Report from the 2007 thermalHUB Community Planning Workshop

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Executive Summary

This report documents the findings from the inaugural Community Planning Workshop for thermalHUB, an evolving web resource and the subject of a new project funded by the US National Science Foundation (NSF) to define the elements of a cyberinfrastructure initiative that will serve the global heat transfer community. Fifty five members (listed here) of the heat transfer community met for two days (10-11 December 2007) on Purdue's campus (West Lafayette, IN USA) to plan the initial prototype implementation of thermalHUB. The discussions focused on defining an initial set of innovative cyberinfrastructure resources for the community. These resources will be consolidated through the thermalHUB.org web portal, whose basic structure is modeled after the successful nanoHUB.org precedent. A major activity of the workshop involved focused, question-driven discussions among small groups of five to nine participants related to each major thrust area of thermalHUB. The following list summarizes the recommendations from each of these groups:

- **Cyberinfrastructure**
  - One of the major areas of content development involves a new community wiki platform. Different wiki editors will be assessed based on their utility for the expected uses on thermalHUB.
  - 500GB of total user space will be made available initially for registered users to store results and content. In addition, 230GB of space will be initially available to host general resources (e.g., simulation tools, wiki content, experimental data).
- **Computational Research Tools**
  - Modeling tools that address multiscale, multiphysics phenomena and process-property-structure relationships are needed by the community and should be encouraged.
  - thermalHUB should provide access to existing freeware codes for heat conduction and computational fluid dynamics, among others, and benchmarking of codes should be emphasized.
- **Computational Learning Tools**
  - At the novice to intermediate levels, a thermal systems simulation tool should be developed, and existing resources for heat transfer correlations and simple finite difference/volume analysis should be made accessible where possible.
  - At the advanced level, solvers for multi-dimensional heat conduction, laminar boundary layers, and radiative exchange should be made available where possible. Among many other potential resources involving sub-continuum heat transfer, these tools were not prioritized because they are highly specialized and typically customized to specific content in graduate-level courses in academia.
- **Community Wiki**
  - thermalHUB should contain a prominently featured solicitation for wiki topics (as a wiki page itself), and wiki pages should typically serve as entries to other thermalHUB components (such as computational tools and experimental databases).

    - The wiki will be particularly useful for consolidating reference material, and the creation and dissemination of collaborative review articles.
- **Online Lectures and Tutorials**
    - Rather than complete course notes, more meaningful and unique contributions would involve course-enhancing materials that could be used on an ad hoc basis by instructors. Demonstrations of experimental methods for undergraduate laboratories and innovative tabletop experiments could serve this purpose well in the form of short (*e.g.*, 10-minute) multimedia clips that support and supplement theory detailed in textbooks.
    - Many institutions are in the process of considering online degrees or are already offering online programs in various forms, and it is likely that this trend will grow in the near future. thermalHUB should proactively respect institution-specific policies regarding online courseware.
- **Experimental Properties and Databases**
    - Compiled data should initially focus on thermal conductivity and diffusivity of small-scale structures (as these are not yet well catalogued), and other properties that are relevant to heat transport or the understanding of heat transport should also be included as thermalHUB evolves. The value of these data will be maximized if the materials are well characterized for purity, phase, and microstructure.
    - Contributors should be encouraged to submit supplemental materials including descriptions of the measurement methods, original measurement data, and data processing procedures. All data should be reviewed by users, and a multi-tier categorization of data quality based on user ratings should be created and implemented.
- **International Partnerships**
    - thermalHUB should be an enabler of international collaborations. Accessibility to information at any time and at any place will enhance the activities of the global community and foster the development of new joint research projects with different groups. As such, international partnerships are critical to the sustainability of thermalHUB.
    - Initial modes of international engagement should include: adoption of tools in courses at international academic institutions; the use of thermalHUB to advertise international conferences and host portions of their content (e.g., keynote lectures), and interactions with multi-national companies by providing common research and learning resources to their engineers.
- **Industrial Partnerships**
    - Engagement with industry will likely be critical to the sustainability of the effort, and concerted efforts should be made to reach out to industrial partners, particularly organizations with large thermal groups. Briefings to individual companies, participation at trade shows, and newsletters should be considered for industry engagement.
    - Areas of particular emphasis for enhancing industrial interest in thermalHUB should include property databases, simple analysis tools, and virtual communities to locate and connect to domain experts.

Introduction

thermalHUB.org is an evolving web resource and the subject of a new project funded by the US National Science Foundation (NSF) to define the elements of a cyberinfrastructure initiative that will serve the global heat transfer community. In Summer 2007, nearly twenty members of the heat transfer community (listed here) collaborated on a successful proposal to the NSF to obtain a two-year planning grant that will support the definition and development of a wide range of innovative cyberinfrastructure resources for the heat transfer community. These resources will be consolidated through the thermalHUB.org web portal, whose basic structure is modeled after the successful nanoHUB.org implementation.

We are now in the planning stage of this exciting resource, and we are reaching out to the global heat transfer community to define the needs and opportunities that cyberinfrastructure might address for our discipline and related ones. As the first major step in this process, a community planning workshop was held (see agenda), and this report contains the findings and recommendations that emerged. The workshop brought together 55 members (listed here) of the heat transfer community for two days (10-11 December 2007) on Purdue's campus (West Lafayette, IN USA) to plan the initial prototype implementation of thermalHUB. The discussions focused on defining an initial set of cyberinfrastructure resources for the community. The resources developed are expected to be rich in content and useful in the activities of heat transfer students, engineers, and researchers. The thermalHUB.org site will be updated frequently as new resources are posted, and we welcome the community's input and contributions to thermalHUB as this initiative moves forward.

thermalHUB Mission Statement

The mission of thermalHUB is to serve the heat transfer community by providing convenient global access to comprehensive, state-of-the-art information, computing, and communications resources that: (a) enhance the efficiency and accuracy of research studies on all types of thermal transport processes across all relevant length and time scales, (b) enable continuous learning by sharing best practices and learning tools with the broad community, from students to experienced engineers and scientists.

