is best learned by doing it rather than hearing about it, and thus suggested that hands-on activities constitute the majority of the program during future tutorials, with presentations interspersed to support the hands-on exercises.

When asked what topics they would have liked to have covered in this tutorial if given more time, the most common response included more information about MPI (See Appendix B for a complete listing of responses). One participant’s comments about what he/she would like to have covered:

“High-level overview of the MPI interface (think pictures rather than code examples and breadth of coverage of available features rather than syntactic differences of C vs. Fortran)....Programming biological problems with tools or languages that are higher-level than MPI. Parallel features (like Map/Reduce) in R and Matlab are steps in the right direction, but are not sufficient. There are research and upcoming industrial languages for parallel programming (e.g. X10 from IBM, Fortress from Sun) that promise to be better for a practitioner who needs to solve a problem rather than create a distributable software package. Such tools may be still in their infancy, but NIMBioS is well-positioned to be the center of expertise in applying them.”

Other themes found in participant responses to this question included parallelization and individual/agent based modeling:

“Parallel bio-applications”

“HPC for hierarchical data. This is a real challenge as subsets of the data aren't independent of each other and so partitioning the problem for parallelization is a real problem. The data clustering example was a nice start in this regard, though what would have been good is to actually go through the strategies in a maybe simplified example and see hands-on what the pitfalls are and how one might go about surmounting the challenge. The authors of BEAST (A. Rambaut, A. Drummon, M. Suchard) and RAxML (A. Stamatakis) should be able to provide excellent material to this - they are actively working on parallelizing ML calculations for trees, for example.”

“A section on distributed individual-based agent-based modeling might have been useful.”

In response to a question about topics participants would like to see at future tutorials, respondents offered up several suggestions. Although most of the suggestions were singular, two respondents indicated they would be interested in a tutorial focused on discussing how to collaborate and share data, and two others indicated they would like a tutorial focused on ideas and resources for using HPC in specific research settings. Some participant comments:

“A venue to discuss collaboration opportunities might be useful.”

“It might be useful to solicit a list of problems that individuals/organizations face which they feel would benefit from use of HPC resources. These people could then be brought together for a workshop or working group, along with HPC specialists, to scope out design/specification documents which could provide a road map for the participants to convert existing applications to HPC ready applications. These case studies could then be used as tutorials later on.”

“I really enjoyed the presentations covering HPC applications -- I would like to see more resources for researchers to get ideas about how to incorporate HPC into their own applications.”

In addition to suggestions for future tutorials, all 20 respondents indicated they would participate in online tutorials to learn more about HPC topics.

Conclusion and Recommendations

The majority of the HPC Tutorial participants found the information presented useful and relevant, but indicated they would like a more hands-on format for future tutorials. While the workshop appeared to meet its main goal of enhancing participant capabilities to leverage HPC resources for biological/computational/mathematical research, participant responses indicated a need for more tutorial offerings on a variety of HPC subjects. The recommendations from analysis of participant survey data are as follows:

- Offer more HPC tutorials on topics specified by participants Appendix B
- Consider offering a “networking” workshop where participants can present on their current HPC research/interests and discuss collaboration opportunities with other researchers
- Consider offering an online HPC tutorial
- Change the tutorial format to include more hands-on activities and demonstrations
- To better understand and meet participant needs, include a question on the tutorial application where applicants can indicate the top three topics they are interested in learning about during the tutorial

Appendix A

HPC Tutorial Respondent Survey

HPC Tutorial Survey

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

NIMBioS will send two reminder emails to tutorial respondents who have not responded to this survey. If you would like to be excluded from these reminder emails, please enter your name below. Your survey results will still remain confidential and your name will not be associated with any of your responses in reporting of survey results.

Name:

Please check the appropriate box to indicate your level of agreement with the following statements about this tutorial:

Strongly agree Agree Neutral Disagree Strongly disagree

This tutorial was appropriate to my level of expertise.

This tutorial met my expectations.

The hands-on exercises were useful.

The presentations were useful.

The instructors were very knowledgeable about their topics.

I would recommend this tutorial to others.

How do you feel about the format of the tutorial?

