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Applying Mathematics: Solving Problems at a National Laboratory

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Pi Mu Espilon Talk, Western Michigan University
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My Background

- **Northwestern University**
  - B.A., Computer Studies, 1994
- **Western Michigan University**
  - M.S., Applied Mathematics, 2001
- **University of Maryland, College Park**
  - Ph.D., Applied Mathematics/Scientific Computation, 2005
- **Sandia National Laboratories**
  - Student Intern, 2001
  - John von Neumann Postdoctoral Fellow, 2005–2007
  - Senior Member of Technical Staff, 2007–Present

- **Interests**
  - Informatics, optimization, linear algebra, machine learning

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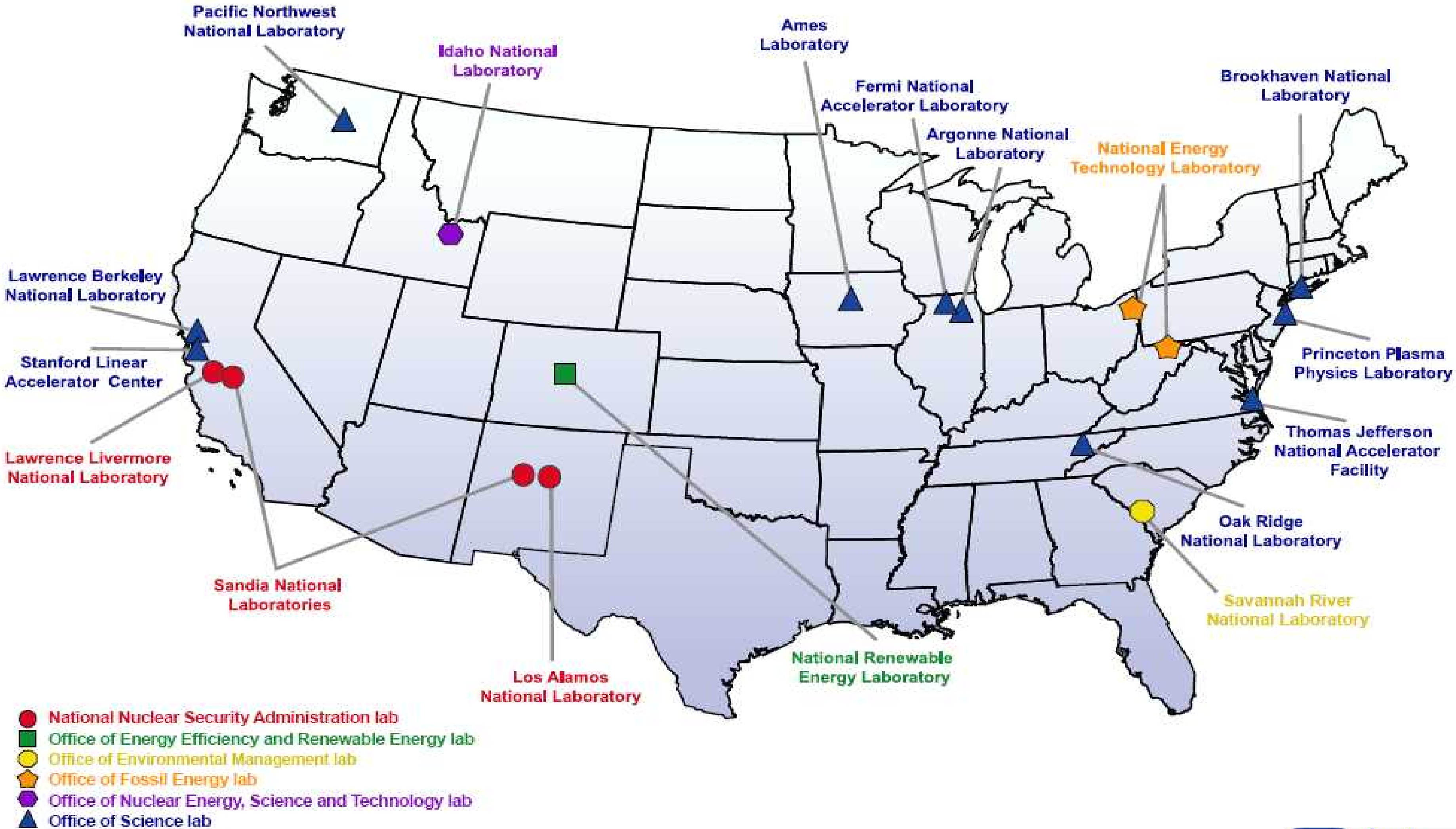

http://www.energy.gov/organization/labs-techcenters.htm

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Mathematics at the Labs

Lab	*Division, Directorate, Center, Department*	*Web Site*
Sandia/NM	Computation, Computers, Information, and Mathematics	www.cs.sandia.gov
Sandia/CA	Computational Sciences and Mathematics Research	csmr.ca.sandia.gov
Argonne	Mathematics and Computer Science	www.mcs.anl.gov
Brookhaven	Computational Science Center	www.bnl.gov/csc
Lawrence Berkeley	High Performance Computing Research Department	hpcrd.lbl.gov
Lawrence Livermore	Center for Applied Scientific Computing	www.llnl.gov/casc
Oak Ridge	Computer Science and Mathematics	www.csm.ornl.gov
Pacific Northwest	Computational Sciences and Mathematics	computing.pnl.gov/csm/

Opportunities for Students

- **Undergraduate**
  - Summer Internships
- **Graduate**
  - Summer Internships
  - Computational Science Graduate Fellowship
  - National Physical Science Consortium Fellowship
    - SNL, LLNL, LANL Sponsorship
- **Postdoctoral**
  - von Neumann (SNL), Wilkinson (ANL), Alvarez (LBL), Householder (ORNL)
  - Project-based positions

Note: most positions require U.S. citizenship

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Important Skills

- **Strong technical proficiency and experience**
  - Mathematics, statistics, computing
  - Work experience important
- **Depth and breadth**
  - Technical leadership in challenging areas
  - May have several different "careers" at a lab
- **Programming skills**
  - Applied research
  - Scripting languages usually not enough
- **Leadership skills**
  - Research teams for most projects
  - Recruitment (students, postdocs, project team members)

Benefits of Working at the Labs

- **Focus on research**
  - Academic-like setting
    - Write scholarly papers
    - Weekly colloquia/seminars
    - Attend conferences
- **Some educational/mentoring opportunities**
  - Summer students, thesis committees, etc.
- **Access to world-class researchers**
  - Both internally and externally
- **Impact of research**
  - Real, challenging, important problems
  - Can impact national science policy

Transitioning from School to Lab

- **Working on a team**
  - Work experiences extremely helpful
    - Summer internships
    - Workshops at IMA, MSRI, SAMSI, IPAM, etc.
- **Mentoring Students**
  - As early as first day
- **Funding**
  - Postdoctoral time covered
  - Proposal writing is essential
- **Transitioning to permanent staff**
  - Postdocs: main recruiting tool for many groups
  - Balancing internal impact and external visibility

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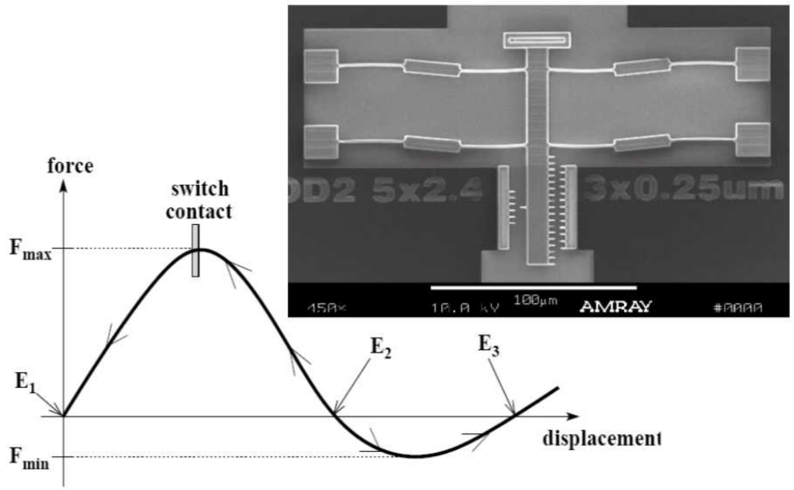
My Path to a Position at Sandia

