Welcome Address – Scott A. Mitchell

Sandia National Laboratories - CSRI Workshop on Combinatorial Algebraic Topology (CAT): software, applications & algorithms
(by invitation only)
29–30 August 2009, Reception Evening 28 August
Hilton Santa Fe, NM
CAT Workshop

- Funders
  - CSRI, ASC, NNSA, DOE, U.S.A. taxpayer
  - Thuc Hoang (DOE), Njema Frazier (DOE)
  - Scott Collis (SNL)
- Organizers
  - Scott Mitchell (idea, proposal)
  - Shawn Martin (logo)
- Note takers – written summary
  - David Day
  - Janine Bennett
- Admin
  - Deanna Ceballos (financial)
  - Bernadette Watts (website)
- 39 Technical participants
  - 18 labs: 16 SNL, 1 LLNL, 1 LBNL
  - 20 univ
  - 1 commercial
# Computer Science Research Institute (CSRI)
CAT workshop’s sponsoring program

<table>
<thead>
<tr>
<th>Measure</th>
<th>2007</th>
<th>2008</th>
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<tbody>
<tr>
<td>Projects</td>
<td>14</td>
<td>3</td>
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<tr>
<td>Workshops</td>
<td>4</td>
<td>7</td>
</tr>
<tr>
<td>Visitors (Institutions)</td>
<td>102 (67)</td>
<td>106 (68)</td>
</tr>
<tr>
<td>Summer Students</td>
<td>43</td>
<td>34</td>
</tr>
<tr>
<td>Sabbaticals</td>
<td>3</td>
<td>2</td>
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<tr>
<td>% Hires having prior CSRI partnerships</td>
<td>73%</td>
<td>80%</td>
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Computer Science Research Institute (CSRI)

- Open environment
  - no guards, gates, guns
  - focus on publications
- Productive place to visit
  - faculty
  - post-docs
  - contracts
- Excellent experience for summer students
  - graduate and some undergrad
  - extensive overview lecture series
- Where I work
  - Scott’s NGC story
Since this is a reception talk…

“How I got interested in topology”

• Algebraic topology Cornell grad-school class – where are the pictures?
  – a doughnut, “applications”, … tried to forget all that, but it came back…
• Hex mesh generation circa 1990’s
  – Q: Given a quadrilateral mesh enclosing a volume, can you fill volume with hexahedra?
    ![Diagram of quadrilateral mesh to hexahedra]
  – Homology and hex-mesh existence proof
      (1993 P. Murdoch rediscovered hex dual = arrangement of surfaces)
      • ball: even #quadrilaterals = necessary and sufficient
      • non-ball w/ embedding in 3d: above +
        The cycles must have even length if they are null-homotopic in volume
      ![Diagram of dual arrangement]

How I got interested in topology

• Meshing circa 1990’s
  – template challenges -> existence proof -> template constructions
  
  tets diced into hexes to semi-structured hex transitions

  Robert Schneiders’s “open problem”

  1995 David Eppstein hexes = O(quads) template transition

  – various challenges for non-ball models -> decomposition by $H_1$ generators finesses in theory, but no tools to do it
  – hex mesh generation via topological arrangements
  – hex mesh improvement “swaps”
  – I could never get the geometry right for anything to be very useful for finite elements…

• 2000 Project leadership -> 2002 management - plead temporary insanity 😊
• 2007 returned to technical work
• 2008 looked around
  – dozens of SNL apps crying out for discrete combinatorial topological solutions!
  – topology community turned computational!

  – Form a small research team, Shawn Martin, David Day, Eric Boman.
  – Get funding for a workshop! Here we are!
CAT Workshop Motivation

- Time right for a CAT workshop
  - Other events
    - Linear algebra factorization
      - Applied Algebraic Topology Minisymposium at the Fifth European Congress of Mathematics, 2008. - 5 speakers
      - IMA shortcourse Applied Algebraic Topology 2009, Carlsson & Ghrist, Henry Adams (also CAT)
    - Computational Geometry, solid modeling
      - SoCG Symp. Comp. Geom, 2009 had 1-3 topo papers
      - CCCG Canadian Conf. Comp. Geom, few papers
    - Visualization, Morse-Smale theory
      - TopolInVis, 2009 Utah 23 talks, 2007 Germany, 2005 Slovakia
    - Math, Mark Brittenham’s “low dimensional topology conference page”
      - 11 annual events (regional?), 6 sessions at AMS meetings, 16 “other” events, 2009
      - http://www.math.unl.edu/~mbrittenham2/ldt/conf.html
      - Bring together researchers from different communities
      - all new to me… but even established groups within an area meet each other for 1st time.
      - Visualization, solid modeling, linear algebra, computational geometry, image analysis,

- Scope is discrete, computation, homology, Morse-Smale

- More CSRI-sponsored workshops possible
  - please send feedback, ideas!
CAT Workshop Goals

• Software, Applications, Algorithms
  – new univ-labs and univ-univ partnerships
    • many forms possible – opportunities on next 4 slides
      – software partnerships
        • Trilinos for parallel linear algebra over finite fields?
      – many SNL topology-ready applications
        • university partnerships to solve?
      – research partnerships
        • univ-labs, univ-univ
  – Identify open problems
    • handle on complexity, scalability
  – Community software plans
Software talks

- **Software**
  The Saturday morning session focuses on existing software efforts for combinatorial algebraic topology. The intended audience is those wishing to use their tools for research framework or application solutions.

