SC2008 Tutorial Proposal

Interoperable Mesh and Geometry Tools for Advanced Petascale Computing

Presented by
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Abstract

Today©s simulations often need advanced software tools to manage the complexities associated with sophisticated geometry, mesh, and field manipulation tasks, particularly as computer architectures move toward the petascale. In this tutorial, we will teach participants about a suite of such tools specifically designed for parallel computation by the Center for Interoperable Technologies for Advanced Petascale Simulation (ITAPS). We start with an overview and introduction of our technology development philosophy which is that such services can be provided as libraries that can be used with minimal intrusion into application codes. We briefly describe several available services including dynamic partitioning, mesh adaptation, mesh quality improvement, and front tracking. Underlying these services are a common data model and interfaces that are key to providing uniform access to all tools. We will teach attendees basic use of the interfaces through simple examples and provide advice on best practices for use of ITAPS software.

Description

Goals and Target Audience. The primary goal for this tutorial is to introduce application scientists to tools and libraries that are available for advanced mesh, geometry, and field manipulations on large-scale parallel computers. These scientists will either have an application code in hand or be planning the development of an application that requires techniques such as adaptive mesh refinement or front tracking to help them reach their scientific goals. The first part of the tutorial will introduce the audience to the wide variety of available software libraries that provide such services and include examples of their use in application codes. The second part of the tutorial will target application scientists who are interested in more details of the ITAPS philosophy and who may be ready to try one or more of the available tools. The detailed discussion of ITAPS interfaces and the hands-on exercises are aimed primarily at this group, but will also give those new to ITAPS technologies a clear view of what's involved in writing, building, and using these packages.

Content Level. 30% beginner, 45% intermediate, 25% advanced

Audience Prerequisites. Attendees should have familiarity with the numerical solution of PDEs on distributed memory computers. Examples will be shown in various programming languages, including Fortran, C, and C++ so specific language background should not matter. To participate in the hands-on portion, a computer with a unix-like operating system and a CD drive is required for software installation. Resources permitting, we are also planning to provide an off-site tutorial server for downloading and building software to ensure a controlled and consistent work environment. All examples will also be projected on the front screen for those without computer or network access.

Duration. Full day is preferred, although this tutorial can be given as either a half or full day. If selected for a half day tutorial, we will focus on the introductory material, and provide an abbreviated description of the interfaces and their use in applications. The hands-on portions of the tutorial will be eliminated.

Relevance. The advent of petascale computing will enable increasingly complex, realistic simulations of PDE-based applications. Numerous software tools are used to help manage the complexity of these simulations, including computer-aided design systems used to represent the geometry of the computational domain, advanced mesh generation tools to discretize those domains, solution adaptive methods (AMR) to improve the accuracy and efficiency of simulation techniques, and parallel tools such as dynamic partitioning to ease implementation on today's computer architectures. However, managing the complexity of interactions between these services on distributed memory comptuers is becoming increasingly difficult, leaving developers little time to focus on the science of their applications. The ITAPS center focuses on providing tools to fill specific technology gaps, along with underlying interfaces providing interoperability between these tools. Mesh- and geometry-based tools which enable PDE simulation continue a trend towards high-performance libraries started by solvers, and we believe these tools will have similar influence on application scientist productivity. We will demonstrate this using examples from applications ranging from accelerator and fusion modeling to nuclear reactor and groundwater flow simulations. These examples will show how scientists are leveraging ITAPS technologies to increase their simulation accuracy, allow them to operate more effectively on complex computational domains, or reduce the total time to solution.

Brief Description of Tutorial.

The tutorial is divided into 6 basic modules as described below:

1. *Overview and introduction:* Introduces students to the need for advanced mesh and geometry libraries for parallel simulation and provides example that motivate their use. We discuss the ITAPS philosophy; namely that such services can be provided in an interoperable way that provides maximum flexibility to the application programmer. We compare the ITAPS approach with other commonly used software development methods.

2. *ITAPS data model: W*e introduce the ITAPS data model and its three core interfaces for mesh geometry, and fields along with the parallel data model for partitions. This abstract data model is based on information flow in PDE simulations and supports a wide array of technologies and usage scenarios. We also describe how the core data types associate with each other through the concept of data relation managers and the building blocks within the data types: namely entities, entity sets, parts, and tags.

