Accurate Solutions of Totally Positive Linear Systems
Application to Generalized Vandermonde Systems

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DEFINITIONS AND GOALS

- Totally Positive (TP) Matrix = All minors positive
- Accurate (Small relative error componentwise) and
  Efficient ($O(n^3)$ or perhaps $O(n^p)$, independent of condition number)
  Solution of $Ax = b$
  - Small componentwise relative forward error:

$$|x_i - \hat{x}_i| \leq O(\epsilon)|x_i|$$

  - Small componentwise relative backward error:

$$|A_{ij} - \hat{A}_{ij}| \leq O(\epsilon)|A_{ij}|$$

- In particular: Totally Positive Generalized Vandermonde Matrices

$$G_\lambda = \begin{bmatrix} x_1^{\lambda_n} & x_1^{1+\lambda_{n-1}} & \dots & x_1^{n-1+\lambda_1} \\ x_2^{\lambda_n} & x_2^{1+\lambda_{n-1}} & \dots & x_2^{n-1+\lambda_1} \\ & & \ddots & \\ x_n^{\lambda_n} & x_n^{1+\lambda_{n-1}} & \dots & x_n^{n-1+\lambda_1} \end{bmatrix},$$

  $0 < x_1 < x_2 < \cdots < x_n$,
  $0 \leq \lambda_n \leq \ldots \leq \lambda_1$ - integer; $|\lambda| = \lambda_1 + \ldots + \lambda_n$
  - Tool to exploit structure: Schur functions

New results

Type of Matrix		$\det(A)$	A^{-1}	Any minor	GENP GEPP	GECP	SVD	NENP	$Ax=b$ Frwrd*	$Ax=b$ Bckwrd*
Cauchy	Any	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	
	TP	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	n^2
Vandermonde	Any	n^2	No	No	No	No	n^3	n^2	No	
	TP	n^2	n^3	Exp	n^2	Exp	n^3	n^2	n^2	n^2
Polynomial Vandermonde Orthogonal Polynomials	Any	n^2	No	No	No	No	n^3		No	
	†	n^2	n^3				n^3		n^3	
Generalized Vandermonde	Any	No	No	No	No	No	No	No	No	No
	TP	Λn^2	Λn^3	Exp	Λn^2	Exp	Exp	Λn^2	Λn^2	Λn^2

Big-O sense

*Forward Bound: $|x-\hat{x}| \leq O(\epsilon)|A^{-1}||b| \Rightarrow |x-\hat{x}| \leq O(\epsilon)|x|$ for A-TP and x checkerboard
Backward Bound: $|A-\hat{A}| \leq O(\epsilon)|A|$, where $\hat{A}\hat{x}=b$.

† $0 < x_1 < \ldots < x_n$ + Other conditions on the signs of the three-term recurrence

$\Lambda = (\lambda_1+1)(\lambda_2+1)^2 \ldots (\lambda_p+1)^2 p$, where $\lambda = (\lambda_1, \ldots, \lambda_p)$.

Outline of this talk

- Model of arithmetic
- Classical method for achieving the goals for simple examples – The Björck-Pereyra Method for Vandermonde Matrices
- How and why it works?
- Application to TP Generalized Vandermonde matrices

How can we lose accuracy in computing in floating point?

- $\mathrm{fl}(a \otimes b) = (a \otimes b)(1+\delta)$ model of arithmetic with no over/underflow
- OK to multiply, divide, add positive numbers
  Proof: $1+\delta$ factors can be factored out
- $x_i \pm x_j$, where x_i and x_j are initial data (so exact)
- $(x_i + y_j)(x_i - y_{j-1})x_{i+1}/(x_{i-1} - y_j)$ - OK
- *Dangerous cancellation* when subtracting approximate results:

```
    .12345xxx
-   .12345yyy
-------------
    .00000zzz
```

- We will compute everything using only allowable expressions
- Explains our interest in TP matrices, minors > 0

Classical Example: Vandermonde Linear Systems

- The Björck-Pereyra methods solve $Vy = b$, where V is Vandermonde:

$$\begin{bmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ 1 & x_2 & \dots & x_2^{n-1} \\ 1 & x_3 & \dots & x_3^{n-1} \\ & & \ddots & \\ 1 & x_n & \dots & x_n^{n-1} \end{bmatrix} \cdot \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} + \\ - \\ + \\ \vdots \\ - \end{bmatrix}$$

  and $0 < x_1 < \dots < x_n$.

