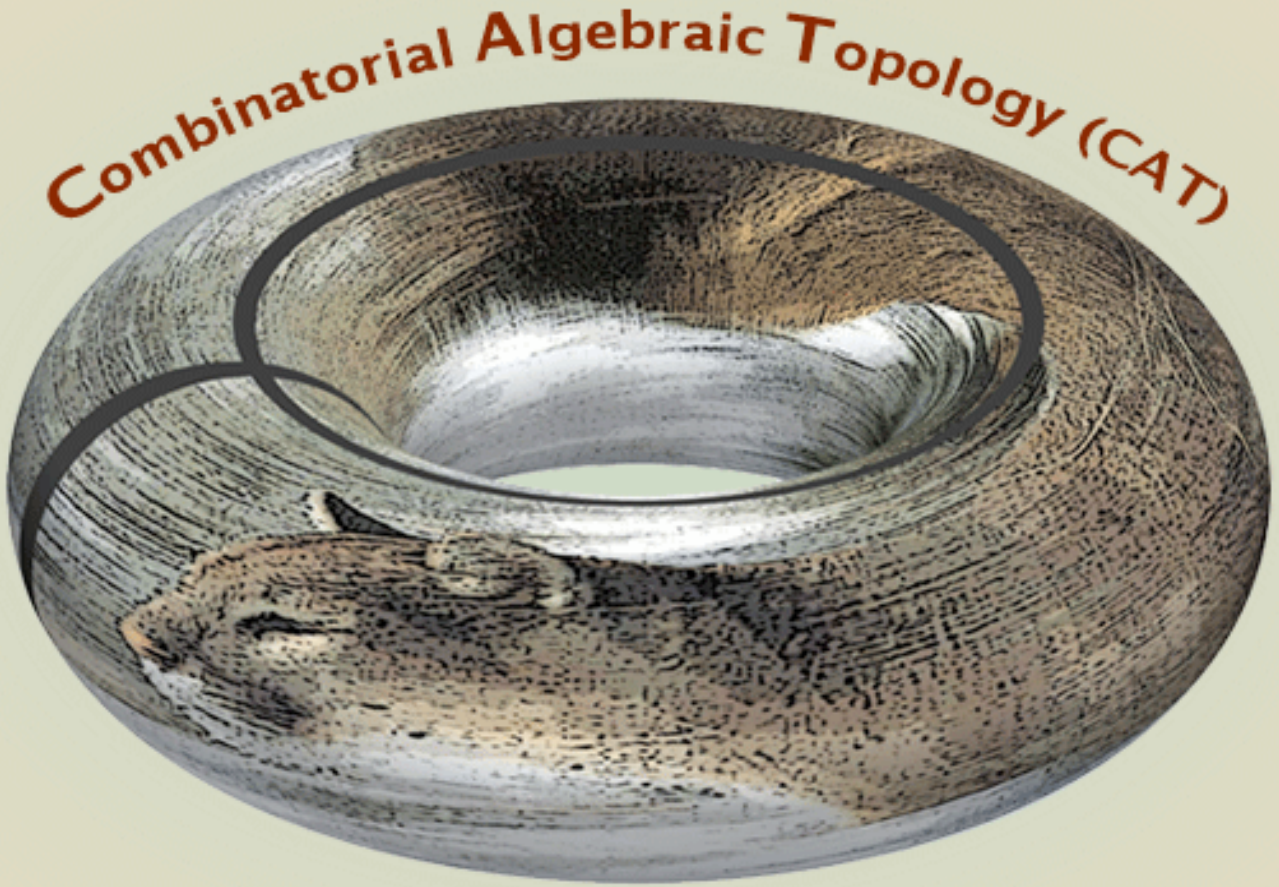


Welcome Address – Scott A. Mitchell

Sandia National Laboratories - CSRI Workshop on

Combinatorial Algebraic Topology (CAT): software, applications & algorithms

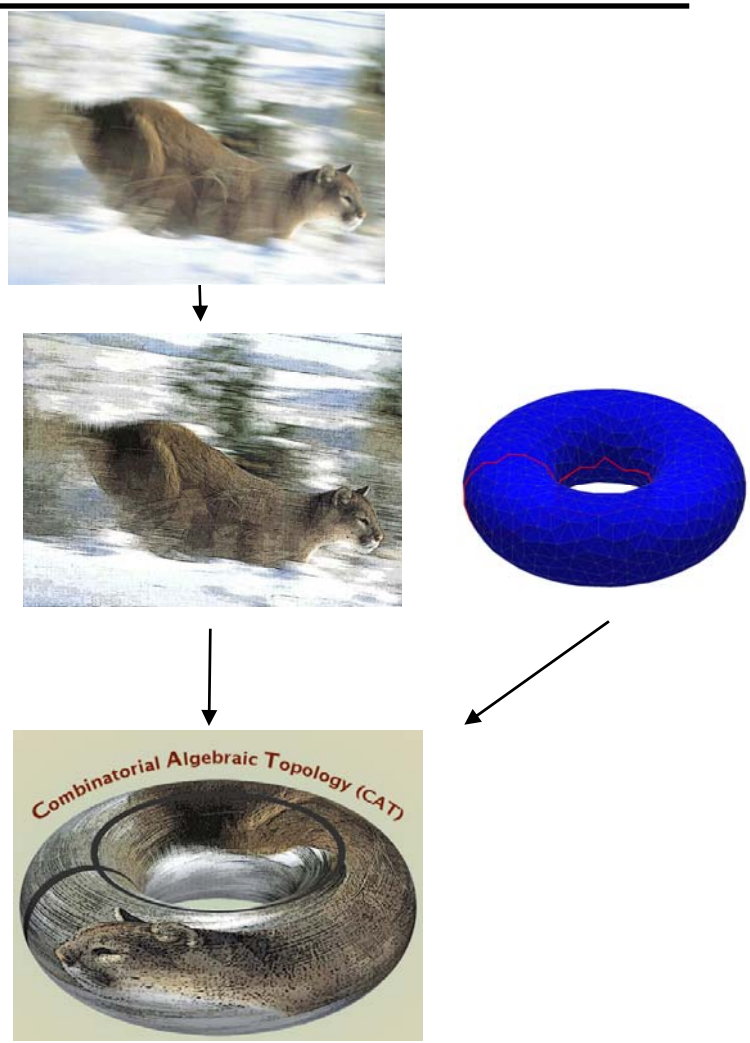
(by invitation only)

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**



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Computer Science Research Institute (CSRI)
CAT workshop's sponsoring program

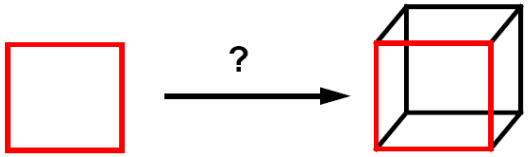
Measure	2007	2008
Projects	14	3
Workshops	4	7
Visitors (Institutions)	102 (67)	106 (68)
Summer Students	43	34
Sabbaticals	3	2
% Hires having prior CSRI partnerships	73%	80%

Computer Science Research Institute (CSRI)

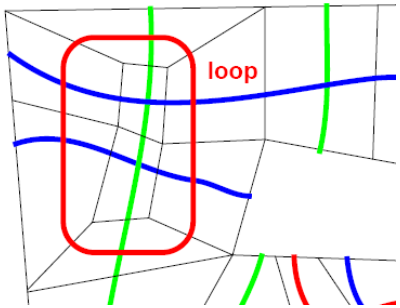
- Open environment
  - no guards, gates, guns
  - focus on publications
- Productive place to visit
  - faculty
  - post-docs
  - contracts
- Excellent experience for summer students
  - graduate and some undergrad
  - extensive overview lecture series
- Where I work
  - Scott's NGC story

Since this is a reception talk…
"How I got interested in topology"

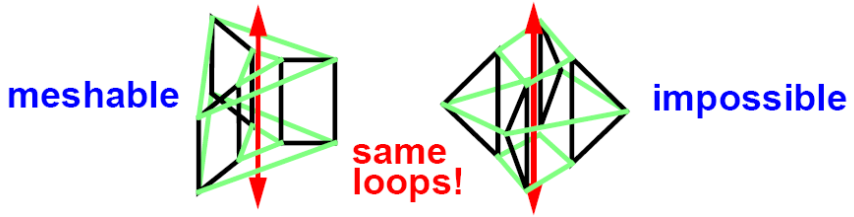
- **Algebraic topology Cornell grad-school class – where are the pictures?**