Workshop Objectives

- Introduce the shared *thermalHUB* concept
- Establish a framework for community involvement,
- Consolidate a detailed set of community-driven research and learning goals,
- Define the critical elements of prototype cyberinfrastructure resources, including:
    - research-grade simulation tools with user-friendly pre- and post-processing interfaces,
    - computational learning tools for use in undergraduate and graduate curricula,
    - a community Wiki resource that provides a user-friendly virtual community forum and that consolidates core concepts in heat conduction, convection, and radiation,
    - multimedia online lectures and tutorials,
    - thermal property databases and experimental networks,

- elements that will enable and simplify international partnerships and collaborations.
- mechanisms to engage industry

Reports from Breakout Groups

A major activity of the workshop involved focused, question-driven discussions among small groups of five to nine participants related to each major thrust area of thermalHUB. The following subsections contain the recommendations from each of these groups.

Breakout: Cyberinfrastructure

Group Members: Kevin Buterbaugh, Michael McLennan (lead), Alan Tackett

What will the wiki area look like? How will it be implemented? How will we integrate it with the existing thermalHUB?

- There are a few existing wiki packages that could form the basis for the thermalHUB wiki. **MediaWiki** (http://www.mediawiki.org/wiki/MediaWiki) is the strongest contender. It is used to implement the popular Wikipedia site, and therefore has a wiki syntax that is widely used and perhaps already familiar to many users. More importantly, it has well-established models for collaborative development and editorial control.
- **PmWiki** (http://www.pmwiki.org/) is another possible choice. PmWiki has an associated plug-in component called WikiPublisher, which allows a user to format the entire content of a wiki as a book, complete with table of contents, references, and so forth. If a similar plug-in were available for MediaWiki, then the combination of MediaWiki/WikiPublisher might be the best choice. Otherwise, PmWiki should receive more consideration. Other wikis, including TWiki and Trac, were discussed and dismissed as quirky or not as powerful.
- Ideally, the wiki software will be hosted on the same Apache web server supporting the existing thermalHUB.org site. The wiki software must be integrated with the **existing thermalHUB LDAP server**, so that the same login/password can be recognized across both parts of the site. As far as users are concerned, there should be a **single sign-on** to access both parts of the site, so their login on one side should be recognized on the other.

What level of user capacity will our current resources allow? How can we supplement/leverage these resources?

- The current thermalHUB.org installation will support up to **100 simultaneous tool sessions**. If usage grows beyond that, we will have to add additional tool execution servers to the rack. Each server costs about $4,000 and should support an additional 300 simultaneous sessions.
- The current thermalHUB.org installation has **230GB of storage space** for all resources and other content uploaded onto the hub. This includes the seminars, tutorials, animations, and publications uploaded via the “Contribute Content” link. Because we are planning to host the

wiki on the same machine as the rest of the thermalHUB.org site, all wiki information would be included in the 230GB of content storage.

- Simulation users on thermalHUB.org have a total of **500GB of storage space** for their simulation results. This space is controlled by a quota system, and different users can have different quotas. If each user has 1GB of storage space, for example, then thermalHUB will support 500 users. If each user has 5GB of storage, then thermalHUB will support only 100 users. In practice, there will likely be a blend of users, many with a small amount of storage, and some with more.

How can partner organizations contribute to CI resources and development activities?

- **Computing cycles** – As part of an NSF grant for Software Development in Cyberinfrastructure (SDCI), the nanoHUB is developing a capability to let other desktop machines and clusters join a network and volunteer their resources for computation. A year from now, this should be as simple as installing a small package on a Linux-based machine and starting a daemon.
- **Distributed data storage** – The Vanderbilt team has created an infrastructure called REDDnet, for handling distributed data repositories. This could be integrated with the hub middleware, providing a way to store large datasets across many different institutions.
- **Distributed backup** – Other universities could also help maintain off-site backups of the thermalHUB database and contributed content.

Breakout: Computational Research Tools

Participants: Jennifer Lukes (lead), Matthew Krane, Darrell Pepper, Ajit Roy, Yuan Zheng, Joan Fuller

Overview

Several questions were posed to the participants to initiate discussion. The questions were intended to identify emerging areas and methods in computational heat transfer research, survey existing industrial and freeware computational heat transfer tools, and find out the types of codes written by the group members. The output of those discussions is listed below.

What are the important emerging application areas for computational heat transfer research?

- The group identified several emerging areas in computational heat transfer research. These generally fell into two categories: topical areas and computational methods. The general topical areas covered energy, building science, materials, interfacial transport processes, electronics cooling, and transportation. Specific subareas within energy included solar energy, turbines, fuel cells, and other ground based sources, and within building science the subareas included fire and combustion, HVAC, thermal comfort, energy efficiency, and sensors for homeland security.

- Aspects of materials research included processing-microstructure-property relationships, computational design of new materials, and materials for energy storage.
- In the area of interfacial transport processes, transport across interfaces in micro- and nanostructured materials, heat exchanger surfaces, and moving (fluid-fluid and fluid-solid) interfaces were identified.
- The group also mentioned active methods for electronics cooling, and transportation-related heat and mass transfer issues in the areas of aerospace, emissions control, and alternative fuels. Most of these topical areas fall into the group members' own research interests; there are likely additional areas viewed as emergent by the broader community.

What are the important emerging techniques in computational heat transfer research?

- Several cross-cutting techniques important to problems in various topical areas were also identified. The techniques determined as most important include multiscale and multiphysics modeling capabilities. In the multiscale modeling area, 'smart' methods to avoid brute force computations were most important, as were methods to enable micro- to macroscale computations and nano- to microscale computations. Multiphysics and coupled phenomena modeling is also very important, and methods enabling inclusion of chemistry, heat transfer, flow, and external magnetic and electric fields will be critical to the development of engineering systems.
- Several other methods also arose in the discussion. New methods to generate models based on limited data sets, for example stochastic and other methods, were identified as an area of need. Also inverse problem solution methods for converting experimental output data into useful properties, for example extraction of thermal conductivity from thermoreflectance data, were identified as important. Open source codes for treatment of moving interfaces, molecular simulation methods, and optimization techniques for achieving desired material microstructures based on processing parameters were also of interest.

What existing tools might be suitable for inclusion?

- The group identified several commercial packages, freeware tools, and downloads currently available to and used by the community. The general commercial packages included COMsol, Ansys, Fluent, CFX, Flow3D, StarCD, Answer, and Accelrys, and the industry specific packages for metals processing included ProCast and Magma. Additionally, the group found the modular function of Simulink to be very appealing; this feature may be useful in the future for building larger systems by coupling separate, independently developed modules.
- Freeware tools and codes included Los Alamos CFD codes, NIST codes (for example Fire Dynamic Simulator), EPA codes for building design, HVAC and heat balances, and NASA codes (formerly free). Google was also mentioned as a frequently used tool to identify other available codes and packages, as was Sourceforge, which is a general repository for freeware codes.