  – In $O(n^2)$ time

  – With small forward error: $|y_i - \hat{y}_i| \le O(\epsilon)|y_i|$

  – With small backward error: If $\hat{V}\hat{y} = b$ then $|V_{ij} - \hat{V}_{ij}| \le O(\epsilon)|V_{ij}|$.

- How does it work?

  – Newton interpolation

The Björck-Pereyra Method (1970)

- Polynomial interpolation: $\begin{array}{c|ccc} x & 1 & 2 & 3 \\ \hline f(x) & 2 & -1 & 14 \end{array}$ by $f(x) = a_1 + a_2 x + a_3 x^2$

  (alternating signs of $f(x)$ for a purpose)

- E.g. solve: $\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2^2 \\ 1 & 3 & 3^2 \end{bmatrix} \cdot \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 2 \\ -1 \\ 14 \end{bmatrix}$.

- GE: $\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 2 & 8 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & \mathit{2} \end{bmatrix}$

- Instead: Newton Interpolation:

x	$f(x)$	$f[\cdot,\cdot]$	$f[\cdot,\cdot,\cdot]$
1	2	2	2
2	-1	$\frac{-1-2}{2-1} = -3$	-3
3	14	$\frac{14-(-1)}{3-2} = 15$	$\frac{15-(-3)}{3-1} = 9$

$$\begin{aligned} f(x) &= 2 - 3(x-1) + 9(x-1)(x-2) \\ &= 2 + 3 + 18 - (3 + 9 + 18)x + 9x^2 \\ &= 23 - 30x + 9x^2 \end{aligned}$$

- No dangerous cancellation

Matrix Interpretation of the Björck-Pereyra Method

- **Matrix version of Newton interpolation**

$$\boldsymbol{y} = \boldsymbol{V}^{-1}\boldsymbol{b} = \begin{bmatrix} 1 & -1 & \\ & 1 & -1 \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ & 1 & -2 \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ & 1 & \\ & -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ -1 & 1 & \\ & -1 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 \\ -1 \\ 14 \end{bmatrix} = \begin{bmatrix} 23 \\ -30 \\ 9 \end{bmatrix}$$

- **Notice:**
  - **Bidiagonal Decomposition of $\boldsymbol{V}^{-1}$ (accurate)**
  - **Checkerboard sign pattern**

  $\Rightarrow$ No dangerous cancellation $\Rightarrow$ High relative accuracy

- **Intrinsic property of all TP matrices**

$$\boldsymbol{A}^{-1} = \begin{bmatrix} 1 & - & \\ & 1 & - \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ & 1 & - \\ & & 1 \end{bmatrix} \cdot \begin{bmatrix} + & & \\ & + & \\ & & + \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ & 1 & \\ & - & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & & \\ - & 1 & \\ & - & 1 \end{bmatrix}$$

Accuracy of the Björck-Pereyra Method for Vandermondes

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & -x_1 & & \\ & 1 & -x_1 & \\ & & 1 & -x_1 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & -x_2 & \\ & & 1 & -x_2 \\ & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & -x_3 \\ & & & 1 \end{bmatrix} \times$$

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & \frac{-1}{x_4-x_1} & \frac{1}{x_4-x_1} \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & \frac{-1}{x_3-x_1} & \frac{1}{x_3-x_1} & \\ & & \frac{-1}{x_4-x_2} & \frac{1}{x_4-x_2} \end{bmatrix} \begin{bmatrix} 1 & & & \\ \frac{-1}{x_2-x_1} & \frac{1}{x_2-x_1} & & \\ & \frac{-1}{x_3-x_2} & \frac{1}{x_3-x_2} & \\ & & \frac{-1}{x_4-x_3} & \frac{1}{x_4-x_3} \end{bmatrix}$$