3. *ITAPS interfaces:* A set of common interfaces that all tools and implementations support is the key component of our design philosophy for interoperable tools. We do not enforce any particular data structure or implementation with our interfaces, requiring only that certain questions about the geometry, mesh, or field data can be answered through calls to a common interface. We provide examples of accessing basic information through these interfaces using both arrays and iterators, how to modify the underlying database, and what is needed to support parallel computations. Finally, we discuss the design decisions made to support language interoperability through both a C interface (which interoperates with C, C++, and Fortran) and through SIDL/Babel (which provides additional interoperability with Java and Python).

4. *ITAPS services and tools:* There are two basic models for use of ITAPS tools in applications and we give a high level description of each. We describe several mesh and geometry services that are available for use including dynamic partitioning, mesh adaptation, front tracking, and mesh quality improvement. In each case we give examples of how applications can benefit from their use.

5. *Using ITAPS: Approaches & Experience*: We provide several case studies of use of ITAPS interfaces in advanced application settings. The first focuses on the insertion of ITAPS mesh adaptation software into a fusion simulation, the second on the use of several ITAPS tools in concert for shape optimization of accelerator cavities, and the third on the development of a new application for nuclear reactor modeling, Based on these and other applications, we provide a list of 'best practices' for use of ITAPS interfaces and software.

6. *ITAPS software:* We provide the necessary information for students to download, use and build ITAPS implementations and tools. We give the status of the available software and show examples of developing and testing a user-specific ITAPS implementation.

Hands-on exercises. A series of individual exercises utilizing ITAPS interfaces and tools in PDE simulations on parallel computers, described in detail below.

Coordination of the Presentation. The ITAPS team has been working together since July of 2001 and has been working to develop tutorial materials since November of 2005. Since that time we have given two half day tutorials at the CCA quarterly meeting (Jan 2006) and the SciDAC 2007 conference (July 2007) which were both positively received by participants. We plan to give two additional half day tutorials before SC08: one at the SciDAC 2008 meeting (July 2008) and the second at the ACTS toolkit meeting (Aug 2008). During this period, we have developed slide materials that are consistent across different presenters; all slides follow the same template for visual consistency, and are presented as a single file from one laptop so that there are no interruptions due to switching of presentations or computers. For each tutorial given to date, we have requested and received feedback and refined our material to reflect this input.

Development Plans. Our tutorial continues to evolve as new technologies and interfaces are defined by various ITAPS working groups. The most substantial addition for SC08 will be a detailed description of the interfaces needed for parallel mesh services. Our hands on exercises will be updated to reflect these additions as well. In the description of ITAPS services, we will focus more heavily on their use in distributed memory environments as well as their performance on large-scale machines.

Description of Hands-On Exercises

Content. Roughly two hours of the tutorial is devoted to a series of in depth examples and hands-on exercises through which the participants will gain a good understanding of the ITAPS data model, interface design philosophy and use of ITAPS implementations and tools in basic applications. At the last hour of the morning session, participants will download, assemble and build a simple "Hello ITAPS" application using a predefined, prebuilt implementation. This ensures they understand the basic structure of an ITAPS application and provides the building block for later exercises. Once this is working correctly, participants will be able to develop a simple driver application that accesses simple mesh information such as vertex coordinate locations and element adjacency information using both array and iterator access. More advanced exercises included for the afternoon hands-on session, include the use of the data relations manager interfaces to work with geometry and meshes together, the use of the parallel interfaces to access off-processor information, and an example use of one of the ITAPS services (for SC08 we will focus on mesh partitioning). We do not expect participants to complete all of these exercises in the time given, but rather to focus on the one or two of most interest to them. Finally, for participants interested in creating their own ITAPS implementation to take advantage of ITAPS tools for their application, we provide a framework and step by step instructions for building and testing the compliance of the implementation. The participants are encouraged to work at their own pace, and to choose the exercises that particularly interest them. A written "Hands-on Guide" will provide detailed, step-by-step instructions for each exercise. The planned exercises are as follows:

1) Assembling an ITAPS application "Hello ITAPS" (from pre-built components)
2) Accessing basic mesh information: vertex coordinate information
3) Accessing basic mesh information: element adjacency information
4) Accessing off processor information in parallel meshes
5) Using an ITAPS service (partitioning a mesh)
6) Using meshes and geometry together: data relations manager
7) Creating an ITAPS implementation and compliance testing

Development Plans for SC08. Many of these exercises have been provided in the past as in depth examples as part of the lecture portion of the ITAPS tutorial. For SC08, we will develop the associated software modules as tutorial material and provide written documentation in the Hands-on Guide.