What kinds of computational codes do you write for your own heat transfer research?

- The group members themselves are involved in code development in a variety of areas. The topical areas include combined convection and radiation modeling, porous media transport, building modeling and design, microstructural evolution, and micro/nanoscale thermal transport. The computational methods involved in most of these include general CFD methods, radiation network models, finite elements, molecular dynamics, boundary elements, and meshless methods.

What important issues should be addressed in existing commercial packages, web-based tools, and your own codes for heat transfer research on thermalHUB?

- Based on the questions above, the group members identified several needs that thermalHUB could fill. For the commercial packages, modules or input files could be added to thermalHUB to provide additional functionality. User-supplied ratings, comparisons, and evaluations of these codes could be added to the site, with mechanisms to prevent self-inflation of ratings. It was also suggested that in exchange for some level of sponsorship, vendors could post commercial codes for trial usage at no (or nominal) cost. Care would have to be taken in this case to avoid excessive commercialism.
- For the freeware and web tools, the group felt it important to collect all links to existing heat transfer web tools and related content in a central location on thermalHUB. User-friendly codes for heat transfer research, for example lattice Boltzmann and molecular dynamics codes, were of interest to the group. Important for such user-posted codes is the ability to validate against known data and benchmark against other codes if they exist. Also needed would be a way to quickly get up to speed on the codes, for example through good documentation and tutorials on how to use the codes. Force field and parameter files for the molecular simulations would also be important. A longer-term goal would be to establish a framework reminiscent of Simulink that could link various thermalHUB modules together (and possibly commercial codes as well) to perform system-level calculations.
- An additional idea would be to pose a challenge problem to the community. This is has been done at several computational heat transfer and related conferences (ICHMT, AIAA, ASME convection, and McWASP—a series of conference on metals casting). The idea is for different groups to attack a problem and post a code for how to solve it. The difficulty in this is to identify a problem of interest to many members of the community. The challenge problem idea will likely not be viable until thermalHUB has a critical mass. At that time thermalHUB could provide a good forum for posting of challenge problems.

Summary

- From the group discussion, a few topics consistently emerged. Multiscale and multiphysics thermal modeling codes were viewed as an important emerging area where thermalHUB may help accelerate research progress. Validation and benchmarking of such codes is crucial.

- Codes for modeling structure-processing-property relationships and advanced methods for constructing models from sparse data are also very important.
- Finally, links to existing commercial and freeware computational heat transfer research codes in a central area on thermalHUB is essential to avoid duplication of effort.

Breakout: Computational Learning Tools

Group Members: Chris Dames, Tim Fisher (lead), David Go (scribe), Abdulmajeed Mohamad, Xiulin Ruan, Kirk Yerkes

What are the most important novice- and intermediate-level learning tools that should be developed for the prototype thermalHUB?

- A **thermal systems simulation tool** was viewed as very desirable because it would engage users from other communities, as well as reinforce basic heat transfer principles (e.g., thermal resistance and capacitance). This tool could easily be tied to the wiki and its prospective organizational structure. The group also articulated a general opinion that thermal systems engineering is underrepresented in undergraduate curricula relative to its importance in practical applications.
- Tools that consolidate and apply **basic heat transfer correlations** would be very useful in an initial effort. For example, Prof. Mills at UCLA offers freeware of this type (see http://www.mae.ucla.edu/academics/faculty/mills.htm), as well as other tools. Some other textbooks also provide such software along with the purchase of a textbook, and while we do not wish to replace these textbook features, these types of tools are very useful in practical engineering problems outside the classroom.
- The group also promoted the possibility of hosting **thermodynamics tools** such as EES (http://www.mhhe.com/engcs/mech/ees/na.html) and recommends making contact with the publisher of this tool. Other possibilities include Simulink™-based tools developed within the community, and the group recommends posting a 'needs' document to attract potential contributors of existing codes.
- The group recommends the deployment of **finite-volume or finite-difference 1D transient conduction** codes. The particular value lies primarily in developing algorithms so that intermediate-level users can develop appreciation of numerical modeling of equations that describe physical phenomena. These tools are already available in various places, including home-grown codes and textbook supplements. Those who have developed open-source or open-use tools should be encouraged to share them on thermalHUB.

What are the most important advanced-level learning tools that should be developed for the prototype thermalHUB?

- Tools that provide **analytical series solutions to conduction problems** would be very valuable in that they would allow users to gain an appreciation of the influence of physical parameters in advanced heat conduction processes. This resource would be particularly useful because many graduate programs no longer teach a full graduate-level course on heat conduction, and this resource could supplement advanced math courses on initial and boundary value problems by providing a collection of heat transfer problems.

- Another important class of tools would involve **semi-analytical solvers for forced convection heat transfer in laminar boundary-layer and pipe flows**. Some home-grown codes exist in this area within the community, and we should seek to incorporate these existing tools into the HUB where possible.
- For computational tools, the group believes that the community should encourage contributions based on the wide range of current graduate topics, such as: 2D FDM/FVM/FEM solvers (e.g., EL2D), lattice dynamics (e.g., DISPERSE, GULP), molecular dynamics, Boltzmann transport equation solvers, lattice Boltzmann solvers, Monte Carlo solvers, density functional theory solvers (e.g., ABINIT), and atomistic Green's function tools. **The group did not seek to prioritize these tools**, because they are highly specialized and typically customized to specific content in graduate-level courses in academia. Ideally, contributions of such tools would come from many different people in the community, and over time, as each tool evolves, instructors at other institutions could choose to modify their course content according to their needs and the maturity of the available codes.

Who will develop these tools?

- The leader of this HUB theme and interested participants should contribute their own codes, and they should also be encouraged to contact people who have already developed suitable codes and invite them to participate.
- In addition, tools at various levels can be developed through undergraduate or graduate student class projects. Some of these tools could be developed in an integrated manner across institutions, or in multiple offerings of a course.

What restrictions, if any, should be placed on the initial group of contributors?