- **Speakers are asked to address the following items**
  - scope, current and planned
  - capabilities, especially:
    - Betti numbers, homology generators, generators meeting application-specific criteria;
    - filtrations & Reeb graphs for sensitivity and transients;
    - Smith Normal Form factorization, other linear algebra capabilities
  - scalability
  - software maturity/usability
  - availability and usage models
  - please try to limit time on reduction, sampling, and initial complex generation
- 35 minutes = 25 talk + 10 discussion
Partnership opportunities, software (snapshots, not a workshop program overview)

- SNL topology-ready software
  - Trilinos large-scale parallel linear algebra
    - general purpose, templated types
    - Heidi Thornquist
  - Workshop answers whether either of these make sense:
    - Trilinos in LinBox or JPlex?
    - Trilinos over finite fields?

![Diagram](image)

- Algorithms
- Matrix Ops
- Scalar Ops

CTT homology
Computational Topology Trilinos
Betti numbers and generators

Trilinos

Anasazi/Belos
null-space, smith-normal form

Tpetra (embedded GMP,...)
Application talks

- **Applications**
  The Saturday afternoon session focuses on laboratory applications, especially those that are not currently using topology, but could. Format consists of an overview talk, together with a discussion session to explore what is possible. The intent is for application owners to engage topology experts for help in solving their problems, with the potential for longer term partnerships.

- **Speakers** are asked to address the following aspects of their applications:
  - geometry, if any
  - dimension: 3d, higher-d, arbitrary-d
  - questions needing solution methods
  - interesting structural features one would like to discover and compute

- **40 minutes = 25 talk + 15 discussion**
Partnership opportunities
(snapshots, not a workshop program overview)

- **SNL topology-ready applications**
  
  Red = talk or person at CAT Workshop
  
  - Morse-Smale for understanding combustion science
    - J. Chen, Ray Grout, Valerio Pascucci, Janine Bennett, David Thompson, ...
  
  - Fracture and fragmentation in meshes
    - Alejandro Mota
  
  - Foam material analysis
    - L. Romero
  
  - Solid Model decomposition and parameterization, defecturing
    - Tamal Dey (non-SNL). also SNL apps
  
  - Sensor networks;
    - R. Ghrist (U. Penn). also SNL apps
  
  - Topology in 2d image analysis
    - Kurt Larson, Carl Diegert
  
  - Discrete combinatorial optimization fitness landscapes (tentative)
    - Jean-Paul Watson, Shawn Martin
  
  - Manifold cutting on system of loops for dimensional reduction, in e.g. image analysis x-ray tomography, molecular conformations
    - Shawn Martin
  
  - Text analysis parameter sensitivity
    - Daniel Dunlavy
  
  - Critical infrastructure network security, Green Grid design
    - W. Hart
  
  - Transportation planning
    - C. Phillips
  
  - Radar and signals analysis
    - Michael Robinson (non-SNL). also SNL apps

Tamal Dey gen $H_1$

Shawn Martin molecular conformation dim. red.

void coalescence graphic from Marian et al. A. Mota

Reflective Particle Tag. K. Larson, C. Diegert
Algorithm talks

• **Algorithmics**
The Sunday morning session focuses on algorithmic challenges. The intended audience is those already familiar with the algorithm basics, rather than application owners.

• Speakers are asked to address one or more of the following aspects of their algorithmic approaches:
  – *algorithmic complexity*, including dependence on genus, dimension, number of vertices, number of simplices, coefficient ring, filtration size, and number of critical points.
    • What's the hope for explicit bounds, tight bounds, and improvements?
  – capabilities for sensitivity analysis and transient features, including Reeb graphs, filtrations, and new math structures
  – application-tailored solutions, e.g. homology generators with specific geometry or cardinality; cycle homotopies
  – visualization techniques that use topology
  – visualization techniques for understanding topology

• 35 minutes = 25 talk + 10 discussion
Labs topology research & development

- SNL
  - Topology for Statistical Modeling of Petascale Data, Jacobi Sets,
    - DoE Office of Science funded 2009
    - P. Pebay, Janine Bennett, David Thompson, M. Rojas, Valerio Pascucci
  - Computational Topology, ASC, homology algorithms and applications
    - Scott Mitchell, Shawn Martin, David Day, Erik Boman, Janine Bennett
    - Optimization manifold exploration, dimensional reduction, molecular conformations
      - Jean-Paul Watson, Shawn Martin
  - Visualization tools, SNL-Univ. Utah partnership to put V. Pascucci’s capabilities in SNL VTK/Titan framework
    - Jason Shepherd, Valerio Pascucci
  - ongoing proposals ...

- LLNL
- LBNL
Panel - summarize

- David Saunders
  Peer-Timo Bremer
  Dmitriy Morozov
  Shawn Martin
  Michael Robinson

- Questions
  - Rank applications in terms of low hanging fruit that topology can pluck.
  - What are the key open problems, or main roadblocks, for advancing algorithms?
    - In particular, comment on scalability, and techniques for high dimensional data. In particular, comment on generalizations of filtrations
  - What new software or software mechanisms/structure would most benefit the community?
    - "New software" means, what techniques would be valuable to have in accessible and general purpose format such as LinBox and Plex? "mechanisms/structure" means, would an open-source effort be helpful? And should general and available versions be developed of Reeb graphs, complex generation methods, or anything else in particular?
Conclusions

• You are at 7,000’ elevation
  – May be hard to sleep
  – Wear sunscreen
  – Drink lots of water
  – Enjoy the guacamole!

• Talk, discuss, meet, participate, brainstorm!

• Slideshow