Presentation Approach. The most effective approach to a hands-on session is to provide the participants with a complete set of written instructions and let them work at their own pace. Instructors roam the room, both answering questions and simply checking on student progress to insure that they're not getting stuck. Some participants will naturally form small groups (2-3 people) to work together on the exercises, while others will work on their own. Participants can pick and choose among the exercises based on their level of experience and interests.

Facilities. To ensure the best use of time during the hands on portion of the tutorial, we request that all participants have a computer with a unix-like operating environment and a CD drive. We will provide all examples, a pre-built implementation, and the Hands-on Guide on CD to participants. We will also endeavor to provide an off-site tutorial server available and provide guest accounts that allow students to work in a more controlled environment. For those that do not have computer or network access we will project the examples on screen and work through them with students providing input.

Detailed Outline of Tutorial

Morning Session

1. Overview and introduction *(lecture format)*
    a. The need for advanced mesh and geometry libraries for parallel simulations
    b. Motivating examples
    c. Overview of the ITAPS philosophy
    d. Comparison with other development approaches
2. ITAPS data model *(lecture format)*
    a. Core data types: Meshes, Partitions, Geometry, and Fields
    b. Basic Building blocks: Parts, Entities, Entity Sets, and Tags
    c. Managing the relationships between core data types
    d. Parallelism in the ITAPS data model
3. ITAPS interfaces *(lecture format)*
    a. Design philosophy and basic tenets
    b. Accessing global (or meta) information
    c. Accessing local information using arrays and iterators
    d. Modifying the underlying parallel database
    e. Parallel operations (communication, ghosting, etc)
    f. Language interoperability through the C interface and through SIDL/Babel
4. Hands-on session: Exercises 1-3 of previous section (Hello ITAPS, information query)

Afternoon Session

5. ITAPS services and tools *(lecture format)*
    a. Two models for ITAPS use in applications
    b. Available ITAPS services (dynamic partitioning, mesh adaptation, front tracking, mesh quality improvement)
    c. *Examples of impact on applications*
6. Using ITAPS: Approaches & Experience *(lecture format)*
    a. Case Study 1: New application for nuclear reactor modeling
    b. Case Study 2: Inserting adaptive mesh refinement into a fusion simulation
    c. Case Study 3: Using several tools in concert for shape optimization of accelerator cavities
    d. Best practices for use of ITAPS software and interfaces
7. ITAPS software *(lecture format)*
    a. Accessing, downloading, and building ITAPS implementations
    b. Accessing, downloading, and building ITAPS services
    c. ITAPS compliance testing
8. Hands-On Session: complete exercises 1-3 of previous section, continued work on advanced exercises 4-8

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Education

- Ph.D., Computer Science, Rensselaer Polytechnic Institute, 1994. Advisor: Joseph Flaherty.
- M.S., Computer Science, Rensselaer Polytechnic Institute, 1989.
- B.S., Computer Science, Wilkes University, 1987.

Professional Experience

- Principal Member of the Technical Staff, Sandia National Laboratories, 2000-present.
  Principal investigator: Zoltan Partitioning and Dynamic Load-Balancing project.
- Acting Manager, Computational Biology Dept., Sandia National Laboratories, 2006-2007.
- Senior Member of the Technical Staff, Sandia National Laboratories, 1996-2000.
- Limited-Term Member of the Technical Staff, Sandia National Laboratories, 1994-1996.
- Research Associate, Computer Science Dept., Rensselaer Polytechnic Institute, 1990-1994.
- Database Programmer, Merck & Co., Inc., 1986-1987.

Research Interests

- Parallel computing, partitioning, load balancing, adaptive methods, graph and hypergraph algorithms, software design for scientific applications, finite element methods.