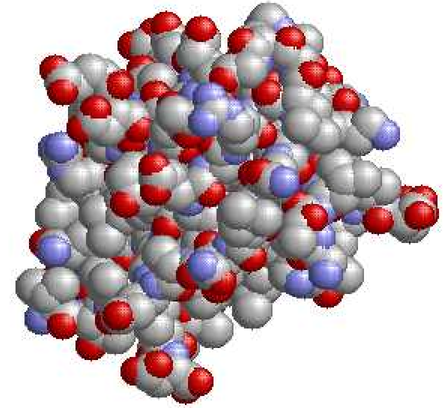
- **Work experience**
  - Internships: Sandia (summer), CCS (1.5 years during Ph.D.)
- **Workshops/conferences**
  - IMA Graduate Workshop, SIAM (4), NIST (2) , GRiD (2), Biosciences (2)
- **Multiple projects**
  - SNL: Multilinear algebra/tensors (text analysis)
  - SNL: PDE preconditioning (chemical equilibrium)
  - SNL: Surrogate-based optimization (MEMS design)
  - SNL/UM: Homotopy optimization methods (protein folding)
  - SNL/UM: Text clustering and summarization (document retrieval)
  - IMA: Nonlinear solvers (RF circuit design)
  - WMU: Linear algebra (structured eigenvalue problems)
- **Skills**
  - C, C++, Java, Matlab, Perl
  - Algorithm design, experimental design and analysis
  - End-to-end code development, code integration, team development, general code development

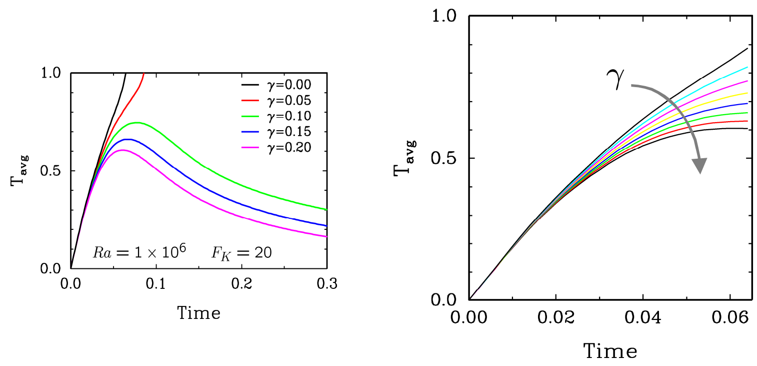
Applications

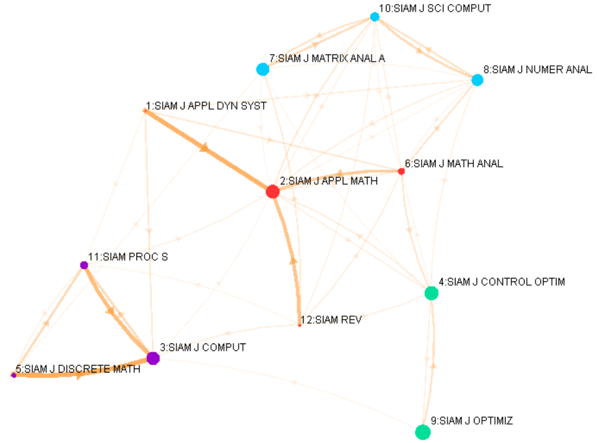
Engineering



Biology







Chemistry

Informatics

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Survey

- Undergraduate/Graduate

- Calculus (1220/30, 1700/10)
- Multivariate Calculus/Matrix Algebra (2720)
- Differential Equations/Linear Algebra (3740)
- Numerical Analysis (5070, 6070)
- Optimization (4080, 6050, 6080)
- Computer Science (programming, algorithms)
- Statistics (sampling, design of experiments)

Homotopies

Definition

A **homotopy** between two continuous functions

$$f^0, f^1 : X \to Y$$

is defined as a continuous function

$$H : X \times [0,1] \to Y$$

such that

$$H(x,0) = f^0(x) \text{ and } H(x,1) = f^1(x)\,, \quad \forall x \in X$$

Examples

$$H(x,\lambda) = \lambda f^1(x) + (1-\lambda) f^0(x)$$ [convex]

$$H(x,\lambda) = f^1(x) - (1-\lambda) f^1(x^0)$$ [global]

$$H(x,\lambda) = \lambda f^1(x) + (1-\lambda)(x-a)$$ [probability-one]

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Solving Nonlinear Systems of Equations

Goal

Given $f^1 : \mathbb{R}^n \to \mathbb{R}^m$, find x such that $f^1(x) = 0$

Homotopy (Continuation, Embedding) Method

1) Initialize: $f^0(x^0) = 0$ [known or trivial solution]

2) Define homotopy: $H(x, \lambda)$

3) Trace equilibrium curve: $H(x, \lambda) = 0$ from $\lambda = 0$ to $\lambda = 1$

Issues

1) Does a smooth curve, $c(\alpha) \in H^{-1}(0)$, exist? [implicit function theorem]

2) Does the curve reach $\lambda = 1$ in a finite length? [problem dependent]

3) How can we numerically trace the curve? [predictor-corrector]

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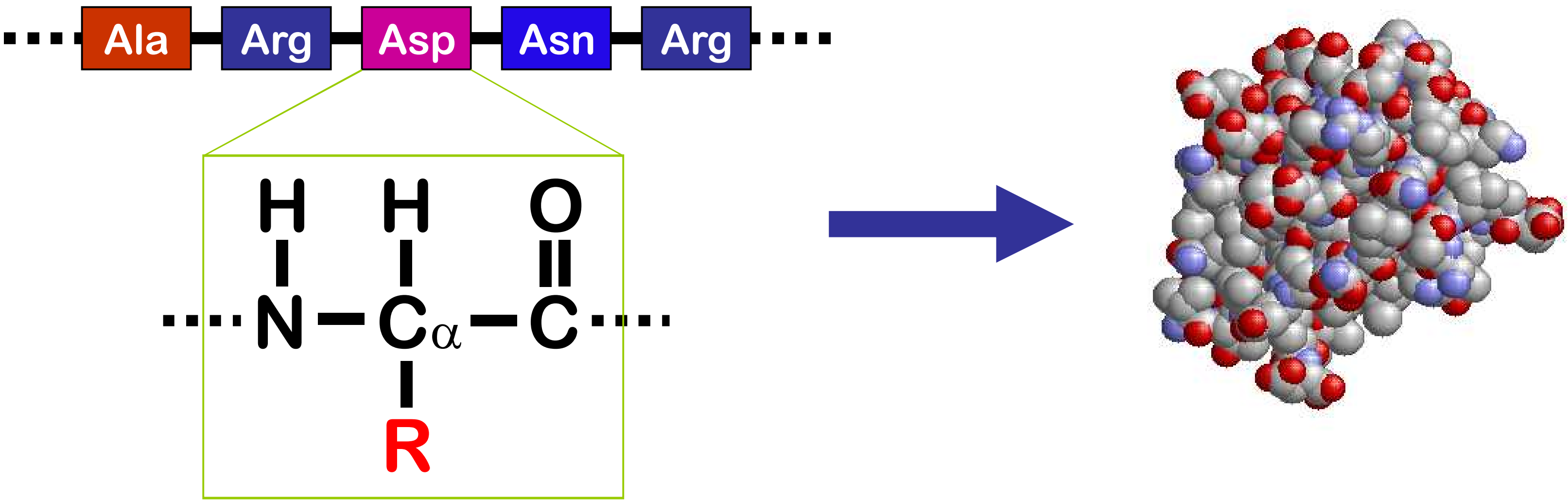
Application: Protein Structure Prediction

Amino Acid Sequence **Protein Structure**



Given the amino acid sequence of a protein (1D), is it possible to predict its native structure (3D)? [energy minimization; Anfinsen, 1971]

