STILL HAVING FUN AFTER 50 YEARS SOME OF JACK'S GREATEST HITS

Jack Dongarra University of Tennessee Oak Ridge National Laboratory University of Manchester



How Did I Get Here?

- Grew up on the southwest side of Chicago.
- Wanted to be a high school science teacher.
- Attending the "normal school" in Chicago that trained teachers, Chicago State University.
- Took many math and science courses.
- The last year in college everything changed.



Argonne's Undergraduate Research Program

- In the Fall of 1971 the Chair of the Department of Physics at Chicago State University, Harvey Left, suggested I apply to the Argonne's Undergraduate Research Program.
 - About 50 undergraduates from around the country are selected to come to ANL for a semester.
 - What I didn't know was that Harvey Left was a college roommate with Jim Pool who was then the head of Applied Math Division at Argonne.
 - So, my last semester at Chicago State was spent as an intern at Argonne.
- When I started at Argonne I had no formal training in computer science with very little programming experience.
 - I was assigned to work with Brian Smith who was leading the EISPACK effort, and I quickly tried to learn all about linear algebra and eigenvalue problems.
 - I realized that computer science was fun and is what I wanted to pursue.
- Applied to Illinois Institute of Technology for a Master's degree in CS.
 - While working on Master's at IIT worked at Argonne one day a week on EISPACK.
 - Wasn't sure I wanted a PhD.
 - When I graduated from IIT with an MS Jim Pool offered me a job at Argonne.













Features: Performance, Portability, and Accuracy			
EISPACK (1970's)	Rely on		
(Translation of Algol to F66)	- Fortran, but row oriented		



NAG Was a Big Influence (a) ANL and Me

- Argonne's MCS Division had a close relationship with NAG.
- My first overseas trip was to visit NAG in 1975 at the invitation of Brian Ford.
- Met up with Wilkinson at National Physical Laboratory and first met Sven.
- Stopped in at Harwell and visited with Iain and John.











SOFTWARE-PRACTICE AND EXPERIENCE, VOL. 9, 219-226 (1979)

Unrolling Loops in FORTRAN*

J. J. DONGARRA AND A. R. HINDS Argonne National Laboratory, Argonne, Illinois 60439, U.S.A.

SUMMARY

The technique of 'unrolling' to improve the performance of short program loops resorting to assembly language coding is discussed. A comparison of the benefit 'unrolling' on a variety of computers using an assortment of FORTRAN compresented.

- Reduces loop overhead
 - Level of unrolling dedicated by the instruction stack size
- Help the compiler to:
 - Facilitates pipelining
 - Increases the concurrence between independent functional units
- Provided ~15% performance improvement

TECHNIQUE

When a loop is unrolled, its contents are replicated one or more times, with appropriate adjustments to array indices and the loop increment. For instance, the DAXPY⁹ sequence, which adds a multiple of one vector to a second vector:

DO 10 I = 1,N Y(I) = Y(I) + A * X(I)10 CONTINUE

would, unrolled to a depth of four, assume the form

M = N - MOD(N,4)DO 10 I = 1,M,4 Y(I) = Y(I) + A * X(I) Y(I+1) = Y(I+1) + A * X(I+1) Y(I+2) = Y(I+2) + A * X(I+2) Y(I+3) = Y(I+3) + A * X(I+3) 10 CONTINUE

Basic Linear Algebra Subprograms for Fortran Usage

C. L. LAWSON Jet Propulsion Laboratory R. J. HANSON Sandia Laboratories D. R. KINCAID The University of Texas at Austin and F. T. KROGH Jet Propulsion Laboratory

A package of 38 low level subprograms for many of the basic operations of numerical linear algebra is presented. The package is intended to be used with Fortran. The operations in the package include dot product, elementary vector operation, Givens transformation, vector copy and swap, vector norm,





Features: Performance, Portability, and Accuracy			
EISPACK (1970's) (Translation of Algol to F66)	Rely on - Fortran, but row oriented		
Level 1 Basic Linear Algebra Subprograms (BLAS)	Standards for: Vector-Vector operations		