Tutorials and Invited Presentations

- Tutorial instructor, SciDAC2007: "Partitioning, Load Balancing and the Zoltan Toolkit" with E.Boman. Tutorial materials available at *http://www.cs.sandia.gov/ kddevin/papers/Zoltan_Tutorial_Slides.pdf*.
- Tutorial instructor, SC2001: "Parallel Partitioning Software for Static, Adaptive, and Multi-phase Computations" with G. Karypis.
- SIAM 2008 Annual Meeting Plenary Speaker.
- SciDAC2007 Plenary Speaker: "Partitioning and Dynamic Load Balancing for Petascale Applications."
- 2005 Salishan Conference on High-Speed Computing: "How to Program on 50,000 Processors."
- 2002 Workshop on Woomen in Applied Mathematics: Research and Leadership: "Load Balancing for Emerging Applications."
- 2001 Workshop on Object-Oriented and Component Technology for Scientific Computing: "Designing Data Management Tools for Parallel Applications."
- Sandia National Laboratories Software Engineering Seminar Series, 2005: "Toolkit Design and Zoltan."
- Sandia National Laboratories Summer Student Seminars, 2001, 2002, 2004.

Synergistic Activities

- Program Committee Member: SC 2008, IPDPS06.
- Minisymposium Organizer and/or Speaker: SIAM Annual Meeting 2008 and 1998; SIAM Parallel Processing Symposium 2008, 2006, 2004; SIAM Computational Science and Engineering 2007, 2005, 2003, 2001; US National Congress on Computation Mechanics 2001, 1999, 1997, 1995; PFEM 2000, PARA 1998, SC 1993.

Selected Papers

- U. Catalyurek, E. Boman, K. Devine, D. Bozdag, R. Heaphy, and L.A. Riesen. "Hypergraph-based Dynamic Load Balancing for Adaptive Scientific Computations." *Proc. Intl. Parallel and Distributed Processing Symp.*, 2007. **Best Algorithms Paper Award winner**.
- A. Pothen, A. Gebremedhin, F. Dobrian, E. Boman, K. Devine, B. Hendrickson, P. Hovland, B. Norris, J. Utke, U. Catalyurek, and M. Strout. "Combinatorial Algorithms for Petascale Science." *SciDAC Review*, Fall 2007.
- K. Devine, E. Boman, R. Heaphy, R. Bisseling, and U. Catalyurek. "Parallel Hypergraph Partitioning for Scientific Computing." *Proc. Intl. Parallel and Distributed Processing Symp.*, 2006.
- K. Devine, E. Boman and G. Karypis. "Partitioning and Load Balancing for Emerging Parallel Applications." *SIAM Parallel Processing for Scientific Computing,* Heroux, Raghavan, Simon, eds. SIAM, 2006.
- K. Devine and B. Hendrickson. "Tinkertoy Parallel Programming: a Case Study with Zoltan." *Internatl. Jrnl. Computational Science and Engrg.*, 2006.
- K. Devine, E. Boman, R. Heaphy, B. Hendrickson, J. Teresco, J. Faik, J. Flaherty, L. Gervasio. "New challenges in dynamic load balancing." *Appl. Numer. Maths.*, 52 (2005) 133-152.
- J. Shadid, R. Tuminaro, K. Devine, G. Hennigan, P. Lin. "Performance of fully coupled domain decomposition preconditioners for finite element transport/reaction simulations." *Jrnl. Computational Physics*, 205 (2005) 24-47.
- J. Teresco, K. Devine, and J. Flaherty. "Partitioning and Dynamic Load Balancing for the Numerical Solution of Partial Differential Equations." In *Numerical Solution of Partial Differential Equations on Parallel Computers*, Bruaset, Bjrstad, Tveito, eds. Springer-Verlag, 2005.
- K. Devine, E. Boman, R. Heaphy, B. Hendrickson, and C. Vaughan. "Zoltan Data Management Services for Parallel Dynamic Applications." *Computing in Science and Engrg.*, 4 (2002) 90-97.
- B. Hendrickson and K. Devine. "Dynamic Load Balancing in Computational Mechanics." *Comput. Methods Appl. Mech. Engrg.*, 184 (2000) 485-500.
- J. Shadid, S. Hutchinson, G. Hennigan, H. Moffat, K. Devine, A. Salinger. "Efficient Parallel Computation of Unstructured Finite Element Reacting Flow Solutions." *Parallel Computing*, 23 (1997) 1307-1325.
- K. Devine and J. Flaherty. "Parallel Adaptive hp-Refinement Techniques for Conservation Laws." *Appl. Numer. Maths.*, 20 (1996) 367-386.