Application: Protein Structure Prediction

Goal

Minimize energy function of ***target*** protein

$$E^1(X^*) = \min_{X \in \mathbb{R}^{3n}} E^1(X), \qquad (E^1 : \mathbb{R}^{3n} \rightarrow \mathbb{R})$$

Homotopy Optimization Method (HOM)

1) Start with (known) lowest energy structure of ***template*** protein:

$$E^0(X^0) = \min_{X \in \mathbb{R}^{3n}} E^0(X)$$

2) Define a ***homotopy*** function deforming template into target:

$$H(X,\lambda) = \rho^1(\lambda)E^1(X) + \rho^0(\lambda)E^0(X)$$ [domain knowledge]

3) Produce sequence of minimizers of $H(X,\lambda)$ starting at $\lambda = 0$ and ending at $\lambda = 1$

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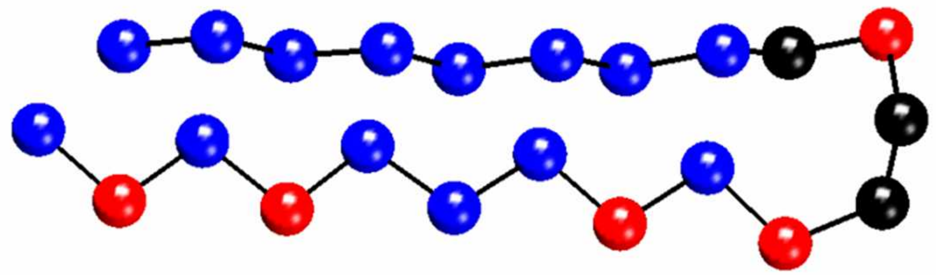
Application: Protein Structure Prediction

Backbone model [Veitshans, *et al.*, 1996]

– Single chain of particles with residue attributes
– Particles model $\mathbf{C}_{\alpha}$ atoms in proteins



Properties of particles

– Hydrophobic, Hydrophilic, Neutral
– Diverse hydrophobic-hydrophobic interactions

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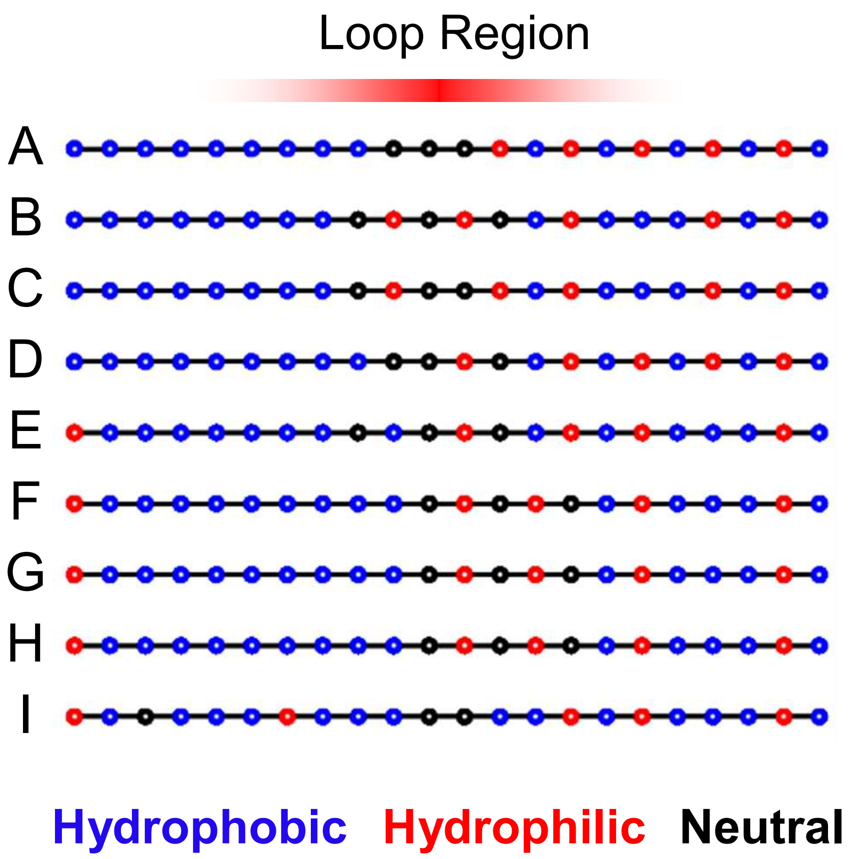
Application: Protein Structure Prediction

Experiment: 9 chains (22 particles) with known structure



Application: Protein Structure Prediction

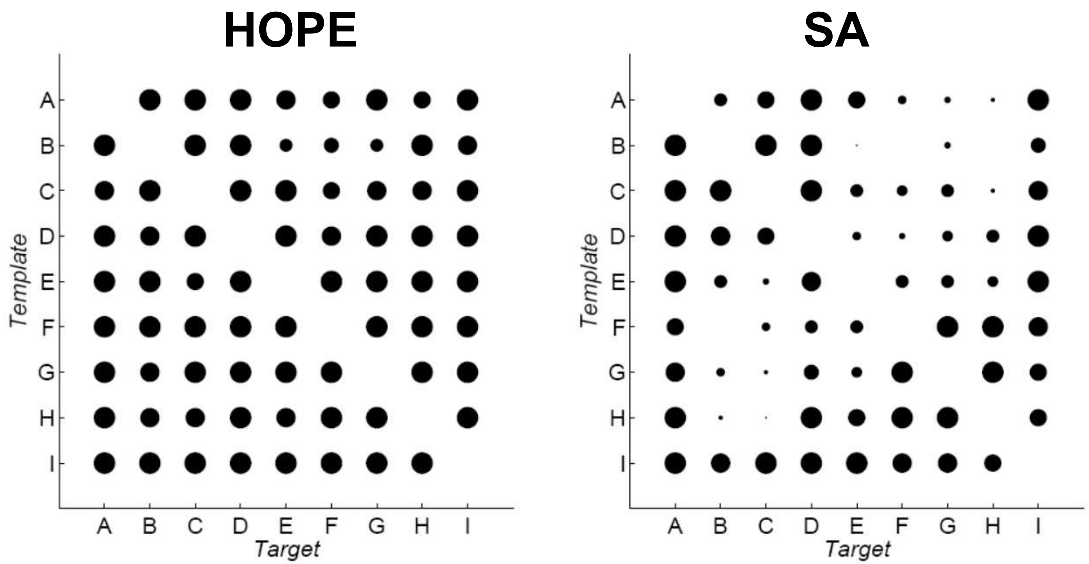
HOPE [Dunlavy, *et al.*, 2005; Dunlavy and O'Leary, 2005]

- HOM using stochastic perturbations, ensembles of minimizers
- Increases probability of finding global minimizer(s)

Ensemble-Based Simulated Annealing [Salamon, *et al.*, 2002]

- Popular optimization method for protein structure prediction

Success of HOPE and ensemble-based simulated annealing (SA) with ensembles of size 16 for each template-target pair. The size of each circle represents the percentage of successful predictions over the 10 runs.



Conclusion: Less work, more accuracy using homotopies

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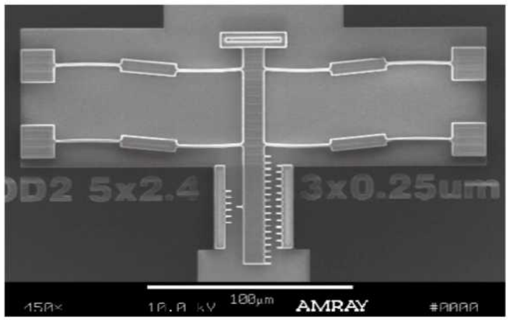
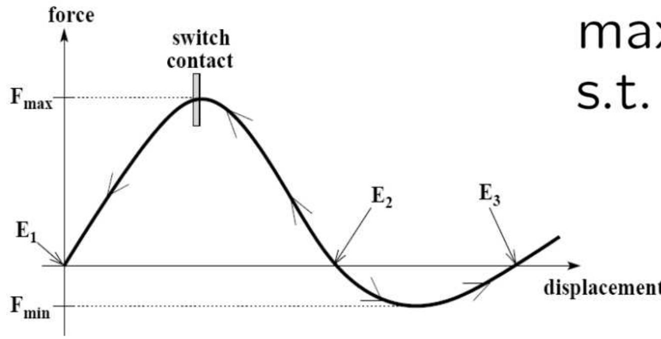
Application: MEMS Design Optimization