- The group felt that no restrictions should be placed on contributors, but that the early contributors should be especially encouraged to set high standards of quality, validation, and documentation.

How will the codes be validated, and should the HUB require some kind of validation test?

- Each new tool should have an entry box related to code validation that each contributor should be asked to complete. This box should also state any known limitations of the code.

How might the community wiki enhance the tools?

- The group recommends that upon code submission, each contributor should be asked to do a search (or perhaps an automatic search could be implemented based on contributor-defined 'tags') on the existing thermalHUB content. Contributors should then be encouraged to enter appropriate links in other wiki pages, as well as links to any online presentations. We note that the Rappture™ development tool now includes the ability to place html links in the user interfaces, and this feature should be exploited as much as possible.
- The tool submission process should automatically generate a wiki page, with at least the contributor-entered tool description as content.

What 'tags' should we use to describe and distinguish our tools?

- Level of rigor: novice, intermediate, advanced
- Heat transfer mode: conduction, convection, radiation, multi-mode
- Scale: system, continuum, nanoscale
- Solution method: analytical, computational
- Other ideas include: base tags on ASME K-committees, use chapter titles from textbooks.

What is the best way to inform the community about these tools?

- A variety of complementary modes of 'marketing' the HUB are envisioned, including: RSS feeds, conference sessions; review papers in community journals; advertisements in journals, magazines; press releases; hosting of a job postings resource; advertisement of learning tools on other parts of the HUB (e.g., on a virtual journal site).

Breakout: Community Wiki

Group members: Ted Bergman, Deyu Li, Nick Roberts, Abhijit Sathe (scribe), Greg Walker (lead)

What is the most effective use of the wiki (educational, reference, literature review, ...)?

- The nature of the content should not be restricted to any particular form. However, the use of the wiki will likely center around encyclopedic content, because this use is most familiar to users. Nevertheless, users are not likely to duplicate content that can be found in other wikis (Wikipedia, for example), so the intent that the wiki can be used for literature review articles, or recent advances in emerging technologies should be emphasized.
- Educational content should not be a priority for the initial wiki entries. This use is not likely to receive as much traffic in the beginning. Of course the community will determine this in the long term and if some users want to supply educational content they should be allowed and encouraged to do so.
- The intent (mission) of the wiki is to provide timely "living" collaborative documents and provide forums for discussion of research in emerging technologies.

How do we get community "buy-in" and participation?

- Education on what the wiki is and how it works will play a large part in the overall success of the wiki as a tool for sharing information on thermalHUB. Even if users are familiar with the wiki concept, they may not appreciate its utility for collaborative documents.
- Users should clearly understand that the wiki is part of thermalHUB and not an extension to Wikipedia. All the content will be visible to the world, but will be specific to what the community deems most important. Only the community will be able to contribute (see following question).
- Credit for contributions is a concept devised to encourage users to contribute to the development of content. In traditional journals, credit is obvious, and contribution is clear. In a wiki article, the authors are not identified explicitly. Moreover, the author's list could contain hundreds of contributors without distinguishing minor editorial changes to major contributions. It has been argued that the quality of the article might actually improve if "credit" for the article were removed. In this case, the author has alternative, presumably more altruistic, intentions to supply content. In addition, the author's contribution is more directly subject to the scrutiny of peers. Therefore, it is not clear whether the community needs credit to encourage contributions.

Should we restrict who can contribute? If so, how do we screen potential contributors and what should the criteria be?

- Initially anyone who has an account on thermalHUB should be allowed to contribute. There is concern that the content can become polluted by miscreants or vindictive users. While we concede that this is possibility, the probability is quite low. Even though anyone can acquire an account without oversight, the mere process should discourage those wishing to vandalize a random site and bots that autonomously post questionable material to any open site. Moreover, all contributions are logged so that malicious editing can be identified and stopped.
- This wiki effort should be regarded as an experiment in community collaboration. (Community in this context is defined as those who have a thermalHUB account.) As such, the wiki should be as open as possible initially to reflect the true sentiments of the community.

Should we maintain editorial control as a way to ensure the accuracy of information and that no copyrighted material is submitted? If so, who will perform this duty?

- No. As with any published scientific materials, errors are inevitable. With a "living" document model, though, the ability to correct the errors is vastly enhanced. In fact, as more people view the documents, the better chance that errors will be found and corrected. Therefore, the content will actually improve in time, which is impossible for traditional archived material.
- This form of peer review is a new model. Everyone has the chance to review the content without the close oversight of an editor. This approach should improve quality.

Should we aggressively plant seed articles (called stubs), or let the community initiate the content?

- No. The community should dictate the preferred style and content of the wiki. Nevertheless, two articles that should be started by the thermalHUB organizers should include a README type of article for thermalHUB in general and a wish list for wiki articles. The README could take the form of an FAQ and should not supplant existing documentation. Perhaps the content should outline the vision of how the wiki interacts with other features of thermalHUB without dictating the type and style of content. The wish list will provide a starting point for folks to begin articles. Anyone who adds an idea to the wish list should be encouraged to also supply the kernel of that article. In this way, users will be encouraged to think about how the wiki can be used and how they can contribute. These two articles could conceivably be the same document.

How do we inform the community about this resource (marketing)?

- The wiki organizers should adopt the "build it and they will come" mentality. Aside from appropriate links to access the content, no aggressive ad campaign should be needed to promote its use.
- A section including "success stories" about thermalHUB in general could include testimonials about the wiki as well.

Breakout: On-line Courses and Tutorials

Group Members: Scott Huxtable, Costas Grigoropoulos (lead), Carl Snyder, Evelyn Wang, Kazuaki Yazawa, Robert Sayer (scribe)

What on-line undergrad-level lectures or tutorials should we develop for the prototype thermalHUB?

- Rather than offering complete course notes, a more meaningful contribution is to develop course-enhancing materials that could be of great benefit to instructors. Demonstrations of experimental methods for undergraduate laboratories and innovative tabletop experiments serve this purpose well. These could be presented effectively in the form of 10 minute-long multimedia clips that support and supplement theory detailed in the texts. Examples could be drawn among topics such as: i) engine operation and combustion processes, ii) energy systems including solar, thermo-electrics, fuel cells, iii) visualization of different boiling modes coupled with experimental measurements, iv) visualization, measurements and analysis of fluid mixing and jets, v) radiation transfer in participating media, vi) analytical techniques and computational modeling, elucidating the nature of transient thermal diffusion, convective and radiation transfer.
- The educational mission can be extended to the development of introductory materials for high school students to provide exposure to heat transfer and thermal sciences. On the other end of the spectrum are lectures and on-line material for retraining that should cover thermal sciences fundamentals. One such example could be the introduction to critical issues in thermal management of electronics, especially in connection to new demands and technical concepts.