Features: Performance, Portability, and Accuracy			
EISPACK (1970's) (Translation of Algol to F66)		Rely on - Fortran, but row oriented	
Level 1 Basic Linear Algebra Subprograms		Standards for: Vector-Vector operations	
LINPACK (1980's) (Vector operations)		Rely on - Level-1 BLAS operations - Column oriented	

An Accidental Benchmarker

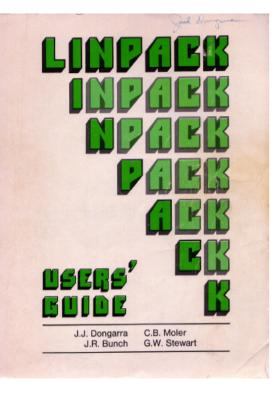
Top 23 List from 1977

Appendix B of the Linpack Users' Guide

• Designed to help users extrapolate execution time for Linpack

software package LINPACK was an NSF Project w/ ANL, UNM, UM, & UCSD First benchmark report from 1977 Worked independentivalid came to Argonne in the summers

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	NCAR 3.5	¥.192	0.56	CRAY-1	ន ន	CFT
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	U. Ill. Chicago	\$4.10	11.9	-IBM 370/158	D	G1





- Encouraged to pursue PhD by many visitors.
- Cleve said he would customize a degree program at the U of New Mexico in the Math Department.
- I was detailed from Argonne to work at Los Alamos (LANL).
 - > Programmed the first Cray-1's.
 - > Found a bug in the Cray-1 HW with the Linpack Ben
- Spent one semester at UNM@LANL, the 2 semesters on UNM campus.
- Cleve was at Stanford on Sabbatical my last year at UNM.
 - The plan was to finish my courses & exan and then join Cleve at Stanford.
- On to Stanford and Serra House.



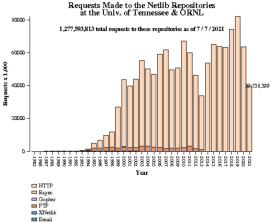




Netlib Mathematical Software & More Over 1.2 B Served

- Began in 1984
 - Eric Grosse @ Bell Labs and JD @ ANL
 - Motivated by need for cost-effective, timely distribution of highquality mathematical software to the community.
- One of the first open source software collections.
- Designed to send, by return electronic mail, requested items. Email to <u>netlib@mcs.anl.gov</u> an in the body of the email: Send dgefa from linpack
- Moderated collection /Distributed maintenance
- Also mail forwarding in 1983 & na-digest started in 1987.



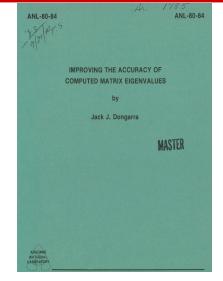


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Exploiting Mixed Precision

- Wilkinson gave a lecture at ANL on the topic of improving λ 's.
- My interest in mixed precision began with my dissertation ...
 - Improving the Accuracy of Computed Matrix Eigenvalues
 - Compute the eigenvalues and eigenvector in low precision then improve selected values/vectors to higher precision for O(n²) ops using the the matrix decomposition
 - Extended to singular values, 1983
 - Algorithm in TOMS 710, 1992



SIAM J. NUMER. ANAL. Vol. 20, No. 1, February 1983 © 1983 Society for Industrial and Applied Mathematics 0036-1429/83/2001-0002 \$01.25/0

IMPROVING THE ACCURACY OF COMPUTED EIGENVALUES AND EIGENVECTORS*

J. J. DONGARRA,† C. B. MOLER‡ and J. H. WILKINSON§

Abstract. This paper describes and analyzes several variants of a computational method for improving the numerical accuracy of, and for obtaining numerical bounds on, matrix eigenvalues and eigenvectors. The method, which is essentially a numerically stable implementation of Newton's method, may be used to "fine tune" the results obtained from standard subroutines such as those in EISPACK [Lecture Notes in Computer Science 6, 51, Springer-Verlag, Berlin, 1976, 1977]. Extended precision arithmetic is required in the computation of certain residuals.