Accuracy ... OK

Other TP matrices? ... Yes. Cauchy

The Björck-Pereyra Method for Cauchy Matrices

- *Cauchy* matrices

$$C_{ij} = \frac{1}{x_i - y_j}$$

- TP, if $x_1 > \ldots > x_n > y_1 > \ldots > y_n$

$$\begin{bmatrix} \frac{1}{x_1-y_1} & \frac{1}{x_1-y_2} & \frac{1}{x_1-y_3} \\ \frac{1}{x_2-y_1} & \frac{1}{x_2-y_2} & \frac{1}{x_2-y_3} \\ \frac{1}{x_3-y_1} & \frac{1}{x_3-y_2} & \frac{1}{x_3-y_3} \end{bmatrix}^{-1} = \begin{bmatrix} 1 & \frac{-(x_1-y_1)}{y_1-y_2} & 0 \\ 0 & \frac{x_1-y_2}{y_1-y_2} & \frac{-(x_1-y_2)}{y_2-y_3} \\ 0 & 0 & \frac{x_1-y_3}{y_2-y_3} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{-(x_2-y_1)}{y_1-y_3} \\ 0 & 0 & \frac{x_2-y_3}{y_1-y_3} \end{bmatrix} \times$$

$$\begin{bmatrix} x_1 - y_1 & & \\ & x_2 - y_2 & \\ & & x_3 - y_3 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{-(x_1-y_2)}{x_3-x_1} & \frac{x_3-y_2}{x_3-x_1} \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ \frac{-(x_1-y_1)}{x_2-x_1} & \frac{x_2-y_1}{x_2-x_1} & 0 \\ 0 & \frac{-(x_2-y_1)}{x_3-x_2} & \frac{x_3-y_1}{x_3-x_2} \end{bmatrix}$$

(Vadim Olshevsky, 1995)

- Unifying Characteristic?

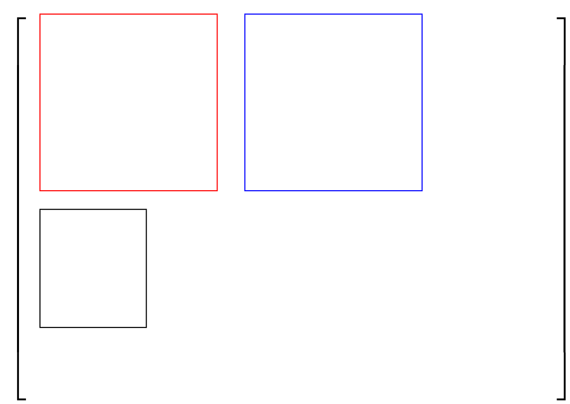
The Connection with Minors

- Which TP matrices permit *accurate* bidiagonal decomposition?
- Each entry is *product of quotients of initial minors*

$$L^{(k)}_{i+1,i} = -\frac{\det(A(i-k+2:i+1,1:k))}{\det(A(i-k+2:i,1:k-1))} \cdot \frac{\det(A(i-k+1:i-1,1:k-1))}{\det(A(i-k+1:i,1:k))}$$

INITIAL MINORS
– Contiguous
– Include first row or column

$A =$



When can we solve TP linear system accurately

- **We can accurately solve TP linear systems iff we can compute accurate initial minors**
- **Initial minors of:**

Cauchy $$\frac{\prod_{i<j}(x_j - x_i)(y_j - y_i)}{\prod_{i,j}(x_i + y_j)};$$ **Vandermonde** $$\prod_{i>j}(x_i - x_j)$$