What on-line grad-level lectures or tutorials should we develop for the prototype thermalHUB?

- In addition to the above mentioned educational enhancement materials that should naturally be of increasing complexity, it is highly appropriate to develop targeted overviews in specialty areas of high current interest and rapid growth rate. These should be developed for different audiences, including graduate students and industry practitioners. Relevant topics may be: i) energy and energy efficiency, ii) thermal sciences and the environment (e.g. greenhouse effects, water resources and management), iii) thermal transport in electronics, iv) thermal aspects in manufacturing including non-traditional materials processing and fabrication, v) nanoscale heat transfer. In this context, it is of interest to convert highlighted review articles to suitable presentation formats. Important lectures from experts including keynotes, invited presentations, and award plenary lectures can be broadcasted through the thermalHUB. Another type of material that could be highly effective for offering a general perspective may be the news magazine style featuring interviews and describing efforts of individual researchers, laboratories, groups, industry and educational institutions. Literature surveys on various topics offering comprehensive lists of resources and available tools (i.e. computational, experimental data) will also be of importance, particularly in cases where the information is difficult to locate without guidance.

Who will contribute the content?

- The workshop participants and coordinators should invite key experts to contribute and spearhead the effort. The program should be open to contributions from the entire Thermal Sciences society, gathering complementary expertise that may be found in different domains. It is important also to solicit international collaborators and call upon the overseas expertise. In any case, the contribution to thermalHUB provides a good opportunity to address the NSF-mandated broader impacts issue creatively in a stream-lined and effective manner. Help must be provided to ensure the professional quality of the materials, taking advantage of the nanoHUB expertise.

What restrictions, if any, do different institutions impose on such course and course-like content?

- The policies depend on the institution and vary from the direct revenue linked to the open access. This may reflect the institutions' fundamental philosophies as well as their publicity strategies. Many institutions are in the process of considering on-line degrees or are already offering on-line programs in various forms. It is likely that this trend will grow in the near future and may have an impact to the structure of the educational system according to some predictions. The professional societies do their own marketing of courses and tutorials that generally represent a stream of revenue. Avoiding the offering of full courses via the thermalHUB mitigates issues related to licensing and intellectual property. Lectures and instruction enhancing materials would be more suited.

Breakout: Experimental Properties and Databases

Group Members: David Cahill, Bara Cola (scribe), Michael Frenkel, Leslie Phinney, Samuel Graham, Lois Gschwender, Stan Setlak, Li Shi (lead), Michael Witt

What materials and properties should be included in thermalHUB?

- The thermophysical properties of many engineering materials are compiled in the CINDAS database; thermalHUB should not attempt to duplicate these valuable resources but should provide links and summaries of the content available in CINDAS and other commercially available databases. There is a great need however for a compilation and clearing-house for data on the thermophysical properties of thin film, nanostructures, and nanostructured materials that are being developed for a wide variety of applications in sensing, information technology, and energy conversion. This user-driven database and bibliography is therefore meant to compliment, not replace, the existing compilations. In addition to data for thin films, nanostructures and nanostructured materials, the thermalHUB compilation should also provide convenient access to bulk materials that are i) commonly used in thermal management; ii) integral to the measurement techniques; and iii) standards that researchers can use to verify their experimental techniques.
- In the short term, i.e., during the planning grant period, the thermalHUB compilation should focus on thermal conductivity and thermal diffusivity, but other properties that are relevant to heat transfer or the understanding of heat transport should also be included as thermalHUB evolves: for example, optical constants in the range of wavelengths that are relevant to thermal transport, and elastic constants or sound velocities. The value of these data will be maximized if the materials are well characterized for purity, phase, and microstructure.
- The commercial databases do not generally include data for thermoelectric transport properties. Because of growing interest in thermoelectric materials for energy conversion, the inclusion of Seebeck coefficient, electrical conductivity and thermoelectric figure of merit in the thermalHUB compilation will be a valuable and unique resource.

How can we motivate the community to submit results to the database?

- Submitting results to the thermalHUB Experimental Properties and Database will promote the visibility of each contributors' research.
- It is recommended that the data submission process will be based on standardized software that will be integrated into the thermalHUB structure with the purpose of facilitating efficient and fast data uploading.
- It is advisable to approach editorial boards and publishers of major periodical journals relevant to the heat transfer community to endorse the submission of new experimental data to the thermalHUB, and also to recommend to the authors to submit their data to thermalHUB at the time of manuscript submission. In the future journals could potentially use this process as a part of their peer review.

- During the planning grant period, we will solicit tutorials on thermal measurement methods and data from experts and post them on the Database as a means to attract contributions from the broad heat transfer community. In particular, in light of the many test techniques used to measure thermophysical properties of materials, the group felt that it would be beneficial to include tutorials on specific techniques to educate and assist the broader community with experimental measurements. First, we will post tutorials on general methods covered in ASTM standards which are generally utilized with bulk materials analysis. The different test methods will be compared and contrasted, showing strengths and weaknesses of each. thermalHUB will work with academia, government labs, and industry to present these tutorials which focusing on applications which are technologically relevant. Techniques will include hot wire methods for powders, flash diffusivity, differential scanning calorimetry, guarded heat plate, etc.
- In addition to tutorials for standard measurement techniques, we will also focus attention on newer methods which are broadly used in our community without the classification of being standardized. This will include methods such as the 3-ω, laser thermoreflectance, scanning probe methods, as well as a host of steady state and AC techniques which utilize unique material structures for property characterization. The purpose of this is to provide newcomers to the field with information on best practices and methods to implement these newer techniques in order to reduce sources of experimental error in their implementation. These tutorials will also assist in helping users select the best testing methodologies when measuring a new material. In addition, uncertainty analysis and issues giving rise to large uncertainties for each method will be explained. Finally, material microstructural information which will be beneficial to measure for samples along with the thermophysical properties will be discussed. Overall, the tutorials will be a tool to assist experimentalists in the generation of new data sets which are needed by the thermal community.