This was a very effective format for learning the material

This was not a very effective format for learning the material (*branch to open-ended response*)

The tutorial format would have been more effective if: _____

How do you feel about the amount of content offered during the tutorial? (check one)

Too little content for the allotted time

Too much content for the allotted time

Amount of content was just right

What topics would you have liked to have covered in this tutorial if given more time?

What was the single *most* useful activity/concept offered during the tutorial?

What was the single *least* useful activity/concept offered during the tutorial?

Do you feel this tutorial will enhance your capabilities to leverage HPC resources for research at the interface of math and biology?

Yes

No (*branch to Please indicate*)

Please indicate how you think the tutorial could be improved to help you leverage HPC resources for your research:

Indicate your overall level of satisfaction with the tutorial:

Very satisfied

Satisfied

Neutral

Dissatisfied

Very dissatisfied

Would you participate in online tutorials to learn more about HPC topics?

Yes

No

What topics would you like to see covered at future NIMBioS tutorials?

Do you currently work under an NSF supported grant?

No

Yes (*branch to Name of grant*)

Name of grant:

Were your housing arrangements during the tutorial arranged by NIMBioS?

Yes (*branch to satisfaction with housing*)

No

Overall, how satisfied were you with your housing arrangements?

Comments about housing arrangements:

Was your transportation to Knoxville arranged by NIMBioS?

Yes (*branch to satisfaction with transportation*)

No

Overall, how satisfied were you with your travel arrangements?

What could NIMBioS have done to make your stay in Knoxville more enjoyable (e.g. better information about nearby attractions, public transportation, etc.)?

Other comments about travel arrangements:

Please indicate your level of satisfaction with the HPC Tutorial accommodations:

Very satisfied *Satisfied* *Neutral* *Dissatisfied* *Very Dissatisfied*

Comfort of the facility in which the tutorial took place
Resources of the facility in which the tutorial took place
Quality of meals
Quality of drinks and snacks provided

Comments about HPC Tutorial accommodations:

Please provide any additional comments about your experience with the HPC Tutorial:

Demographics

I am a(n): (check one that best describes you)

Undergraduate student

Graduate student

Postdoctoral researcher

University faculty—teaching/research

University faculty—teaching only

University faculty—research only

University staff (*all university/student answers branch to Describe your institution:*)

Business/industry employee

Non-profit organization employee

Describe your institution: (check all that apply)

2-year college/university

4-year college/university

Minority serving institution

Women's only institution

Please give a 2-5 word description of your main area of business/education/research (e.g. mathematical immunology, high school science teacher, etc.):

Gender: (check one)

Male

Female

Are you Hispanic or Latino? (check one)

Yes

No

What is your racial background? (check all that apply)

American Indian or Alaska Native

Native Hawaiian or other Pacific Islander

Asian

Black or African American

White

Appendix B

Open-ended Responses

The tutorial format would have been more effective if: (n=2)

There need to be *much* more time for hands-on sessions. Programming knowledge and know-how is best learned and most effectively retained by doing it, not by hearing about it. My suggestions would be to give the hands-on sessions in fact the majority of the time - lectures in between can introduce the learning goals, give an overview and hints, and then participants can work through the material in a hands-on way through exercises.

MPI and other parallel programming lectures were allotted less time and concentrated on explaining concepts (with minimal, if at all, use of code examples), while hands-on sessions were given more time and were more structured (interspersed with 5min mini-lectures based on the code examples).

What topics would you have liked to have covered in this tutorial if given more time? (n=13)

Miscellaneous (6)

This is difficult to say, as codes and application areas can be so drastically distinct. If the participants were from a more focused application area, then taking an real example code through the profiling and scaling process seems like it would be quite useful. This would provide opportunities to see different algorithms, approaches and libraries that may be of use to coders in that application domain.

Perhaps three more hours of dedicated lab time to complete , the examples. , Also, a session on COTS cluster solutions such as ROCKS.

Perhaps a more in-depth discussion on small cluster computing, which can be used as a "stepping stone" to the HPC arena.

Identifying the roles of a software architect in exploiting the HPC for biological and other scientist who may be new to HPC.