Introduction. The calculation of an eigenvalue λ and the corresponding eigenvector x (here after referred to as an eigenpair) of a matrix A involves the solution of the nonlinear system of equations

 $(A-\lambda I)x=0.$



WHY MIXED PRECISION?

- There are many reasons to consider mixed precision in our algorithms...
 - Less Communication
 - Reduce memory traffic
 - Reduce network traffic
 - Reduce memory footprint
 - More Flop per second
 - Reduced energy consumption
 - Reduced time to compute
 - Accelerated hardware in current architecture.
 - Suitable numerical properties for some algorithms & problems.



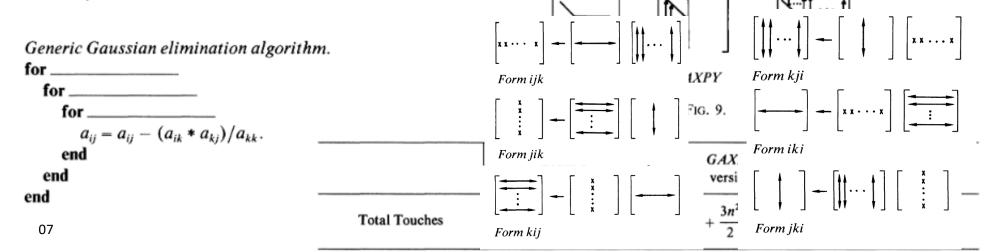
Did A Brief Postdoc at IBM Watson – IJK Paper

SIAM REVIEW Vol. 26, No. 1, January, 1984 © 1984 Society for Industrial and Applied Mathematics 0036-1445/84/2601-0003 \$01.25/0

IMPLEMENTING LINEAR ALGEBRA ALGORITHMS FOR DENSE MATRICES ON A VECTOR PIPELINE MACHINE*

J. J. DONGARRA, † F. G. GUSTAVSON ‡ AND A. KARP§

Abstract. This paper examines common implementations of linear algebra algorithms, such as matrixvector multiplication, matrix-matrix multiplication and the solution of linear equations. The different versions are examined for efficiency on a computer architecture which uses vector processing and has pipelined instruction execution. By using the advanced architectural features of such machines, one can usually achieve maximum performance, and tremendous improvements in terms of execution speed can be seen over conventional computers. Generic matrix multiplication algorithm. for _____ = 1 to _____ for _____ = 1 to _____ for _____ = 1 to _____ $c_{ij} = c_{ij} + a_{ik} * b_{kj}$ end end end



Argonne Math & CS Division 1986



Back row: Jim Boyle (w/picture of Larry Wos), John Gabriel, Ken Dritz, Joe Cook, Bob Veroff, Hans Kaper, Paul Messina, Bernie Matkowsky, Jim Cody, James Lyness, Wayne Cowell, Bert Garbow, Ken Hillstrom, Brian Smith, ? Seated: JD, Rusty Lusk, Mike Minkoff, Larry Leaf, Jorge More', Danny Sorensen, Bruce Char, Doris Pool, Judy Beumer





Features: Performance, Portability, and Accuracy			
EISPACK (1970's) (Translation of Algol to F66)		Rely on - Fortran, but row oriented	
Level 1 Basic Linear Algebra Subprogram	ns (BLAS)	Standards for: Vector-Vector operations	
LINPACK (1980's) (Vector operations)		Rely on - Level-1 BLAS operations - Column oriented	
Level 2 & 3 BLAS - ATLAS	$\begin{array}{c} \text{GEMV:} \end{array} \overbrace{p}^{\text{GEMA:}} \\ A \\$	Standards for: Matrix-Vector & Matrix-Matrix operations	

An Extended Set of FORTRAN Basic Linear Algebra Subprograms

JACK J. DONGARRA Argonne National Laboratory JEREMY DU CROZ and SVEN HAMMARLING Numerical Algorithms Group, Ltd. and RICHARD J. HANSON Sandia National Laboratory

ACM Transactions on Mathematical Software, Vol. 14, No. 1, March 1988, Pages 1-17.