Who will manage and oversee the database?

- The Database needs to be user-driven in order to be sustainable.
- During the planning stage, staff support will be needed to develop standardized software for automatic formatting of the submitted data.
- The breakout group discussed the need for a Database manager who will oversee the data review process.

How will the submitted data be reviewed before the data are accepted officially into the database?

- Contributors will be encouraged to submit supplemental materials including descriptions of the measurement methods, original measurement data, and data processing procedures. All data will be reviewed by users of the Database.
- The Database will be divided into a two-tier structure. As-submitted data will be placed into one tier. Submitted data rated highly by the users will be officially accepted into another tier by the Database manager.

How can we engage the community to review the submitted results and use the database?

- The Database will serve as a convenient resource for the users to find reliable thermal properties data. The database should be searchable by type of material, property, measurement technique, and a general data 'quality' tag.
- It is important that early contributors set high standard for their submitted data.

Should round-robin tests be part of the initial prototype?

- The consensus reached by the experimental breakout session regarding round robin tests is that thermalHUB-sponsored round robin tests are a low priority at this time. The focus of the current efforts should be collecting and stockpiling existing databases and sources of data, both commercial and freely available. Also, investigators participating in round robin testing through organizations such as ASTM, NIST, ONR, etc. will be encouraged to post their data from these efforts on thermalHUB. When this data are assembled and can be evaluated, a need for a round robin test may be determined based on observations of discrepancies in the data for a particular type of material or experimental technique. In this way, the experimental properties and database can provide direction and guidance for future research efforts to collect particular data and develop and refine measurement techniques and procedures.
- There was discussion of including a thermal test structure for a Center for Integrated Nanotechnologies (CINT) Cantilever Discovery Platform. A design submission will be made at the end of 2007, and a thermal test structure can be added to the design by CINT researchers. CINT is a Department of Energy funded user facility, and fabricated chips are available to users for free once a proposal has been submitted and approved. Based on discussions with CINT staff, parts could be made available for thermalHUB round robin testing. Since a thermal test structure can be added to the current design at this time at no cost, it was viewed as an opportunity worth pursuing. Two membrane structures were discussed with: 1) Metal patterned to create a central heater with neighboring heater lines and 2) a four point probe, 3-omega structure. Leslie Phinney will communicate with CINT researchers in order to finalize a thermal test structure design for the CINT Cantilever Discovery Platform chip design.

What 'tags' should be used to describe and distinguish the content?

- Content type: data set, tutorial, data analysis tool, lecture, etc.
  Property: thermal conductivity, thermal diffusivity, heat capacity, thermal expansion coefficient, optical properties, etc.
- Experimental conditions: temperature range, pressure range, steady state, transient, etc.
  Technique: three omega, electrical resistance, photoacoustic, transient thermal reflectance, pump-probe, laser flash, ellipsometry, etc.

- Material type: metal, semiconductor, insulator, dielectric
  Processing details: LPCVD, evaporation, sputtered, CVD, etc.
  Test sample type: suspended membrane, microbridge, film, nanostructure, etc.
  Material: silicon, silicon dioxide, aluminum, gold, etc.

Breakout: International Partnerships

Group Members: Faruk Arinc, Stefan Bertsch (scribe), Andrei Federov, Eckhard Groll, Arvind Krishna, M. Pinar Mengüç (lead), Ray Viskanta,

The objective of the International Partnership theme is to determine effective ways of engaging the international community with the thermalHUB activities. Other than the obvious benefits of globalization and reaching wider audiences, the following benefits are expected:

- Through thermalHUB, accessibility to information will be easier by a wider community of researchers, who will eventually contribute more to thermal sciences.
- It will be easier for US researchers to find better and more qualified students.
- International interactions will accelerate the identification of new problems and new solution methodologies.
- International participation may help to sustain thermalHUB partially.
- thermalHUB will help in finding better ways of teaching courses in different international academic institutions
- Face-to-face and virtual thermal science conferences can be tied to thermalHUB, which will allow wider on-line participation and savings in publication and meeting costs.
- International industry, which is more application oriented, will benefit from recent and more extensive research findings available through thermalHUB.

The following specific questions were asked by the group members. The discussions surrounding these questions will lead our future efforts on international partnerships:

Why do we want to emphasize international partnerships?

- There is significant thermal science research and development activity in the United States; yet, in many international institutions, academic and industrial, there is also substantial amount of fundamental and applied research being carried out. It is to the benefit of all researchers, in the US and overseas, to collaborate and share their research findings. With the globalization of trade, there is more need to have international partnership to enhance scientific and engineering understanding and development. We believe that thermalHUB will allow this integration in a seamless manner.
- With the help of thermalHUB, we will be able to establish an infrastructure for collaboration. Accessibility to information, at any time, at any place, in consistent way will enhance the activities of each and every researcher. In addition, thermalHUB will help in the development of new joint research projects with different groups.

- Thermal sciences research in the US has always benefited from the infusion of international graduate students. thermalHUB will allow inspiring students all over the world to find mentors in the US academic institutions. By the same token, many US engineering students will become aware of the research and job opportunities all around the world. Information within thermalHUB will allow them to collaborate with other groups around the globe.
- With these possibilities on the horizon, the international activities of thermalHUB will be crucial to its success and sustainability.

Which international academic/research institutions and universities are likely to take part in our collaborative efforts? (where to start)

- thermalHUB is all-inclusive. We will encourage all academic and industrial institutions, in the US or in any other part of the world, to use its resources extensively. We are hoping that in the long run the research and education partnerships will be started by individual researchers who are part of the thermalHUB community. However, in the beginning, we will encourage all the participants to actively pursue joint research and education activities using the thermalHUB platform.
- To this end, we plan to combine the existent research and education collaborations with our thermalHUB activities. These initial partnerships will serve as demonstrative examples of collaborations, but they will not be limiting at all.
- The education partners of Purdue University, University of Kentucky, Karlsruhe University, and Middle East Technical University, and industrial partners of Delphi will be among to first attempt of these partnerships (just because of the affiliations and interests of the group members.)

How should we inform the community about the international partnerhip activities of thermalHUB?