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Research Interests

- Mesh Component Interfaces and Software
- Mesh Quality Improvement Techniques
- Adaptive Mesh Refinement
- Numerical algorithms and software
- Component Software Systems

Education

Ph.D.	Applied Mathematics, University of Virginia, 1992
M.A.M.	Applied Mathematics, University of Virginia, 1990
B.A.	Mathematics, Edinboro University of Pennsylvania, 1988

Professional Experience

3/06-present	Computational Mathematics Group Leader, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory (LLNL), Livermore, CA
8/03–present	Research Program Manager for the Office of Science and MICS Point of Contact, Center for Applied Scientific Computing, Lawrence Livermore National Laboratory (LLNL), Livermore, CA
10/02–8/03	Principle Member of Technical Staff, Computer Systems and Enabling Technologies Group, Sandia National Laboratories (SNL), Albuquerque, NM
1999-2002	Computer Scientist, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL
1999-2002	Fellow, Computation Institute, The University of Chicago, Chicago, IL
1994-1999	Assistant Computer Scientist, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL
1997, 1998	Lecturer, Mechanical Engineering Department, University of Illinois at Chicago, Chicago, IL
1992-1994	Postdoctoral Appointee, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL

Teaching Experience

- “ITAPS Tools for Geometry Mesh and Field Manipulation”, Co-Instructor, SciDAC ’07, Tutorials Workshop, MIT, June 2007
- “Terascale Simulation Tools and Technologies”, Co-Instructor, CCA Quarterly Meeting, San Francisco, January 2006
- “Adaptive methods”, Short course organizer, SIAM CSE 03, San Diego, February, 2003
- “Terascale Simulation Tools and Technologies”, ACTS Toolkit Meeting, Berkeley, CA 2003, 2004
- Lecturer, Mechanical Engineering Department, University of Illinois at Chicago, Chicago, IL, (1997, 1998)

Selected Publications and Presentations

Interoperable mesh and geometry tools for advanced petascale simulations, L.A. Diachin, A.C. Bauer, B. Fix, J. Kraftcheck, K. Jansen, X. Luo, M. Miller, C. Ollivier –Gooch, M.S> Shephard, T. Tautges, H. Trease, **Journal of Physics Conference Series, SciDAC 2007**, (Editor, David Keyes, et. al.), IOP Publishing, Volume 78, 2007.

Parallel Adaptive Simulations on Unstructured Meshes, M.S. Shephard, K.E. Jansen, O. Sahni, L.A. Diachin, **Journal of Physics Conference Series, SciDAC 2007**, (Editor, David Keyes, et. al.), IOP Publishing, Volume 78, 2007.

Parallel PDE-Based Simulations Using the Common Component Architecture, (with L. C. McInnes, B. A. Allan, R. Armstrong, S. J. Benson, D. E. Bernholdt, T. L. Dahlgren, M. Krishnan, J. A. Kohl, J. W. Larson, S. Lefantzi, J. Nieplocha, B. Norris, S. G. Parker, J. Ray, and S. Zhou), **Numerical Solution of PDEs on Parallel Computers** (Editors A. M. Bruaset and A. Tveito), Springer, pages 327-384, 2006.

Parallel Adapative Mesh Refinement, (with Richard Hornung, Paul Plassmann, Andrew Wissink), **Parallel Processing for Scientific Computing** (Editors Mike Heroux, Padma Raghavan, and Horst Simon), SIAM, pages 143-162, 2006.

A Comparison of Two Optimization Methods for Mesh Quality Improvement, (with Patrick Knupp, Todd Munson, Suzanne Shontz), **Engineering with Computers**, Volume 22, pages 61-74, 2006.

Parallel Components for PDEs and Optimization: Some Issues and Experience, (with Boyana Norris, Satish Balay, Steven Benson, Paul Hovland, Lois McInnes, and Barry Smith), **Parallel Computing**, 28(12), 1811-1831, 2002.

Tetrahedral Mesh Improvement Via Optimization of the Element Condition Number, (with Patrick Knupp), **International Journal for Numerical Methods in Engineering**}, Volume 53, pages 1377-1391, 2002.

Local Optimization-based Simplicial Mesh Untangling and Improvement, (with Paul Plassmann), **International Journal of Numerical Methods in Engineering**, Volume 49, Issue 1-2, July, 2000, pages 109-125.

A Cost/Benefit Analysis of Simplicial Mesh Improvement Techniques as Measured by Solution Efficiency (with Carl Ollivier-Gooch), **International Journal of Computational Geometry and Applications**, Volume 10, Number 4, 2000, pages 361-382.

Comparative Visualization Techniques to Analyze Aluminum Smelting Furnace Efficiency in a Virtual Reality Environment (with Tim Urness), to appear **Transactions of ASME, Journal of Manufacturing Science and Engineering**, submitted January 1999.