A Set of Level 3 Basic Linear Algebra Subprograms

JACK J. DONGARRA University of Tennessee and Oak Ridge National Laboratory JEREMY DU CROZ and SVEN HAMMARLING Numerical Algorithms Group, Ltd. and IAIN DUFF Harwell Laboratory

ACM Transactions on Mathematical Software, Vol. 16, No. 1, March 1990, Pages 1-17.

Summer's in East Hagbourne & Oxford

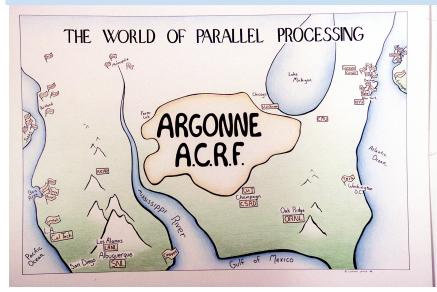


Argonne's Parallel Menagerie



Several radically different parallel architectures, from shared to distributed memory; from vector to dataflow to bit parallel processors

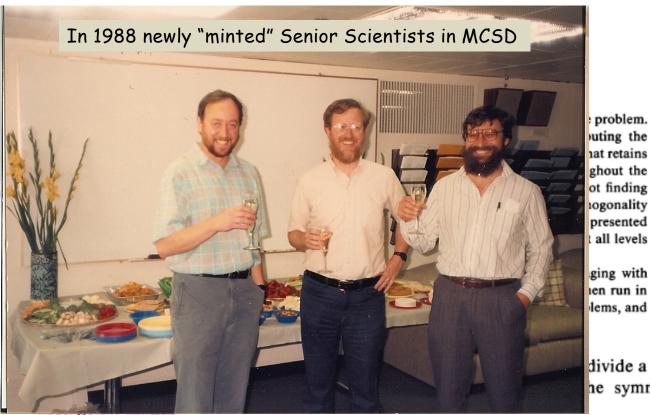
Thinking Machines CM-2, w/16,384 procs. Active Memory Technology DAP-510, w/1024 procs. BBN TC 2000 (Butterfly II), w/32 procs. Cydrom Cydra 5, VLIW architecture Denelcor HEP, w/4 PEMs Intel iPSC/d5 hypercube w/32 procs. Sequent Balance 21000, w/24 procs. Encore Multimax, w/20 procs. Intel iPSC/d4 hypercube, w/16 vector procs. Alliant FX/8, w/8 vector procs. Ardent Titan graphics supercomputer, w/4 vector procs.



6

SIAM J. SCI. STAT. COMPUT. Vol. 8, No. 2, March 1987

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(2.1)
$$T = \begin{pmatrix} T_1 & \beta e_k e_1^T \\ \beta e_1 e_k^T & T_2 \end{pmatrix} = \begin{pmatrix} \hat{T}_1 & 0 \\ 0 & \hat{T}_2 \end{pmatrix} + \theta \beta \begin{pmatrix} e_k \\ \theta^{-1} e_1 \end{pmatrix} (e_k^T, \theta^{-1} e_1^T)$$

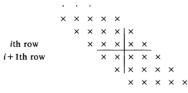


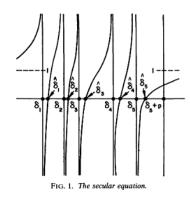
This algorithm can be generalized to handle band matrices as well. Instead of performing a rank-one tearing to split the matrix into two independent subproblems, we proceed by making (m+1)m/2 rank-one changes designed to split the matrix, (m is the half bandwidth, m = 1 for tridiagonal matrices).

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ging with ien run in lems, and

divide a given he symmetric





In 1989 Decided to Move to Tennessee

Bob Ward and Mike Heath made me an offer I couldn't refuse Moved and setup shop: "Innovative Computing Laboratory"



















Based on the block Householder work of Charlie VL and Chris B...