- Current projects utilizing Kraken/TeraGrid, - NanoHub

* a little more information about obtaining accessing to HPC resources, * a little more information about the differences between related technologies, such as grid, * a little more information about educational or instructional resources about HPC

MPI (3)

MPI and OpenMP hybrid techniques

More MPI

- High-level overview of the MPI interface (think pictures rather than code examples and breadth of

coverage of available features rather than syntactic differences of C vs. Fortran.) - This is provided MPI will still remain a major topic, see next. , - Programming biological problems with tools or languages that are higher-level than MPI. Parallel features (like Map/Reduce) in R and Matlab are steps in the right direction, but are not sufficient. There are research and upcoming industrial languages for parallel programming (e.g. X10 from IBM, Fortress from Sun) that promise to be better for a practitioner who needs to solve a problem rather than create a distributable software package. Such tools may be still in their infancy, but NIMBioS is well-positioned to be the center of expertise in applying them.

Parallelization (2)

parallel bio-applications

HPC for hierarchical data. This is a real challenge as subsets of the data aren't independent of each other and so partitioning the problem for parallelization is a real problem. The data clustering example was a nice start in this regard, though what would have been good is to actually go through the strategies in a maybe simplified example and see hands-on what the pitfalls are and how one might go about surmounting the challenge. The authors of BEAST (A. Rambaut, A. Drummon, M. Suchard) and RAxML (A. Stamatakis) should be able to provide excellent material to this - they are actively working on parallelizing ML calculations for trees, for example.

Modeling (2)

Optimal control and individual/agent-based modeling using HPC.

A section on distributed individual-based agent-based modeling might have been useful.

What was the single *most* useful activity/concept offered during the tutorial? (n=14)

Hands-on exercises (8)

The hands-on session on Monday afternoon.

Real time experience on kraken.

Hands-on Tutorial

Hands on working on Kraken with sample MPI code

Basics of HPC and machine architecture and hands-on exercises

The MPI programming exercise AND the 'from the trenches' perspectives, of Christian Halloy and others on how to port existing applications , into the MPI environment.

The MPI exercises to build on the MPI overview.

MPI tutorial

Miscellaneous (2)

Among NIMBioS presentations, Eric Carr's and Tabitha Samuel's

overview of parallel features in MATLAB and R.

* exposure to teragrid and freely available resources

HUBs (3)

The guest lecture on HUBzero.

HUBs, GPUs and the discussions

For me it was the presentation on Science Gateways, and Nano Hub in particular. The Rappture toolkit described at that site will be quite useful.

Profiling (2)

I found the analysis and profiling session very interesting.

High Performance profiling

What was the single *least* useful activity/concept offered during the tutorial? (n=6)

They were all pretty good, but if I HAD to select one, , it would be the discussion on MATLAB programming.

the science portal or hub presentation (it was vague as to why this was important as it related to HPC, except that it utilized HPC resources on the backend).

The lectures that went into excruciating details on the API calls.

Some background and introductory material would have been sufficient if supplied in print. The presenters probably could have jumped to advanced topics much quicker.

I could not pick one: all presented material was appropriate for this tutorial.

CS grad student presentations on clique/graph processing. The topics appeared disjointed and very narrowly focused. While interesting theoretically, perhaps using "real world" problems to illustrate these concepts would have been more helpful.

Please indicate how you think the tutorial could be improved to help you leverage HPC resources for your research: (n=1)

Well... I think this tutorial was above my level and therefore I think it would be nicer if it was longer and about more basic topics. However, I am delighted about the possibilities that I was exposed during this tutorial

What topics would you like to see covered at future NIMBioS tutorials? (n=13)

Miscellaneous (9)

MPI, Dense Lin Algebra

More of basics.

More in-depth MATLAB PCT topics.

Infectious disease modeling

How about a session focusing on simulation models used in Ecology, (such as the Optimal Control talk)? Many Ecologists would be interested, in this.

Effective and authentic use of HPC in the classroom.

Detailed HPC topics that will be modular in nature and will help the learning process. For eg: Understanding MPIs is a major topic. In a similar way one could start with LINUX/CLI/UNIX concepts keeping biologist in mind.

Parallelizing calculations over hierarchical data structures, such as trees. Loop parallelization.

Bioinformatics

Collaboration (2)

A venue to discuss collaboration opportunities might be useful.