Interactive Simulation and Visualization of Massless, Massed, and Evaporating Particles (with Darin Diachin, Daniel Heath, Jim Herzog, William Michels), **Institute of Industrial Engineers Transactions**, Volume 30, Number 7, Kluwer Academic Publishers,1998, pages 621--628.

Tetrahedral Mesh Improvement Using Face Swapping and Smoothing (with Carl Ollivier-Gooch), **International Journal for Numerical Methods in Engineering**, Volume 40, J. Wiley and Sons, 1997, pages 3979--4002.

A Parallel Algorithm for Mesh Smoothing, (with Mark Jones and Paul Plassmann), **SIAM Journal of Scientific Computing**, Volume 20, No. 6, pp 2023-2040, 1999.

Collaborative Virtual Environments used in the Design of Pollution Control Systems (with Darin Diachin, Daniel Heath, James Herzog, William Michels, and Paul Plassmann), **The International Journal of Supercomputer Applications**, Volume 10.2, November 1996, pages 223--235.

The RSCG Algorithm on Distributed Memory Architectures, (with James M. Ortega) **Journal of Numerical Linear Algebra with Applications**, Volume 2(5), September-October 1995, pages 404-414.

The Scalability of Mesh Improvement Algorithms (with Mark Jones and Paul Plassmann), Algorithms for Parallel Processing (Editors Michael Heath, Abhiram Ranade, and Robert Schreiber), **IMA Volumes in Mathematics and Its Applications**, Volume 105, Springer-Verlag, 1998, pages 185--212.

A Comparison of Inexact Newton and Coordinate Descent Mesh Optimization Techniques, (with P. Knupp, T. Munson, and S. Shontz), **Proceedings of the 13th International Meshing Roundtable**, Williamsburg, VA, September, 2004.

The Mesquite Mesh Quality Improvement Toolkit, (with M Brewer, L. Diachin, P. Knupp, T. Leurent, and D. Melander), **Proceedings of the 12th International Meshing Roundtable**, Santa Fe, NM September, 2003.

A Survey of Optimization Software for Mesh Shape-Quality Improvement Problems (with Patrick Knupp, Todd Munson, and Suzanne Shontz), **Proceedings of the 11th International Meshing Roundtable**, May 2002.

Local Optimization-based Untangling Algorithms for Quadrilateral Meshes, (with Paul Plassmann) **Proceedings of the 10th International Meshing Roundtable**, Newport Beach, California, October 2001.

Tetrahedral Element Shape Optimization via the Jacobian Determinant and Condition Number, (with Patrick Knupp) **Proceedings of the Eighth International Meshing Roundtable**, Lake Tahoe, California, October, 1999.

Adaptive Multiresolution Visualization of Large Data Sets Using Parallel Octrees (with Ray Loy), **SC99 Conference Proceedings**, Portland, Oregon, November 1999.

A Computational Study of the Effect of Unstructured Mesh Quality on Solution Efficiency (with Michael Batdorf and Carl Ollivier-Gooch), **AIAA 97-1888**, 13th Annual AIAA Computational Fluid Dynamics Conference, Snowmass, Colorado, July 1997.

On Combining Laplacian and Optimization-based Mesh Smoothing Techniques, **Trends in Unstructured Mesh Generation**, ASME Applied Mechanics Division, Volume AMD-Vol 220, 1997, pages 37--44.

A Comparison of Tetrahedral Mesh Improvement Techniques (with Carl Ollivier-Gooch), **Proceedings of the Fifth International Meshing Roundtable**, Pittsburgh, Pennsylvania, October 1996, pages 87--100.

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Professor of Civil and Environmental Engineering

Honors and Awards

Samuel A. and Elisabeth C. Johnson, Jr. Professorship from Rensselaer Polytechnic Institute
Computational and Applied Sciences Award of the US Association for Computational Mechanics
Past President and Fellow of the US Association for Computational Mechanics
Fellow of the International Association for Computational Mechanics
Fellow of the American Society of Mechanical Engineers
Associate Fellow American Institute for Aeronautics and Astronautics
Best paper award for 1997 for the *Int. J. of Numerical Methods for Heat & Fluid Flow*
Editor of *Engineering with Computers*
Editorial Board Member: *Computer Methods in Applied Mechanics and Engineering, Int. J. for Numerical Methods in Engineering, International Journal Multiscale Computational Engineering, Computers & Structures, Integrated Computer-Aided Engineering*

Teaching: Professor Shephard has developed and taught courses in numerical methods and scientific computing at Rensselaer for nearly 30 years. He has developed and delivered a number of and has delivered short courses at SIAM, USACM, Meshing Round table, DOE SciDAC meetings as well as at other universities and for private groups. Topic covered in these various short courses include: finite element theory and methods, automatic mesh generation, adaptive finite element analysis, parallel mesh generation and adaptation, and simulation-based engineering.