- We will send an informative e-mail to all research and education institutions outlining our plans (and hopes) for international partnerships through the thermalHUB platform. The International Centre for Heat and Mass Transfer (ICHMT) will be an important part of this phase of community awareness activities. Dr. Arinc will lead the way to inform all researchers participating in the ICHMT conferences. In addition, we will give short presentations about the thermalHUB activities at every International conference run by ICHMT, ASME and other professional societies.

How can we make the “hub” attractive to other countries?

- It is important to make thermalHUB useful, relevant and attractive so that it can be sustained over the years. This requirement is not only for the US contributors, but also for all international participants. We should emphasize that: (a) the content is always compelling, (b) the provided information is selective and coherent (no information overload); (c) the content is always dynamic (compared to static textbooks); (d) the hub is democratic due to its rating and open access approach; (e) provide new ideas for future international partnership and participations.

How can establish meaningful and potentially sustainable relationship between thermalHUB and different international funding agencies?

- It is important to assure the sustainability of thermalHUB in the long run. This requires extensive support of its activities and the recognition of its usefulness to the research community. By showing the value of the research and education tools available to both the academic and industrial institutions, we will prove the broader impact of the thermalHUB platform.
- We are hoping that the international funding agencies will recognize the impact of thermalHUB to their communities, and will allow additional funding for their students, researchers, and industrial partners to continue contributing to thermalHUB in the coming years.

How can we combine our cyber efforts with education in non-US programs?

- With the use of the thermalHUB platform, we will increase awareness of new research and education tools. thermalHUB could also allow the sharing of course resources so that undergraduate students can take courses while they attend other universities.

Is there any reason/way to explore the potential of thermalHUB for mechanical (and other) engineering programs in non-US universities?

- Fundamental and applied thermal science research and education efforts are related to many engineering problems that are crucial in different international locations. We anticipate that thermalHUB will enhance research on energy, food processing, medical and pharmaceutical applications, electronics cooling, and nanoscale engineering, among others. In several countries, researchers who work on these challenging problems do not have a convenient resource to help them for the thermal science issues. Availability of the research and educational content in thermalHUB will allow them to solve their problems more efficiently, and meanwhile it will foster the new international collaborations.
- thermalHUB can also enable the wide-spread use of codes and standards around the globes in a consistent way. Initially this effort will be passive, indicating different web pages about the existent codes and standards. We anticipate that in the long run the availability of coherent information will motivate further collaborations toward standardization of international codes.

How will we measure the success and impact of international partnerships?

- It is important to have quantitative data to discern the effectiveness of our activities in international partnership with the thermalHUB platform. We will monitor the impact of our activities during the next few years by counting (a) the hits from other countries, b) the amount of content provided by the international academic and industrial organizations, c) the number of actual partnerships started with the help of thermalHUB, (d) the citations and publications resulted from thermalHUB-related activities.

What are the potential pitfalls in international partnerships?

- Cultural sensitivity is crucial in posting different messages on thermalHUB. We will monitor potential problems that could be caused by language differences. In addition, international differences in intellectual property rights need to be addressed, and potential international legal issues should be ironed out. However, we note that, as for the nanoHUB model and other web-based technical communities, the responsibilities regarding intellectual property and copyright issues will rest with individual users through a Terms of Use agreement with each user (see http://thermalhub.org/content/21?task=view).

Breakout: Industrial Partnerships

Group Members: Dick Chu, Suresh Garimella (lead), Jay Gore, Brian Iverson (scribe), Mark Juds, Frank Mason

What do you view as industry's role in the thermalHUB?

- Industry users can post tutorials and/or case studies as learning tools for researchers/students
- A corporation may be willing to host (with other industry leaders) a 2-day seminar to define state of the art for thermal management technology and design practice:
    - Record and post presentations
    - Possibly introduce the field to different audiences (K-12, university, …)
- Industry may not be a primary target, but it can help to sustain the effort. Tying them in early and along the way may be necessary.
- The industrial component should not compete or duplicate efforts of others; rather, it should involve others with similar thrusts.

What can thermalHUB do for industry?

- It may provide a corporate library of sorts, especially to smaller companies.
- Thermophysical property databases are very important all through the design process.
- It could provide software design tools, simulation tools, models, etc., and simple analysis tools that can reduce computation/analysis time.
- It may provide the ability to look up and connect to researchers working in a given area, i.e., a virtual community.
- It may provide a forum for comparing notes to arrive at the best methods or improve existing tools.
- New experimental techniques and corresponding results could be posted, e.g., non-intrusive temperature measurements.
- It should provide a link / resource where similar research could be done or is currently being done.

How should we inform/reach industry?

- Consider using sponsored conferences / tradeshows, press releases, trade magazines, … to promote and find contributors.
- Consider a "show and tell" tour in key regions.
- Tap into thermal interest groups that have monthly meetings, e.g., the Corporate Cooling Council at IBM.
- Through introduction of thermalHUB in classroom settings to students who will later work in industry.
- Begin work with existing strong connections (CTRC example) and recruit other academics with strong existing connections in other sectors (energy/fuel cells, etc.).
- Focus on a few industry sectors early on even for impact, though the academic work may be broad all along.

How can we attract industry?

- Important and relevant information is really what will draw them.
- Consider an email progress report/newsletter to key persons and groups.
- Define a metric to determine whether or not we are connecting with industry.
- Can thermalHUB be all things to all people?
    - Yes in the long run, but maybe early on we focus on a few sectors where we have more connection (including international ties, graduate student participation) and then build from there.

Which companies should we connect with?

- Consider starting with the larger companies who have thermal groups.
    - Intel, AMD, HP, Apple, Microsoft (data center cooling), GE, Siemens
- Contact Air Force Materials Lab (AFM) at Wright Patterson and similar other places. They have been charged with disseminating property data.
- Contacting companies should come after substantive content has already been posted.
- Need to have a few ambitious and achievable targets. Sandia has been running a "challenge" program.
- Short term goals and long term vision.

What can industry do for the thermalHUB?

- Major companies could consider equipment donations as the effort develops.
- A group of companies could put together a tutorial seminar set regarding the state of the art for the thermal design.
- Post industrial case studies

- It is understood that industry should offer support and not simply expect free benefits.

Conclusion

Based on the foregoing breakout reports, a list of short-term (i.e., 6-month) action items will be established by the thermalHUB Executive Committee. This list will guide the thermalHUB development activities through Summer 2008, when a panel session and associated meetings will be held at the Summer Heat Transfer Conference to assess progress to date and to establish a new set of action items.