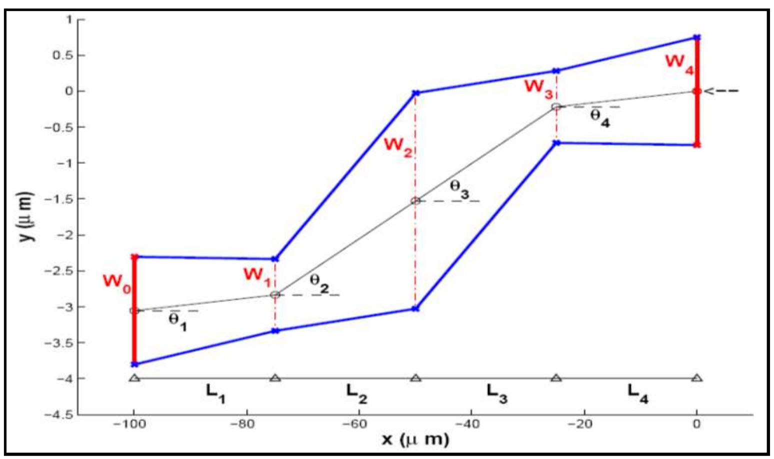
Microelectromechanical Systems (MEMS) Design

Bi-stable Switch



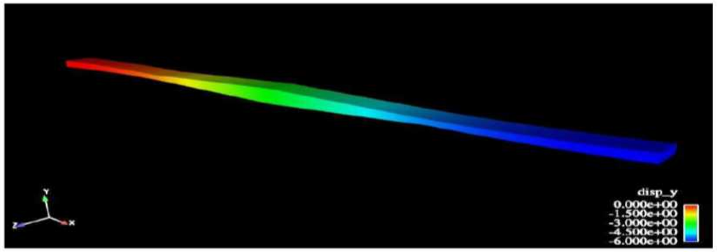


$$
\begin{array}{llll}
\max & F_{\max}(\mathbf{d}) & & \\
\text{s.t.} & E_2(\mathbf{d}) & \leq & 8 \\
 & S_{\max}(\mathbf{d}) & \leq & 3000 \\
 & F_{\min}(\mathbf{d}) & = & -5.
\end{array}
$$



13 design variables: $d=(W_i, L_i, \theta_i)$

Force (F), displacement (E), and stress (S) computed using finite element analysis



[evaluations ~ O(hours)]

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MEMS: Constraint Relaxation

- **Original Problem**

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g_l \le g(x) \le g_u \\ & h(x) = 0 \\ & x_l \le x \le x_u \end{aligned}$$

- **Constraint Relaxation**

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & g_l \le G(x,\lambda) \le g_u \\ & H(x,\lambda) = 0 \\ & x_l \le x \le x_u \end{aligned}$$

$$G(x,\lambda) = G(x) + (1-\lambda)b_G$$

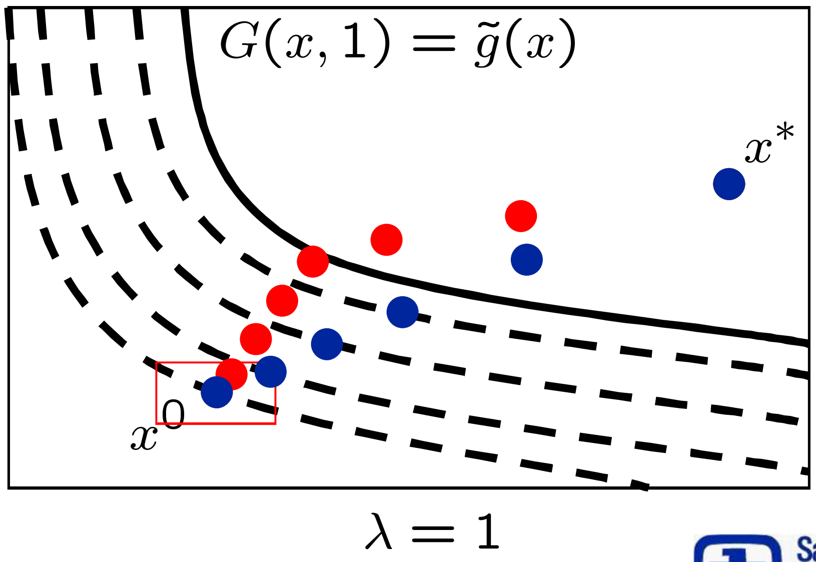
$$H(x,\lambda) = H(x) + (1-\lambda)b_H$$

b_G, b_H chosen s.t.

$$g_l \le G(x^0, 0) \le g_u$$

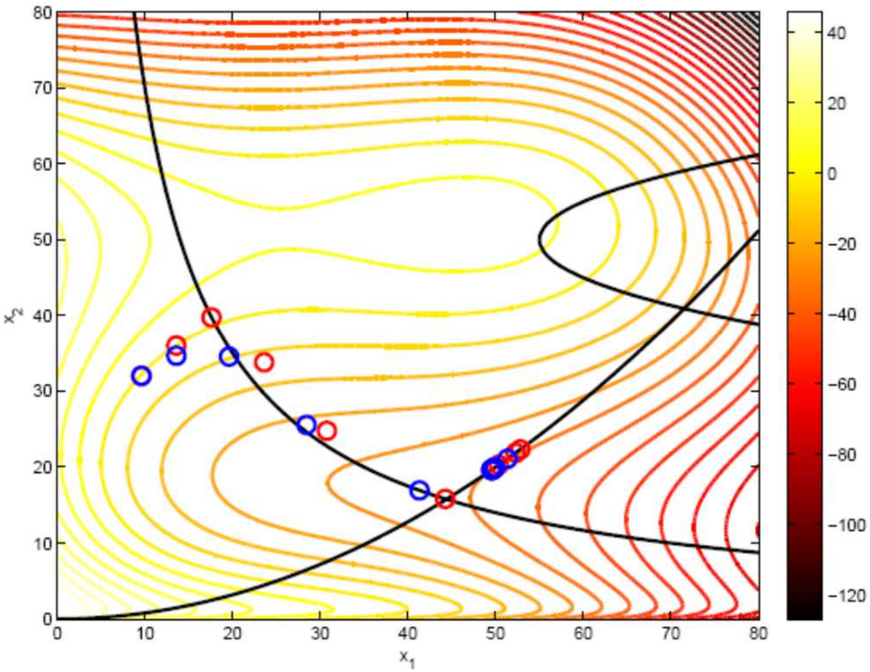
$$H(x^0, 0) = 0$$

[adaptation of Perez, *et al*, 2004]

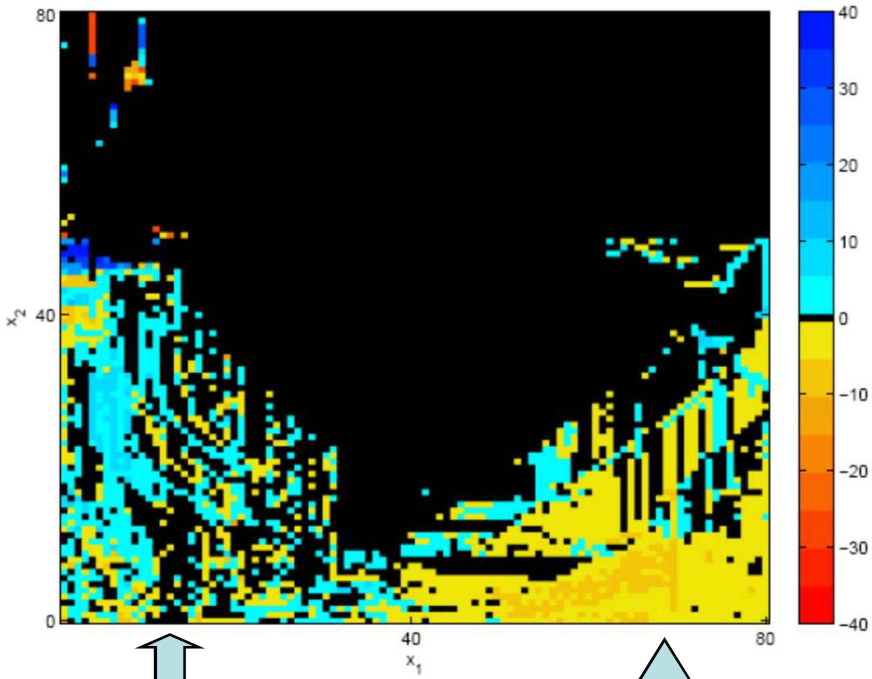


MEMS: Effect of Constraint Relaxation

Sample homotopy constraint relaxation



10^6 starting points on uniform grid



Optimal/feasible directions differ by < 90°.
Relaxation beneficial to achieve balance.