- **Other classes?**

New results: TP Generalized Vandermonde Matrices

- TP Matrices with initial minors that are easy to compute accurately
  Vandermonde and Generalized Vandermonde

$$V = \begin{bmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ 1 & x_2 & \dots & x_2^{n-1} \\ & & \ddots & \\ 1 & x_n & \dots & x_n^{n-1} \end{bmatrix}, \qquad G_\lambda = \begin{bmatrix} x_1^{\lambda_n} & x_1^{1+\lambda_{n-1}} & \dots & x_1^{n-1+\lambda_1} \\ x_2^{\lambda_n} & x_2^{1+\lambda_{n-1}} & \dots & x_2^{n-1+\lambda_1} \\ & & \ddots & \\ x_n^{\lambda_n} & x_n^{1+\lambda_{n-1}} & \dots & x_n^{n-1+\lambda_1} \end{bmatrix},$$

  where $0 < x_1 < x_2 < \cdots < x_n$, $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$, $|\lambda| = \lambda_1 + \ldots + \lambda_n$

- Initial Minors for G_λ?

$$\det(G_\lambda) = \det(V) \cdot s_\lambda(x_1, x_2, \ldots, x_n)$$

- s_λ - called Schur function
  - Polynomial with positive integer coefficients
  - Widely studied in combinatorics [Macdonald], group representation theory

- Example:

$$\det \begin{bmatrix} 1 & x_1^2 & x_1^4 \\ 1 & x_2^2 & x_2^4 \\ 1 & x_3^2 & x_3^4 \end{bmatrix} = \det \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \cdot (2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1^2x_3 + x_1x_3^2 + x_2^2x_3 + x_2x_3^2)$$

Accuracy and Efficiency for TP Generalized Vandermonde Matrices

- **Example:**

$$\det \begin{bmatrix} 1 & x_1^2 & x_1^4 \\ 1 & x_2^2 & x_2^4 \\ 1 & x_3^2 & x_3^4 \end{bmatrix} = \det \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \end{bmatrix} \cdot (2x_1x_2x_3 + x_1^2x_2 + x_1x_2^2 + x_1^2x_3 + x_1x_3^2 + x_2^2x_3 + x_2x_3^2)$$

- **Accuracy?**
  - $\det(V) = \Pi_{i>j}(x_i - x_j)$ - YES.
  - s_λ - polynomial with nonnegative coefficients - YES.
- **Efficiency?**
  - $\det(V) = \Pi_{i>j}(x_i - x_j)$ - OK.
  - $s_\lambda(x_1, x_2, \ldots, x_n)$?
    * We are only interested in subtraction-free algorithms, thus:

$$\left.\begin{array}{l} s_\lambda = f(\text{elementary symmetric polynomials}) \\ \text{Jacobi} - \text{Trudi identity} \end{array}\right\} - \text{useless}$$

    * Have to evaluate as polynomial ...
    * ... which has exponentially many terms – $n^{|\lambda|}$

Computing the Schur Function

- Def: $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_n)$ is a partition of $|\lambda| = \lambda_1 + \lambda_2 + \cdots + \lambda_n$
- Schur functions are indexed by partitions $s_\lambda(x_1, \ldots, x_n)$
- Generalize the elementary symmetric functions
- Example:

  $s_{(2)}(x_1, \ldots, x_n) = \sum_{i \leq j} x_i x_j =$

  $= x_1 x_1 + (x_1 + x_2)x_2 + (x_1 + x_2 + x_3)x_3 + \ldots + (x_1 + \ldots + x_n)x_n$
- Cost: $3n$, although $s_{(2)}$ has n^2 terms.
- Same trick generalizes. Recursion + memoization. Macdonald:

$$s_\lambda(x, y) = \sum_{\mu < \lambda} s_\mu(x) s_{\lambda/\mu}(y),$$

  x, y - sets of indices
- Complexity reduces

$$\text{from} \quad O\left(n^{|\lambda|}\right) \quad \text{to} \quad \Lambda \cdot n,$$