Block reduction of matrices to condensed forms for eigenvalue computations

Jack J. DONGARRA* and Danny C. SORENSEN**

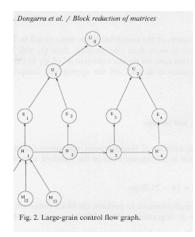
Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL 60439, U.S.A.

Sven J. HAMMARLING

Numerical Algorithms Group Ltd., Wilkinson House, Jordan Hill Road, Oxford, United Kingdom OX2 8DR

Received 11 February 1988 Revised 7 October 1988

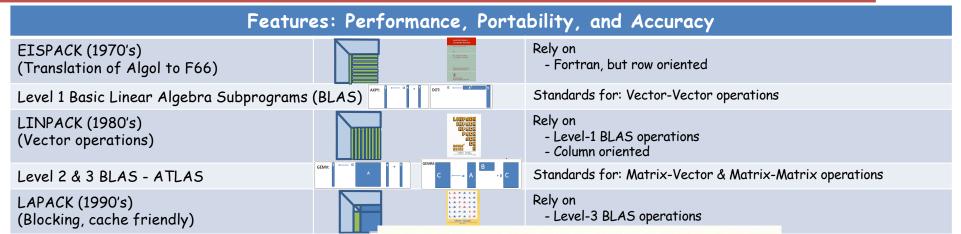
Abstract: In this paper we describe block algorithms for the reduction of a real symmetric matrix to tridiagonal form and for the reduction of a general real matrix to either bidiagonal or Hessenberg form using Householder transformations. The approach is to aggregate the transformations and to apply them in a blocked fashion, thus achieving algorithms that are rich in matrix-matrix operations. These reductions to condensed form typically comprise a preliminary step in the computation of eigenvalues or singular values. With this in mind, we also demonstrate how the initial reduction to tridiagonal or bidiagonal form may be pipelined with the divide and conquer technique for computing the eigensystem of a symmetric matrix or the singular value decomposition of a general matrix to achieve algorithms which are load balanced and rich in matrix-matrix operations.



23









Missing C. Bischof, S. Blackford, A. McKinney, D. Sorensen



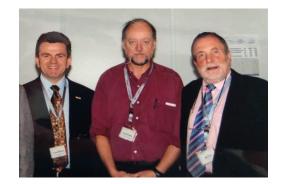


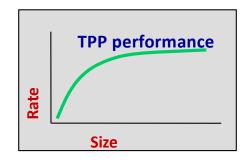


Top500 Since 1993

- Since 1978 I maintained a LINPACK Benchmark list.
- Hans Meuer and Erich S. had a list of fastest computers ranked by peak performance
- Listing of the 500 most powerful computers in the World
- Yardstick: Performance for *Ax=b, dense problem*

Maintained and updated twice a year SC'xy in the States in November









PVM

Parallel Computing was off and running, but no standards existed.

- Al Geist and Vaidy Sunderam started the project in the summer of 1989 at ORNL.
 - Version 1 was used internally at ORNL and not released.
- Liz Jessup came to ORNL as the Householder Fellow, July 1990 - July 1991

Bob Manchek

- Bob was hired by ICL to rewrite PVM and work on extending a DAG based programming system built on PVM called SCHEDULE.
- PVM was done by 6 people in the mountains of Tennessee.
- Many message passing systems in use.
- Clear a standard was needed.