Optimal/feasible directions opposed.
Relaxation harmful since feasibility must ultimately take precedence.

Application: MEMS Design Optimization

Experiments using Constraint Relaxation (CR)

- Surrogate-based optimization (SBO) + trust region [DAKOTA]
- Sequential quadratic programming (SQP) [NPSOL, DOT]
- Problems
  - Barnes Problem (common engineering test problem for SBO methods)
  - Constrained and Unconstrained Testing Environment (CUTE)
  - MEMS Bi-stable switch design

Results [Eldred and Dunlavy, 2006]

- Barnes: helps in some parts of domain, hinders in others
  - Angle between directions of descent and greatest constraint reduction
- CUTE: helps most for problems with equality constraints
  - Constraint satisfaction a challenge for SQP
- MEMS: leads to **3X** reduction in computation!!!

Conclusion: CR via homotopies can lead to reduced computation

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Application: Chemical Equilibrium

Extended Frank-Kamenetskii Explosion Model

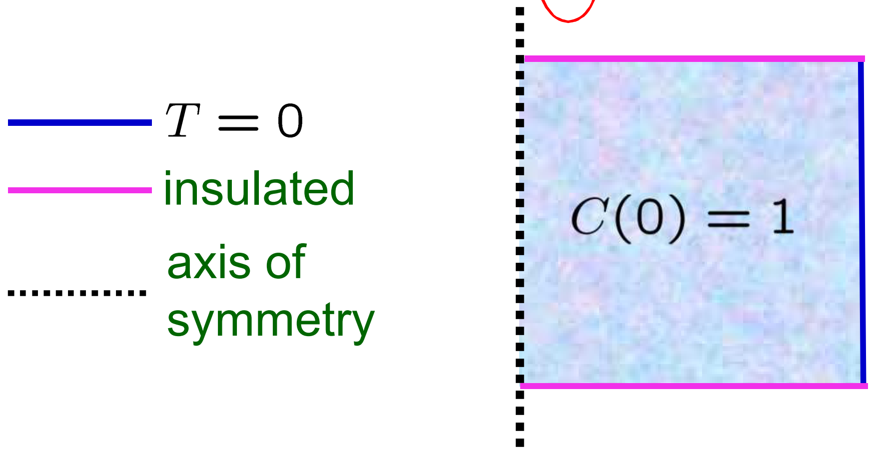
- Includes reactant consumption term
- 5 scalar PDEs, 5 unknowns: v_x, v_y, P, T, C

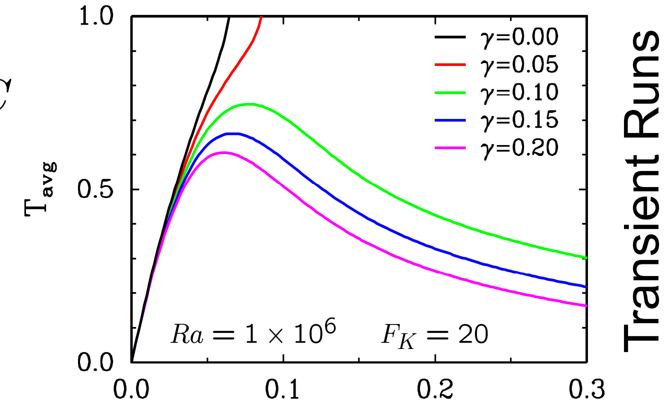
$$\frac{dv}{dt} + v \cdot \nabla v = -\nabla P + \nabla^2 v + RaTe_z$$

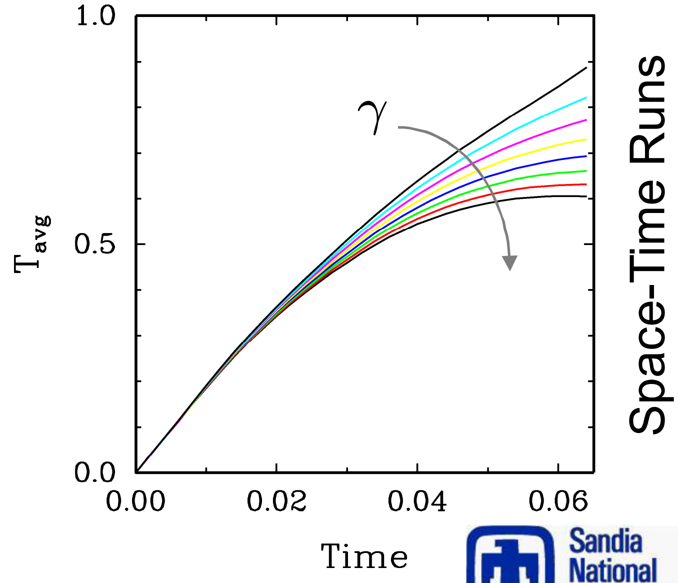
$$\nabla \cdot v = 0$$

$$\frac{dT}{dt} + v \cdot \nabla T = \nabla^2 T + F_K C e^T$$

$$\frac{dC}{dt} + v \cdot \nabla C = \nabla^2 C - \gamma F_K C e^T$$







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Application: Chemical Equilibrium

Space-Time Formulation of Transient PDEs

Transient simulation: $\mathbf{B}\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \lambda)$

Backward Euler: $\mathbf{B}\frac{\mathbf{x}_1 - \mathbf{x}_0}{\Delta t} - \mathbf{f}(\mathbf{x}_1, \lambda) = 0 \Rightarrow \mathbf{B}\frac{\mathbf{x}_2 - \mathbf{x}_1}{\Delta t} - \mathbf{f}(\mathbf{x}_2, \lambda) = 0 \Rightarrow \cdots$

Instead, solve for all solutions at once: $\mathbf{g}(\mathbf{y}, \lambda) = 0$

where $\mathbf{y} = [\mathbf{x}_1\ \mathbf{x}_2\ \cdots\ \mathbf{x}_n]^T$ and $\mathbf{g}_i = \mathbf{B}\mathbf{x}_i - \mathbf{B}\mathbf{x}_{i-1} - \Delta t \mathbf{f}(\mathbf{x}_i, \lambda)$

- -

With Newton solver, direction is found by solving: $(\mathbf{J} \equiv \nabla \mathbf{f})$

$$\begin{vmatrix} (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 & 0 \\ -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 & 0 \\ 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 & 0 \\ 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) & 0 \\ 0 & 0 & 0 & -\mathbf{B} & (\mathbf{B} - \Delta t\mathbf{J}) \end{vmatrix} \begin{vmatrix} \Delta\mathbf{x}_1 \\ \Delta\mathbf{x}_2 \\ \Delta\mathbf{x}_3 \\ \Delta\mathbf{x}_4 \\ \Delta\mathbf{x}_5 \end{vmatrix} = \begin{vmatrix} -\mathbf{g}_1 \\ -\mathbf{g}_2 \\ -\mathbf{g}_3 \\ -\mathbf{g}_4 \\ -\mathbf{g}_5 \end{vmatrix}$$

Efficient solves of this system are key to success!

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Application: Chemical Equilibrium

Explosion Model Experiments

- Finite element method [MPSalsa]
  - 2M unknowns
  - 1024 processors

Results [Dunlavy and Salinger, 2006]

- Need good initial guess to solve space-time systems
  - Transient simulation for first parameter value, then continuation
- Preconditioners
  - Several developed to leverage spatial/temporal parallelism
  - At least 20% more efficient to solve space-time systems

Conclusion: Continuation of space-time systems more efficient than transient simulations when preconditioners are used.