  - **a doughnut, "applications", … tried to forget all that, but it came back…**
- **Hex mesh generation circa 1990's**
  - **Q: Given a quadrilateral mesh enclosing a volume, can you fill volume with hexahedra?**



  - **Homology and hex-mesh existence proof**
    - **Thurston newsgroup posting 1993. Mitchell STACS paper 1995.**
  - **A: Yes.** Dualize surface mesh into arrangement of discrete curves cycles.
    (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



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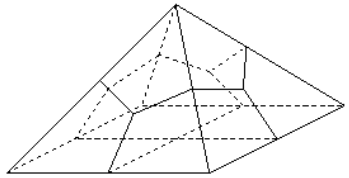
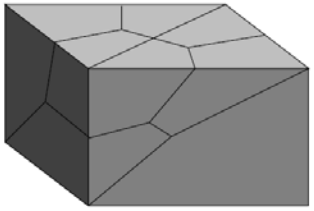
How I got interested in topology

- **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

1998 Mitchell "geode" 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!**

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CAT Workshop Motivation

- Time right for a CAT workshop
  - Other events
    - Linear algebra factorization
      - Algebraic Topological Methods in Computer Science "satellite conference" of European Congress of Mathematics, 2008. - 8 speakers
      - 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
      - TopoInVis, 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!