Professional Contributions: Mark S. Shephard's professional activities have focused on technologies to improve the reliability and level of automation of advanced numerical simulations to support their application by engineers and scientist. His research activities have lead to well recognized and applied contributions on the areas of automatic mesh generation of CAD geometry, automated and adaptive analysis methods, and parallel adaptive simulation technologies. This research has been supported by government agencies (over 65 grants from 13 agencies) and industry (funding from 44 companies). Professor Shephard has published over 250 papers and graduated 24Ph.D's.

As part of his professional activities Mark S. Shephard founded Rensselaer's Scientific Computation Research Center that has brought together faculty form seven academic departments and three schools at Rensselaer to perform research on the development and application of advanced simulation technologies. These research activities have included collaborations with more that ten other universities over the past decade.

Mark S. Shephard is a co-founder, board member and technical advisor to Simmetrix Inc., a computer-aided engineering company dedicated to producing the technologies and associated software components to enable simulation-based engineering. Simmetrix is currently researching, developing and providing advanced simulation automation and simulation-based design technologies to CAE and Fortune 500 companies, and universities.

Fifteen Recent Publications

1. M. S. Shephard and E. S. Seol, "Flexible Distributed Mesh Data Structure for Parallel Adaptive Analysis", *Advanced Computational Infrastructures for Parallel and Distributed Adaptive Applications*, Wiley, 2008.
2. M.S. Shephard, M.A. Nuggehally, B. FranzDale, C.R. Picu, J. Fish, O. Klaas, J. Tourtellott and M.W. Beall, "Component Software for Multiscale Simulation", *Bridging the Scales in Science and Engineering*, Oxford University Press, 2008.
3. M.A. Nuggehally, C.R. Picu, M.S. Shephard and J. Fish, "Adaptive model selectionprocedure for concurrent multiscale problems", *Journal of Multiscale Computational Engineering*, 5(5):369-386, 2007.
4. L.-Q. Lee, V. Akcelik, S. Shen, L. Ge, E. Prudencio, G. Schussman, R. Uplenchwar, C. Ng, K. Ko, X-J. Luo and M.S. Shephard, Enabling technologies for petascale electromagnetic accelerator simulation, *Journal of Physics: Conference Series*, 78-012040, 5 pages, 2007.
5. J. Fish, M.A. Nuggehally, M.S. Shephard, C.R. Picu, S. Badia, M.L. Parks and M. Gunzburger, "Concurrent AtC coupling based on a blend of the continuum stress and the atomistic force", *Comp. Meth. Appl. Mech. Engng.*, 196:4548-4560, 2007.
6. Lankalapalli, S., Flaherty, J.E., Shephard, M.S. and Strauss, H., "An Adaptive Finite Element Method for Magnetohydrodynamics", *Journal of Computational Physics*, 225 (1):363-381, 2007
7. M.S. Shephard, K.E. Jansen, O. Sahni and L.A. Diachin, Parallel Adaptive Simulations on Unstructured Meshes, *Journal of Physics: Conference Series*, 78-012053, 2007.
8. L. Diachin, A. Bauer, B. Fix, J. Kraftcheck, K. Jansen, X. Luo, M. Miller, C. Ollivier-Gooch, M. S. Shephard, T. Tautges and H. Trease, "Interoperable mesh and geometry tools for advanced petascale simulations", *Journal of Physics: Conference Series*, 78-012015,6 pages, 2007.
9. De, S., Fish, J., Shephard, M.S., Keblinski, P. and Kumar, S.K., "Multiscale modeling of polymer rheology", *Physical Review E*, 74(3)030801(1)-030801(4), 2006.
10. Seol, E.S. and Shephard, M.S., "Efficient distributed mesh data structure for parallel automated adaptive analysis", Engineering with Computers, 22(3-4):197-213, 2006.
11. Dey, S., Datta, D., Shirron, J.J. and Shephard, M.S., "p-version FEM for structural acoustics with a-posteriori error estimation", *Comp. Meth. Appl. Mech. Engng*., 195:1946-1957, 2006.
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Timothy Tautges was trained in nuclear engineering with an emphasis on parallel computing. His two main research areas are hexahedral mesh generation and component-based application of mesh and geometry in scientific computing applications. After receiving his Ph.D. from the University of Wisconsin (thesis topic: parallel nuclear severe accident simulation), he worked on severe accident modeling at the CEC Joint Research Center, Ispra, Italy, and Sandia National Laboratories. Later he joined the Cubit mesh generation project at Sandia, where he performed research on unstructured hexahedral mesh generation. He ultimately lead the Cubit project for two and a half years, during which the project reduced the overall time to mesh for complex hexahedral meshes by over a factor of 3. He was responsible for the development and open-source releases of the Common Geometry Module (CGM) and a Mesh-Oriented datABase (MOAB). After moving to Argonne in 2006, Tim took on the responsibility for mesh and geometry infrastructure for the SHARP reactor simulation project. He also is the Argonne Principle Investigator on the SciDAC ITAPS project.