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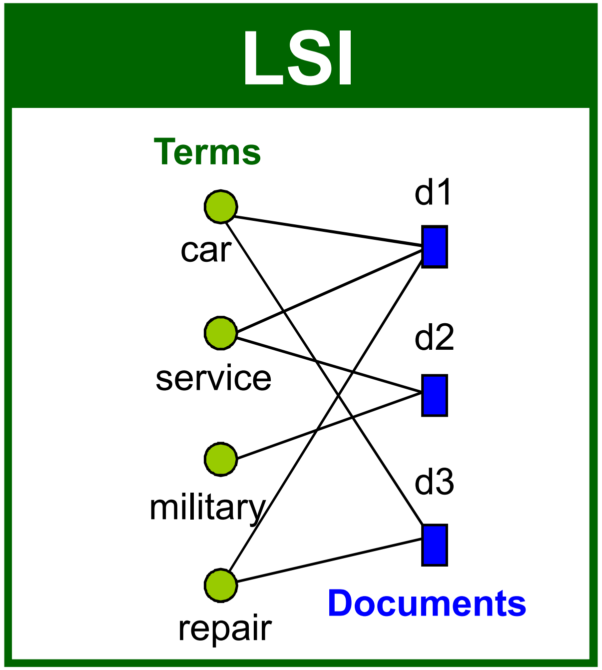
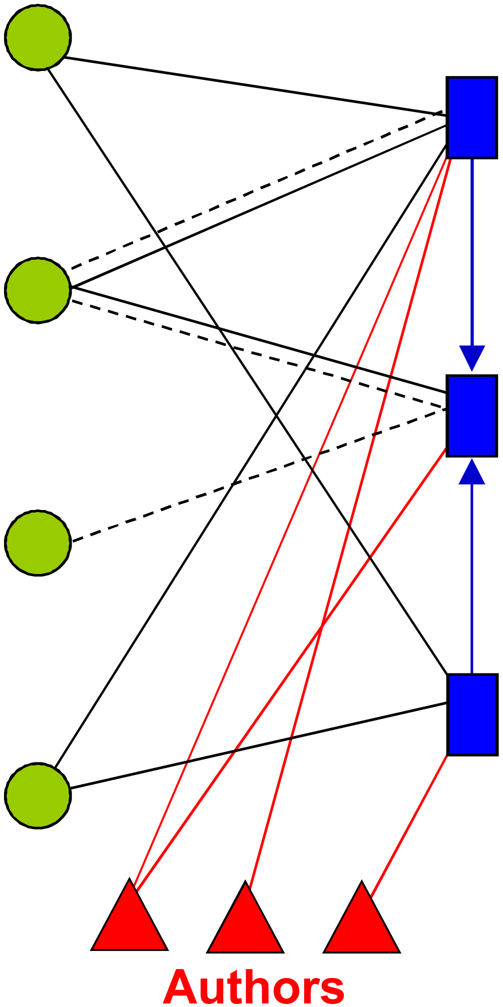
Application: Informatics

- **Network analysis and bibiliometrics**
- **PageRank** [Brin & Page, 1998]
  - Transition matrix of a Markov chain: $\mathbf{M}$
  - Ranks: $\mathbf{M}\mathbf{r} = \mathbf{r}$
- **HITS** [Kleinberg, 1998]
  - Adjacency matrix of the Web graph: $\mathbf{L}$
  - Hubs: $\mathbf{L}\mathbf{L}^T\mathbf{y} = \mathbf{y}$
  - Authorities: $\mathbf{L}^T\mathbf{L}\mathbf{x} = \mathbf{x}$



- **Latent Semantic Indexing (LSI)** [Dumais, et al., 1988]
  - Vector space model of documents (term-document matrix): $\mathbf{A}$
  - Truncated SVD: $\mathbf{A} \approx \mathbf{T}\mathbf{\Sigma}\mathbf{D}^{\mathsf{T}} = \sum_{r=1}^{k} \sigma_r \, \mathbf{t}_r \mathbf{d}_r^T$
  - Maps terms and documents to the "same" *k*-dimensional space

Multilinear Algebra, More Complex Graph Analysis



- **Nodes (one type) connected by multiple types of links**
  – Node x Node x Connection
- **Two types of nodes connected by multiple types of links**
  – Node A x Node B x Connection
- **Multiple types of nodes connected by a single link**
  – Node A x Node B x Node C
- **Multiple types of nodes connected by multiple types of links**
  – Node A x Node B x Node C x Connection
- **Etc…**

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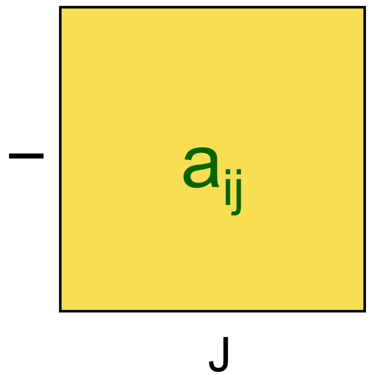
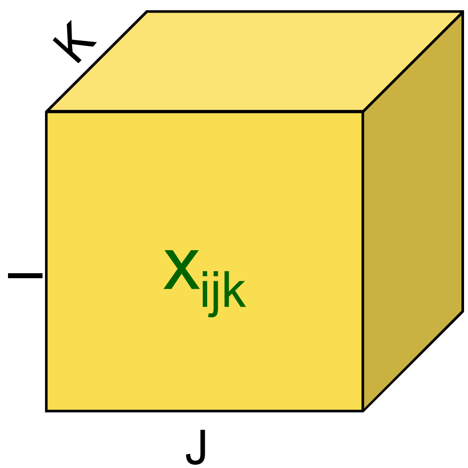
Tensors (Multidimensional Arrays)

Notation	
s	scalar
$\mathbf{a}$	vector
$\mathbf{B}$	matrix
$\mathcal{X}$	tensor

An I x J matrix



An I £ J £ K tensor



- **Other names for tensors…**
  - Multi-way array
  - N-way array
- **The "order" of a tensor is the number of dimensions**
- **Other names for dimension**
  - Mode
  - Way
- **Example**
  - The matrix **A** (at left) has order 2.
  - The tensor $\mathcal{X}$ (at left) has order 3 and its 3^{rd} mode is of size K.

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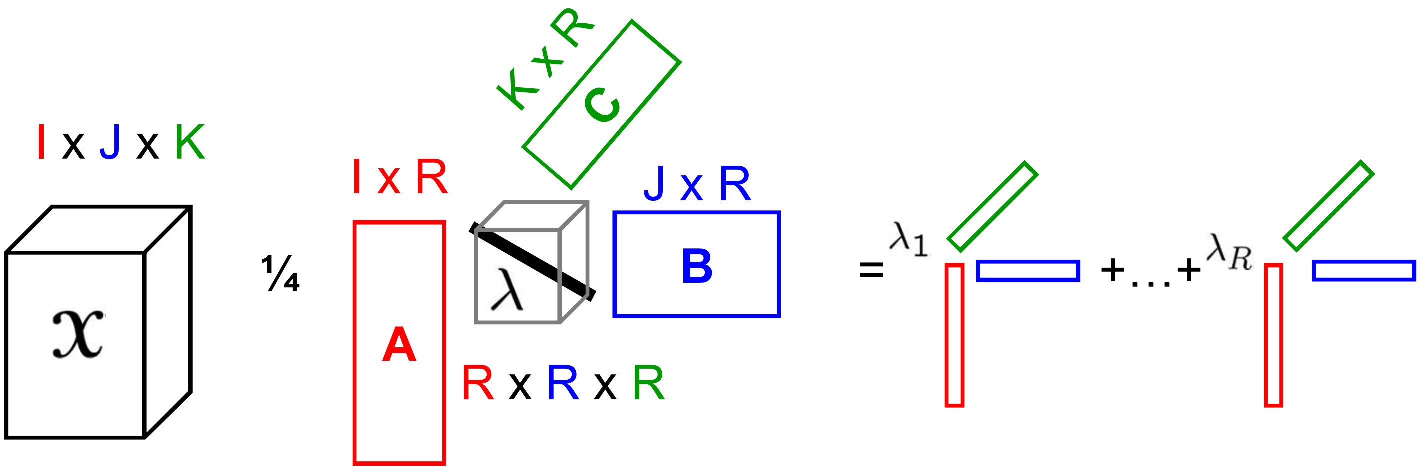
CANDECOMP/PARAFAC (CP) Decomposition



$$\mathcal{X} \approx [\![\boldsymbol{\lambda} \,; \mathbf{A}, \mathbf{B}, \mathbf{C}]\!] = \sum_r \lambda_r \, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$$