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CAT Workshop Goals

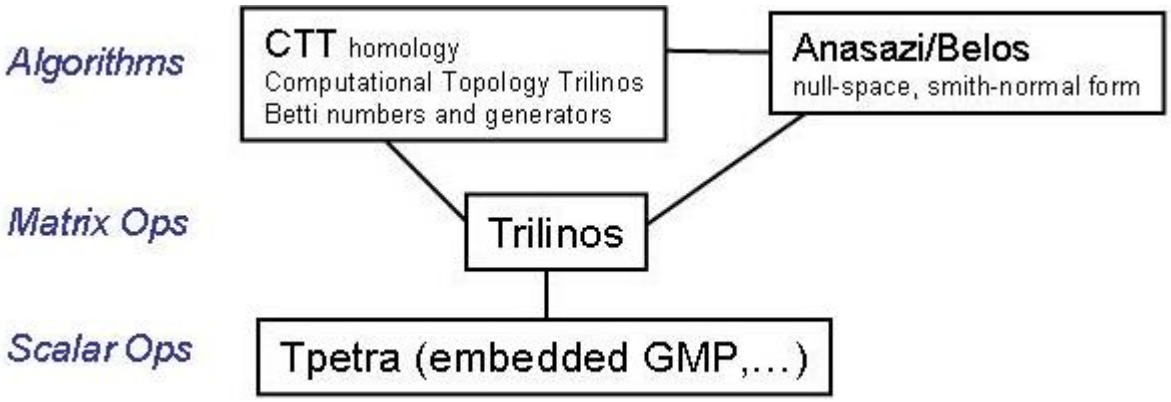
- **Software, Applications, Algorithms**
  - **new univ-labs and univ-univ partnerships**
    - **many forms possible – opportunities on next 4 slides**
      - **software partnerships**
        - **Trilinos for parallel linear algebra *over finite fields?***
      - **many SNL topology-ready applications**
        - **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?**



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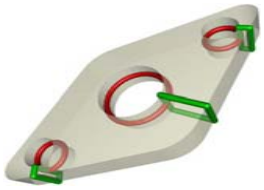
Application talks

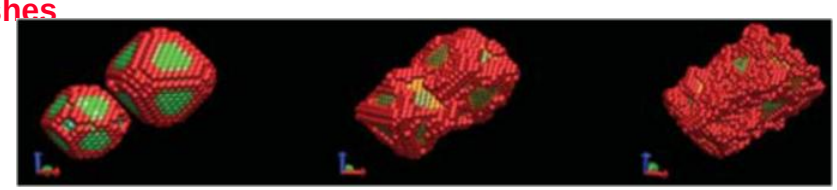
- **Applications**
  The Saturday afternoon session focuses on laboratory applications, especially those that are not currently using topology, but could. Format consists of an overview talk, together with a discussion session to explore what is possible. The intent is for application owners to engage 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, defeaturing**
    - **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**

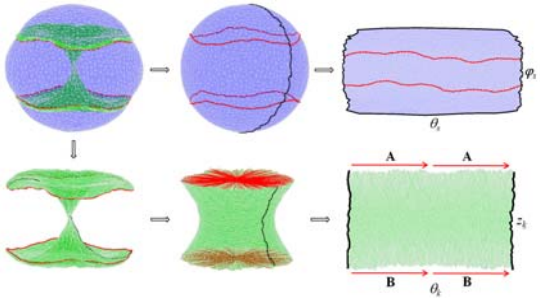


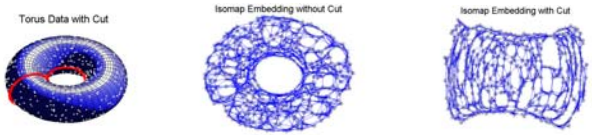
Tamal Dey gen H_i



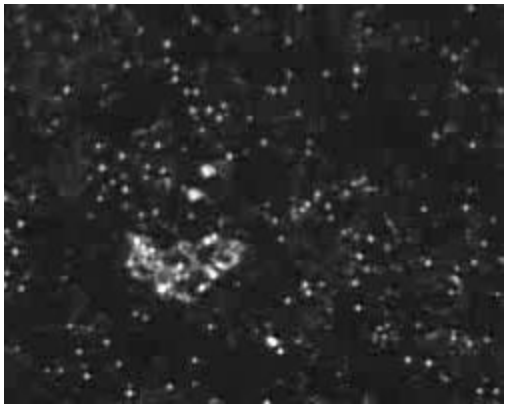
void coalescence graphic from Marian et al. A. Mota

Shawn Martin molecular conformation dim. red.





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

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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

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