Appendix: Workshop Agenda

Dates: 10-11 December 2007

Location: Purdue University, West Lafayette, IN USA

Day 0: 9 December 2007 (Sunday)

Visitors arrive by evening

Day 1: 10 December 2007 (Monday)

Morning (7:30 am to noon)—Burton D. Morgan Center

0730-0800	Registration and continental breakfast
0800-0815	Welcome
	Leah Jamieson, John A. Edwardson Dean of Engineering
	George Adams, Associate Director for Programs, Network for Comp. Nanotechnology
0815-0830	Introductions, and workshop format and goals (T. Fisher)
0830-0900	Examples of successful cyberinfrastructure (G. Klimeck)
0900-1000	Tutorial on Powerpoint voice-overs and Rappture (M. McLennan)
1000-1015	thermalHUB CI demonstration (M. McLennan)
1015-1030	Break (including opportunity for attendees to register on thermalHUB)
1030-1200	Moderated panel discussion on community needs
	5-minute overviews of theme areas
	Cyberinfrastructure: M. McLennan
	Computational Research Tools: J. Lukes
	Computational Learning Tools: T. Fisher
	Online Lectures and Tutorials: C. Grigoropoulos
	Community Wiki: G. Walker
	Properties Database & Experimental Network: L. Shi
	International Partnerships: P. Menguc
	Industrial Partnerships: S. Garimella
	Group discussion (T. Fisher-moderator)

Lunch

1200-1330	Birck Nanotechnology Center atrium

Afternoon (1:30 pm to 5:00 pm)—Burton D. Morgan Center

1330-1345	Explanation of breakout session purpose and format (T. Fisher)
1345-1500	Breakout sessions in theme areas—Breakout rooms in Morgan and Birck Centers
	Panelists to lead question-guided discussions
1500-1530	Break
1530-1630	Breakout session, writing of brief reports from breakout sessions
1630-1700	Delegate survey/questionnaire (G. Walker)
1700-1800	(optional) Tour of Birck Nanotechnology Center (B. Cola)

Evening Dinner and Reception—Birck Nanotechnology Center

1800-2100	Dinner, with invited speaker (T. Sands, BNC Director)

Day 2: 11 December 2007 (Tuesday)

Morning (7:30 to 11:30 am)—Burton D. Morgan Center

0730-0800	Continental breakfast
0800-0930	Summary presentations from each breakout group
0930-1000	Break
1000-1030	Summary of survey results (G. Walker)
1030-1130	Final feedback from attendees, action items, concluding remarks (T. Fisher)

Lunch

1130-1300	Box lunch, in Birck Nanotechnology Center atrium

Afternoon (1:00 pm to 3:00 pm—Coordinating Committee only, including the Advisory Board and Executive Committee)—Birck Nanotechnology Center

1300-1500 Meeting of the Coordinating Committee

- Committee charter and organization (Fisher)
- Meeting frequency and communications protocols (Fisher)
- Establishment and certification of user policies (McLennan, Walker)

Appendix: List of Workshop Participants

Adams	George	Purdue University
Alexeenko	Alina	Purdue University
Arinc	Faruk	Int'l Centre for Heat and Mass Transfer
Bergman	Ted	University of Connecticut
Bertsch	Stefan	Purdue University (student)
Buterbaugh	Kevin	Vanderbilt University
Cahill	David	University of Illinois
Chu	Dick	IBM
Cola	Bara	Purdue University (student)
Dames	Chris	UC Riverside
Fedorov	Andrei	Georgia Tech
Fisher	Timothy	Purdue University
Frenkel	Michael	NIST
Fuller	Joan	AFOSR
Garimella	Suresh	Purdue University
Go	David	Purdue University (student)
Gore	Jay	Purdue University
Graham	Samuel	Georgia Tech
Grigoropoulos	Costas	University of California, Berkeley
Groll	Eckhard	Purdue University
Gschwender	Lois	Air Force Research Laboratory
Huxtable	Scott	Virginia Tech
Iverson	Brian	Purdue University
Juds	Mark	Eaton Corporation
Krane	Matthew	Purdue University
Krishna	Arvind	Delphi
Li	Deyu	Vanderbilt University
Lukes	Jennifer	University of Pennsylvania
Mason	Frank	CINDAS LLC
Mchale	John	Purdue University (student)
McLennan	Michael	Purdue University
Menguc	Pinar	University of Kentucky
Mohamad	Abdulmajeed	University of Calgary
Murthy	Jayathi	Purdue University
Pepper	Darrell	University of Nevada, Las Vegas
Phinney	Leslie	Sandia National Laboratories
Pilon	Laurent	UCLA
Roberts	Nicholas	Vanderbilt University (student)
Roy	Ajit	Air Force Research Laboratory
Ruan	Xiulin	Purdue University
Sands	Tim	Purdue University
Sathe	Abhijit	Purdue University (student)
Sayer	Robert	Purdue University (student)

Setlak	Stan	CINDAS LLC
Shi	Li	University of Texas, Austin
Snyder	Carl	Air Force Research Laboratory
Tackett	Alan	Vanderbilt University
Viskanta	Ray	Purdue University
Walker	Greg	Vanderbilt University
Wang	Evelyn	MIT
Witt	Michael	Purdue University
Xu	Xianfan	Purdue University
Yazawa	Kazuaki	Sony Corporation
Yerkes	Kirk	Air Force Research Laboratory
Zheng	Yuan	Purdue University

Appendix: NSF Proposal Team

- Gang Chen (MIT)
- Chris Dames (UC-Riverside)
- Andrei Fedorov (GaTech)
- Timothy Fisher (Purdue)
- Suresh Garimella (Purdue)
- Costas Grigoropoulos (UC-Berkeley)
- Scott Huxtable (VaTech)
- Deyu Li (Vanderbilt)
- Jennifer Lukes (Penn)
- Arun Majumdar (UC-Berkeley)
- Michael McLennan (Purdue)
- Pinar Menguc (Kentucky)
- Jayathi Murthy (Purdue)
- Laurent Pilon (UCLA)
- Xiulin Ruan (Purdue)
- Li Shi (UT-Austin)
- Raymond Viskanta (Purdue)
- Greg Walker (Vanderbilt)
- Xianfan Xu (Purdue)