- **CANDECOMP** = Canonical Decomposition [Carroll & Chang, 1970]
- **PARAFAC** = Parallel Factors [Harshman, 1970]
- Core is *diagonal* (specified by the vector λ)
- Columns of **A**, **B**, and **C** are **not** orthonormal
- If R is *minimal*, then R is the **rank** of the tensor [Kruskal 1977]
- Can have rank($\mathcal{X}$) > min{I,J,K}

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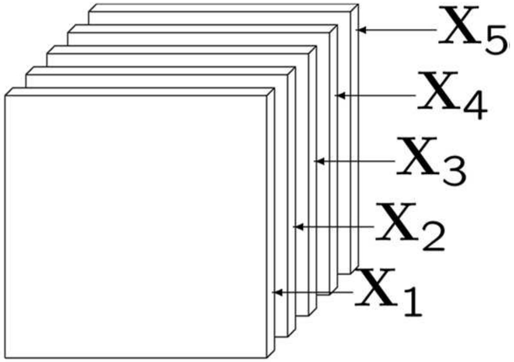
SIAM Journal Data: Tensor Construction



Frontal Slices $\mathbf{X}_k$

Slice (k)	*Description*	*Nonzeros*	$\sum_i \sum_j x_{ijk}$
1	Abstract Similarity	28476	7695.28
2	Title Similarity	120236	33285.79
3	Keyword Similarity	115412	16201.85
4	Author Similarity	16460	8027.46
5	Citation	2659	5318.00

- $\mathbf{X}_1 = \mathbf{T}^{\mathsf{T}}\mathbf{T}$ where $t_{ij} = f_{ij} \log_2(N/N_i)$ for terms in the **abstracts**
  - f_{ij} is the frequency of term **i** in document **j**
  - N_i is the number of documents that term **i** appears in
- $\mathbf{X}_2 = \mathbf{T}^{\mathsf{T}}\mathbf{T}$ for terms in the **titles**
- $\mathbf{X}_3 = \mathbf{T}^{\mathsf{T}}\mathbf{T}$ for terms in the author-suppplied **keywords**
- $\mathbf{X}_4 = \mathbf{W}^{\mathsf{T}}\mathbf{W}$ where $w_{ij} = \begin{cases} 1/\sqrt{M_j} & \text{if author } i \text{ wrote document } j \\ 0 & \text{otherwise,} \end{cases}$
- $x_{ij5} = \begin{cases} 2 & \text{if document } i \text{ cites document } j \\ 0 & \text{otherwise.} \end{cases}$

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SIAM Journal Data: Document Similarity

Link Analysis: Hubs and Authorities on the World Wide Web,
C.H.Q. Ding, H. Zha, X. He, P. Husbands, and H.D. Simon, *SIREV*, 2004.

- **CP decomposition, R = 10:** $\mathcal{X} \approx [\![\boldsymbol{\lambda} \, ; \mathbf{A}, \mathbf{B}, \mathbf{C}]\!] = \sum_{r=1}^{10} \lambda_r \, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$
- **Similarity scores:** $\mathbf{S} = \frac{1}{2}\mathbf{A}\mathbf{A}^{\mathsf{T}} + \frac{1}{2}\mathbf{B}\mathbf{B}^{\mathsf{T}}$

Interior Point Methods	**(Not related)**
Sparse approximate inverses	**(Arguably distantly related)**
Graph Partitioning	**(Related)**

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SIAM Journal Data: Document Similarity

Link Analysis: Hubs and Authorities on the World Wide Web,

C.H.Q. Ding, H. Zha, X. He, P. Husbands, and H.D. Simon, *SIREV*, 2004.

- **CP decomposition, R = 30:** $\mathcal{X} \approx [\![\boldsymbol{\lambda} \,; \mathbf{A}, \mathbf{B}, \mathbf{C}]\!] = \sum_{r=1}^{30} \lambda_r \, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$
- **Similarity scores:** $\mathbf{S} = \frac{1}{2}\mathbf{A}\mathbf{A}^{\mathsf{T}} + \frac{1}{2}\mathbf{B}\mathbf{B}^{\mathsf{T}}$

Score	*Title*
0.000563	Skip graphs
0.000356	Random lifts of graphs
0.000354	A fast and high-quality multilevel scheme for partitioning irregular graphs
0.000322	The minimum all-ones problem for trees
0.000306	Rankings of directed graphs
0.000295	Squarish k-d trees
0.000284	Finding the k-shortest paths
0.000276	On floor-plan of plane graphs
0.000275	1-Hyperbolic graphs
0.000269	Median graphs and triangle-free graphs

Graphs (Related)

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SIAM Journal Data: Disambiguation

- **CP decomposition, R = 20:** $\mathcal{X} \approx [\![\boldsymbol{\lambda}\, ; \mathbf{A}, \mathbf{B}, \mathbf{C}]\!] = \sum_{r=1}^{20} \lambda_r \, \mathbf{a}_r \circ \mathbf{b}_r \circ \mathbf{c}_r$
- **Computed centroids of top 20 authors' papers (** $\mathbf{g}_A, \mathbf{g}_B$ **)**
- **Disambiguation scores:** $\mathbf{s} = \frac{1}{2}\mathbf{A}\mathbf{g}_A + \frac{1}{2}\mathbf{B}\mathbf{g}_B$
- **Scored all authors with same last name, first initial**

Before Disambuguation		*After Disambuguation*	
Papers	*Author*	*Papers*	*Author*
17	Du Q	17	Du Q
15	Kunisch K	16	Chan TF
15	Zwick U	16	Manteuffel TA
14	Chan TF	16	McCormick SF
13	Klar A	15	Kunisch K
13	Manteuffel TA	15	Zwick U
13	McCormick SF	13	Klar A
13	Motwani R	13	Golub GH
12	Golub GH	13	Motwani R
12	Kao MY	12	Kao MY