  where

$$\Lambda = (\lambda_1 + 1)(\lambda_2 + 1)^2 \ldots (\lambda_p + 1)^2$$

New results

Type of Matrix		$\det(A)$	A^{-1}	Any minor	GENP GEPP	GECP	SVD	NENP	$Ax=b$ Frwrd*	$Ax=b$ Bckwrd*
Cauchy	Any	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	
	TP	n^2	n^2	n^2	n^3	n^3	n^3	n^2	n^2	n^2
Vandermonde	Any	n^2	No	No	No	No	n^3	n^2	No	
	TP	n^2	n^3	Exp	n^2	Exp	n^3	n^2	n^2	n^2
Polynomial Vandermonde Orthogonal Polynomials	Any	n^2	No	No	No	No	n^3		No	
	†	n^2	n^3				n^3		n^3	
Generalized Vandermonde	Any	No	No	No	No	No	No	No	No	No
	TP	Λn^2	Λn^3	Exp	Λn^2	Exp	Exp	Λn^2	Λn^2	Λn^2

Big-O sense

*Forward Bound: $|x-\hat{x}| \leq O(\epsilon)|A^{-1}||b| \Rightarrow |x-\hat{x}| \leq O(\epsilon)|x|$ for A-TP and x checkerboard
Backward Bound: $|A-\hat{A}| \leq O(\epsilon)|A|$, where $\hat{A}\hat{x}=b$.

† $0 < x_1 < \ldots < x_n$ + Other conditions on the signs of the three-term recurrence

$\Lambda = (\lambda_1+1)(\lambda_2+1)^2 \ldots (\lambda_p+1)^2 p$, where $\lambda = (\lambda_1, \ldots, \lambda_p)$.

Conclusions

- **TP Structured linear systems can be solved very accurately, if initial minors factor**
- **Implies accurate A^{-1}**
- **New application: Generalized Vandermonde Matrices**
- **New accurate algorithm for computing the Schur function**
  - **Extends to computing Jack polynomials**
- **Not in this talk: Accurate SVDs of**
  - **Some Polynomial Vandermonde Matrices**
  - **Weakly Diagonally Dominant M-matrices**

Open Problems

- **Totally Positive Matrices in general appear impossible. Proof?**
- **Characterize which structured matrices permit accurate and efficient linear algebra**