Professional Preparation

Ph.D., *Nuclear Engineering & Engineering Physics*, University of Wisconsin, 1990.

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Professional History

Computational Scientist, Argonne National Laboratories, 2006-present.

Adjunct Professor, Engineering Physics, University of Wisconsin, 2000-present.

Principal Member Technical Staff, Sandia National Laboratories, 1992-2006.

Visiting Scientist, CEC Joint Research Centre, Ispra, Italy, 1990-1991.

Research Interests

Hexahedral Mesh Generation, Component-Based Scientific Computing, CAD-Based Radiation Transport.

Selected Meshing Journal Papers

T. Tautges, P. Knupp, J. Kraftcheck, H. J. Kim, *Interoperable Geometry and Mesh Components for SciDAC Applications*, Journal of Physics Conference Series, 16:486-490, Institute of Physics Publishing, 2005.

M. Wang, T. Tautges, D. Henderson, L. El-Guebaly, X. Wang, "Three-Dimensional Modeling of Complex Fusion Devices Using CAD-MCNPX Interface", Fusion Science & Technology, Vol 47, No. 4, pp1079-1083, 2005.

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D. White, T. Tautges, “Automatic Scheme Selection for Toolkit Hex Meshing”, Int. J. Numer. Meth. Engr., 49, pp127-144, 2000.

T. Tautges, T. Blacker, S. Mitchell, “The Whisker Weaving Algorithm: A Connectivity-Based Method for Constructing All-Hexahedral Finite Element Meshes”, Int. J. Numer. Meth. Eng., 39, pp3327-3349, 1996.

Selected Conference Papers

T. Tautges, “Applications of the TSTT Geometry, Mesh, and Relations Interfaces”, SIAM Conference on Computational Science & Engineering (CSE07), Costa Mesa, CA, Feb. 19-23, 2007.

T. Tautges, H. J. Kim, “Parallel Hex Mesh Generation: An Overview”, SIAM Conference on Parallel Processing for Scientific Computing, San Francisco, CA, Feb. 22-24, 2006.

Short Courses Taught

“ITAPS Tools for Geometry, Mesh, and Field Manipulation” (co-instructor), SciDAC 2007 Tutorials Workshop, MIT, June 29, 2007.

“Geometry, Mesh Components for Scientific Computing”, 15th International Meshing Roundtable, Birmingham, AL, Sept. 17-20, 2006.

“Geometry”, 13th International Meshing Roundtable, Williamsburg, VA, Sept. 19, 2004.

“Geometry & CAD”, 12th International Meshing Roundtable, Santa Fe, NM, Sept. 13, 2003.

“Automatic Detail Reduction for Design-Based Mesh Generation”, 8th International Conference on Numerical Grid Generation in Computational Field Simulations, Honolulu, HA, June 2, 2002.

“Mesh Generation for High Performance Computing Part II: Mesh Generation for Massively Parallel-Based Analysis” (co-instructor), Supercomputing 2000, November 5, 2000.

“Geometry Issues in Mesh Generation”, 9th International Meshing Roundtable, New Orleans LA, October 2, 2000.

“New Advances and Open Issues in Hexahedral Mesh Generation”, 8th International Meshing Roundtable, Lake Tahoe CA, October 10, 1999.