Data Sharing, Collaboration Computing

Using HPC in research (2)

It might be useful to solicit a list of problems that individuals/organizations face which they feel would benefit from use of HPC resources. These people could then be brought together for a workshop or working group, along with HPC specialists, to scope out design/specification documents which could

provide a road map for the participants to convert existing applications to HPC ready applications. These case studies could then be used as tutorials later on.

I really enjoyed the presentations covering HPC applications -- I would like to see more resources for researchers to get ideas about how to incorporate HPC into their own applications.

Award title: (n=4)

SGER: A Novel Multi-Scoring Functions Sampling Approach to Improve Protein Modeling Resolution and It's Applications in Protein Loop Structure Prediction (CCF-0829382)

NSDL Pathways.

National Center for Ecological Analysis and Synthesis

iPlant Collaborative

Institution at which award is held: (n=4)

University of Arizona

UC Santa Barbara

Shodor

North Carolina A&T State University

Comments about housing arrangements: (n=1)

Hotel is nice, but wireless Internet did not work all of the time.

What could NIMBioS have done to make your stay in Knoxville more enjoyable (e.g. better information about nearby attractions, public transportation, etc.)? (n=3)

Not much. All my needs were met!, Oh, ONE thing: I did not receive the emails that told everyone (else) when , the Monday session was to begin. Despite calls and emails to Eric Carr. So , I was late to the first session, something I don't like to have happen. , So, a bit more attention to getting the word out!

None

Everything was fine.

Other comments about travel arrangements: (n=0)

Comments about HPC Tutorial accommodations: (n=1)

Overall, a good tutorial

Please provide any additional comments about your experience with the HPC Tutorial: (n=0)

Please give a 2-5 word description of your main area of business/education/research (e.g. mathematical immunology, high school science teacher, etc.): (n=17)

Miscellaneous (8)

Computational Protein Structure Modeling

HPC solutions in the area of large-scale social network agent-based simulations.

applied and computational mathematics

Adaptive Finite Element, Non conforming Methods

geospatial information system

Computational Biophysics

systems manager for iPlant Collaborative

mathematical study of phase transitions

Computational ecology/biology (3)

Computational Ecology

computational biology

computational biology education k-college

Modeling of infectious diseases (2)

I am interested in modeling infectious disease transmission on managed dairy herds and evaluating the effectiveness of control measures such as culling intervention and vaccination.

Agent based modeling of infectious diseases

Engineering (2)

Math Models and Simulations in Environmental/civil engineering.

Mechanical Engineering, particularly Computational Fluid Dynamics(CFD)

Informatics support for evolutionary biology (2)

Informatics support and cyber infrastructure for evolutionary biology

informatics support for evolutionary biology

Appendix C

List of Participants

Participants

Last name	First name	Institution
Aristotelous	Andreas	University of Tennessee
Banks	David	University of Tennessee
Bryant	Stephanie	RTI International
Diglio	Simoni	RTI International
Ganapathi	Laxminarayana	RTI International
Gapeyev	Vladimir	National Evolutionary Synthesis Center (NESCent)
Gewecke	Nicholas	University of Tennessee
Krause	Jeff	Shodor
Lapp	Hilmar	National Evolutionary Synthesis Center (NESCent)
Li	Yaohang	North Carolina A&T State University
Lu	Zhao	National Evolutionary Synthesis Center (NESCent)
Naswa	Sudhir	University of Tennessee
Ortega	Davi	University of Tennessee
Reeves	Rick	NCEAS
Roberts	Douglas	RTI International
Saum	Michael	University of Tennessee
Sekachev	Mikhail A	University of Tennessee
Skidmore	Edwin	IPLANT COLLABORATIVE
Solano	Eric	RTI International
Wei	Yaxing	ORNL

Presenters

Last name	First name	Institution
*Berry	Michael W	University of Tennessee
*Carr	Eric	University of Tennessee
Duke-Sylvester	Scott	Emory University
Eblen	John	University of Tennessee
*Ferguson	Jim	NICS
Halloy	Christian	NICS
*Langston	Mike	University of Tennessee
Loftis	Bruce	NICS
McLennan	Michael	Purdue University
Rogers	Gary	University of Tennessee
Tomov	Stan	University of Tennessee
Wong	Kwai Lam	NICS
Yost	Christal	NICS

*Organizer of event