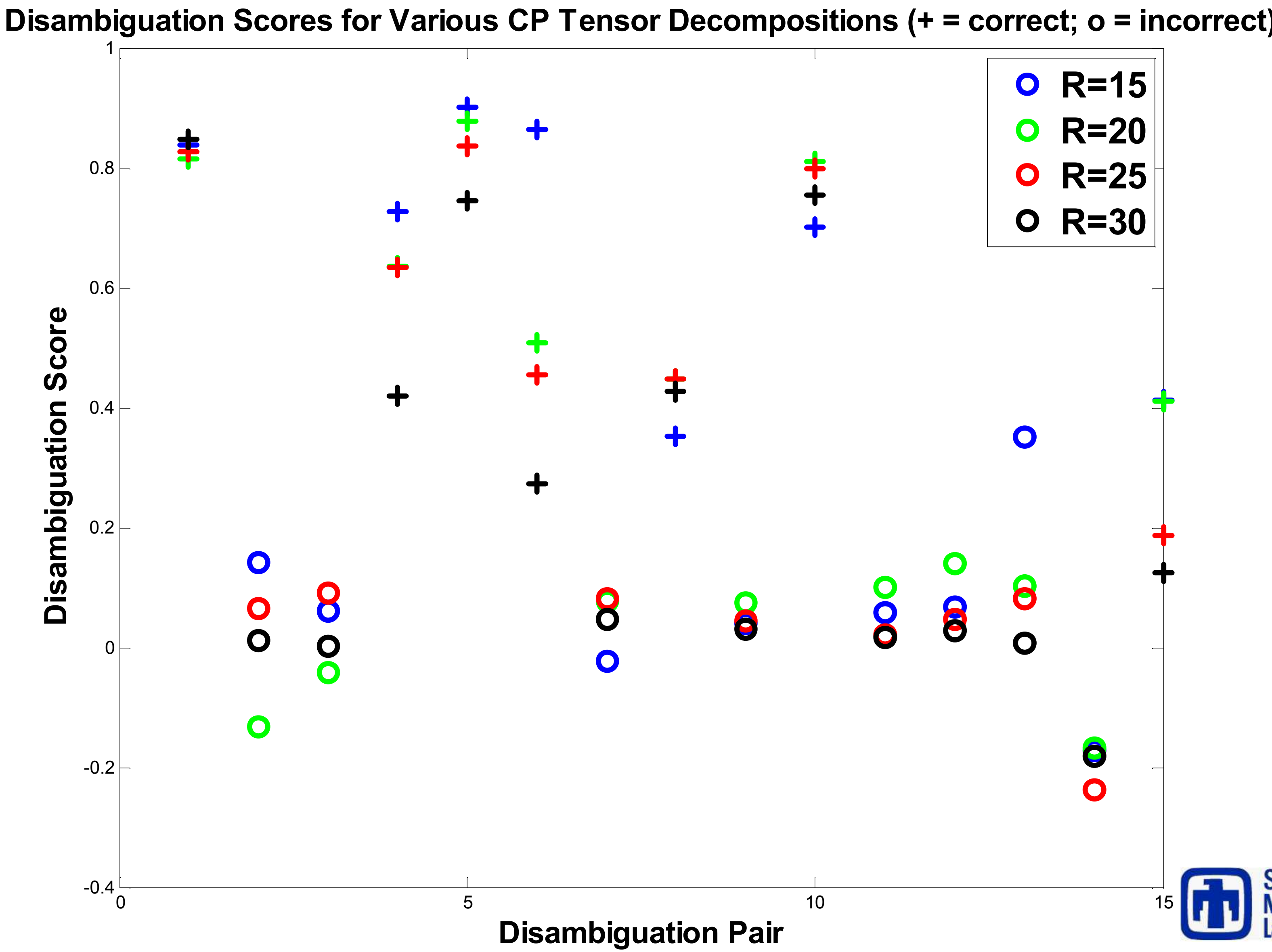
T Chan (2), TM Chan (4)

T Manteufel (3)

S McCormick (3)

G Golub (1)

SIAM Journal Data: Disambiguation



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SIAM Data: Journal Prediction

- **CP decomposition, R = 30, vectors from B**
- **Bagged ensemble of decision trees (n = 100)**
- **10-fold cross validation**
- **43% overall accuracy**

ID	*Journal Name*	*Size*	*Correct*	*Mislabeled as*
1	SIAM J APPL DYN SYST	1%	0%	2 (44%)
2	SIAM J APPL MATH	11%	58%	6 (10%)
3	SIAM J COMPUT	11%	56%	11 (20%)
4	SIAM J CONTROL OPTIM	11%	60%	2 (10%)
5	SIAM J DISCRETE MATH	5%	15%	3 (47%)
6	SIAM J MATH ANAL	8%	26%	2 (29%)
7	SIAM J MATRIX ANAL A	8%	56%	10 (19%)
8	SIAM J NUMER ANAL	12%	50%	10 (16%)
9	SIAM J OPTIMIZ	7%	66%	4 (16%)
10	SIAM J SCI COMPUT	13%	36%	8 (21%)
11	SIAM PROC S	9%	32%	3 (38%)
12	SIAM REV	3%	5%	2 (34%)

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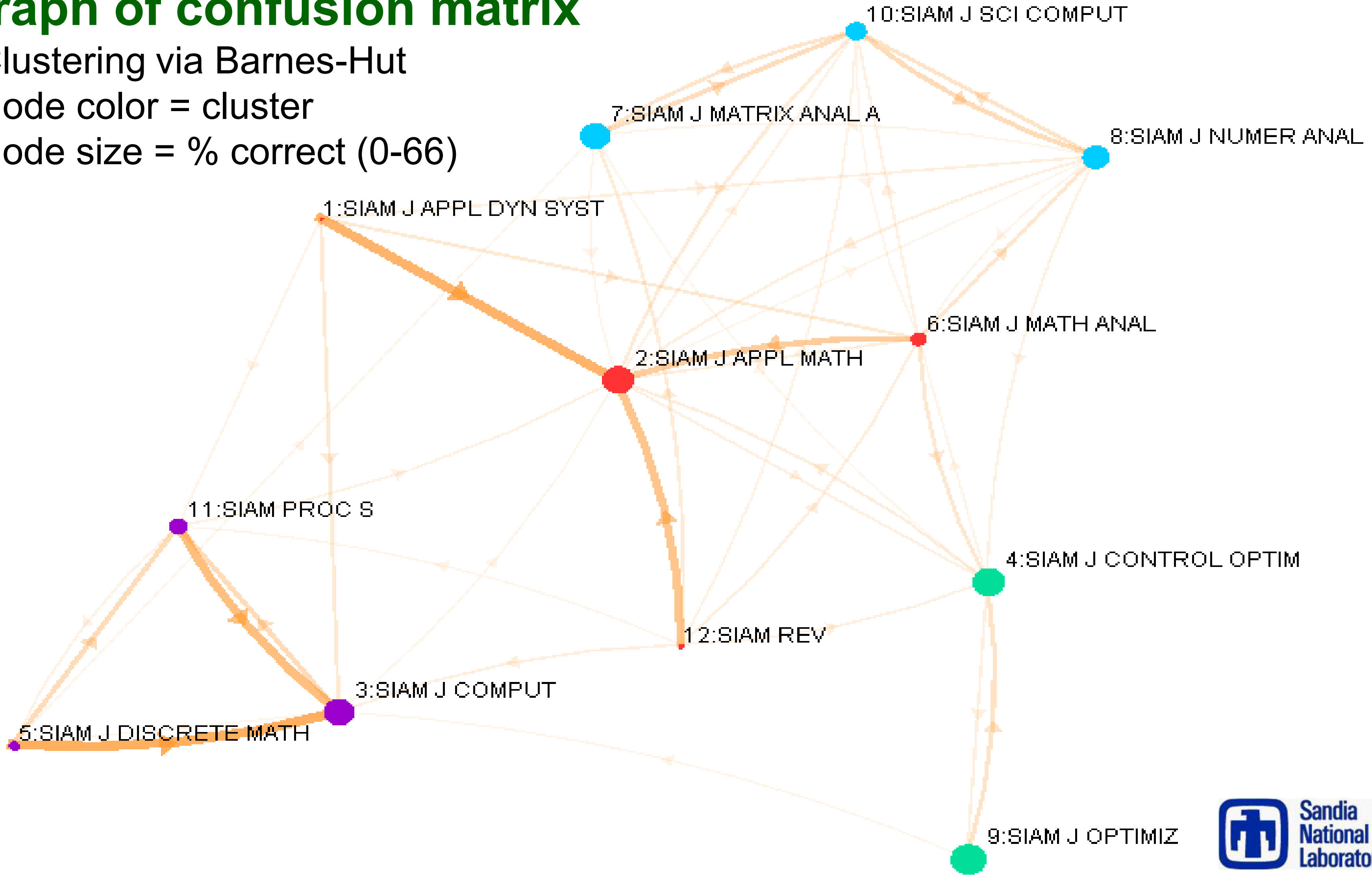
SIAM Data: Journal Prediction

Graph of confusion matrix

- Clustering via Barnes-Hut
- Node color = cluster
- Node size = % correct (0-66)



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Other Tensor Applications at Sandia

- **Tensor Toolbox (MATLAB)** [Kolda/Bader, 2007]
  http://csmr.ca.sandia.gov/~tgkolda/TensorToolbox/
- **TOPHITS (Topical HITS)** [Kolda, 2006]
  - HITS plus **terms** in dimension 3
  - Decomposition: CP
- **Cross Language Information Retrieval** [Chew et al., 2007]
  - Different **languages** in dimension 3
  - Decomposition: PARAFAC2
- **Temporal Analysis of E-mail Traffic** [Bader et al., 2007]
  - Directed e-mail graph with **time** in dimension 3
  - Decomposition: DEDICOM

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Thank You

Applying Mathematics: Solving Problems at a National Laboratory

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