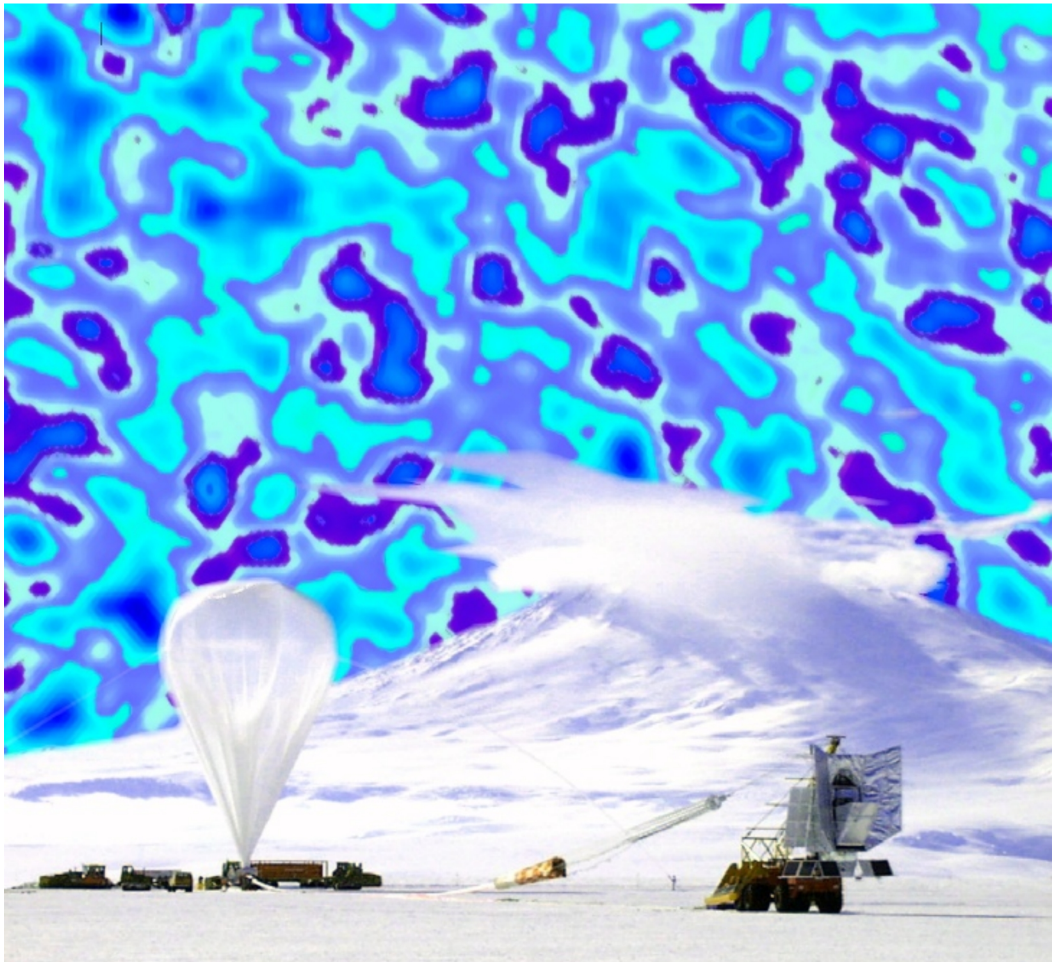
Resources

- **These slides:** `www.math.berkeley.edu/~plamen/hh02.pdf`
- **Reports:**
  - **Plamen Koev, Accurate and Efficient Computations with Structured Matrices, UC Berkeley Ph.D. thesis.**
  - **J. Demmel and P. Koev, Necessary and sufficient conditions for accurate and efficient rational function evaluation and factorizations of rational matrices. In *Structured matrices in mathematics, computer science, and engineering. II (Boulder, CO, 1999)*, pages 117–143. Amer. Math. Soc., Providence, RI, 2001.**
  - **J. Demmel and P. Koev, Accurate and Efficient Matrix Computations with Totally Positive Generalized Vandermonde Matrices Using Schur Functions,** `www.math.berkeley.edu/~plamen/hagen.ps`
  - **J. Demmel, M. Gu, S. Eisenstat, I. Slapničar, K. Veselić, and Z. Drmač. Computing the singular value decomposition with high relative accuracy. *Lin. Alg. Appl.*, 299(1–3):21–80, 1999.**
    `www.cs.berkeley.edu/~demmel/DGESVD.ps`
  - **J. Demmel, Accurate SVDs of structured matrices. *SIAM J. Mat. Anal. Appl.*, 21(2):562–580, 1999.**
    `www.netlib.org/lapack/lawns/lawn130.ps`

Other Interests

- **Large scale parallel applications of structured matrices, e.g.**

Computing the Power Spectrum of the Cosmic Microwave Background Radiation



- **Lowered complexity from $O(n^3)$ to $O(n^{3/2})$**

Other Interests (2)

- Computer Arithmetic
  - Impact of model of arithmetic on algorithms
    e.g. $(1+\delta)$ vs. IEEE
  - Harry Diamond's Theorem and the Table Maker's Dilemma
    f
    $g = f^{-1}$,
    $H = G \circ F$,
    $H(H(H(x))) = H(H(x))$
  - Proved validity when f non strictly convex and IEEE arithmetic rounding to nearest even
- Computational noncommutative algebra
  - Polynomial Identities in Matrix Algebras
  - All identities of degree $2k+2$ in $M_k(\mathrm{Z})$ follow from the *Standard Identity* of Amitzur-Levitzky of degree $2k$.