PVM

ORNL/TM-12231

Engineering Physics and Mathematics Division Mathematical Sciences Section

A PROPOSAL FOR A USER-LEVEL, MESSAGE-PASSING INTERFACE IN A DISTRIBUTED MEMORY ENVIRONMENT

Jack J. Dongarra [‡]§ Rolf Hempel ¶ Anthony J. G. Hey [†] David W. Walker §

- Department of Computer Science 107 Ayres Hall Knoxville, TN 37996-1301
- [†] Department of Electronics and Computer Sciences University of Southampton Southampton, SO9 5NH United Kingdom
- ¶ Gesellschaft f
 ür Mathematik und Datenverarbeitung mbH P. O. Box 1316 D-5205 Sankt Augustin 1 Germany
- Mathematical Sciences Section
 Oak Ridge National Laboratory
 P.O. Box 2008, Bldg. 6012
 Oak Ridge, TN 37831-6367

The Center for Research on Parallel Computation at Rice University

Chameleon P4 P4 CEGMSG Chameleon P4 CONND CCMND CCMND CCMND

Draft report in November 1992 Many meeting involving the community MPI standard introduced in 1994









Features: Performance, Portability, and Accuracy			
EISPACK (1970's) (Translation of Algol to F66)		Rely on - Fortran, but row oriented	
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LINPACK (1980's) (Vector operations)		Rely on - Level-1 BLAS operations - Column oriented	
Level 2 & 3 BLAS - ATLAS	$[GEMV:] \longrightarrow \alpha \qquad A \qquad F + V \qquad GEMM: C \qquad - \alpha \qquad A \qquad + \beta$	 Standards for: Matrix-Vector & Matrix-Matrix operations 	
LAPACK (1990's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations	
PVM and MPI		Standards for: Message passing	
ScaLAPACK (2000's) (Distributed Memory)		Rely on - PBLAS Mess Passing	





Features: Performance, Portability, and Accuracy			
EISPACK (1970's) (Translation of Algol to F66)		Rely on - Fortran, but row oriented	
Level 1 Basic Linear Algebra Subprograms		Standards for: Vector-Vector operations	
LINPACK (1980's) (Vector operations)	Literaes Records Becker Acce Acce Acce Acce Acce Acce Acce Ac	Rely on - Level-1 BLAS operations - Column oriented	
Level 2 & 3 BLAS - ATLAS	$GEMV: \boxed{ \begin{array}{c} \bullet \\ \bullet \end{array}} \xrightarrow{\alpha} \left(\begin{array}{c} \bullet \\ \bullet \end{array} \right) \xrightarrow{\alpha} \left(\begin{array}{c} \bullet \\ \end{array} \right) \xrightarrow{\alpha} \left(\begin{array}{c} \bullet \end{array} \right) \xrightarrow{\alpha} \left(\begin{array}{c} \bullet \\ \end{array} \right) \xrightarrow{\alpha} \left(\begin{array}{c} \bullet \end{array} \right)$	Standards for: Matrix-Vector & Matrix-Matrix operations	
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ScaLAPACK (2000's) (Distributed Memory)		Rely on - PBLAS Mess Passing	
PLASMA / DPLASMA / MAGMA (2010's) (Many-core friendly & GPUs)		Rely on - DAG/scheduler - block data layout	
PaRSEC		Standards for: Scheduling	

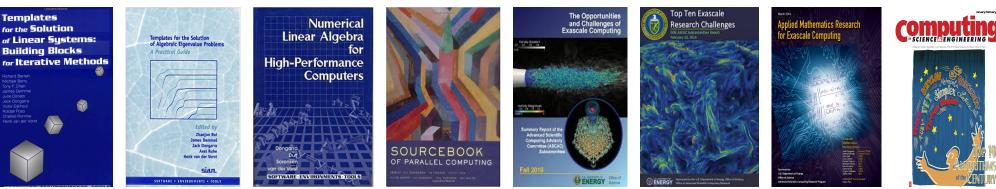




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LINPACK (1980's) (Vector operations)	Literates Litera	Rely on - Level-1 BLAS operations - Column oriented	
Level 2 & 3 BLAS - ATLAS	$GEMV: \boxed{\begin{array}{c} & \\ & \\ \end{array}} \xrightarrow{\alpha} \\ A \\ \end{array} \xrightarrow{\alpha} + \overbrace{}^{\alpha} \\ C \\ \xrightarrow{\alpha} \\ C \\ \xrightarrow{\alpha} \\ \end{array} \xrightarrow{\alpha} A \\ \xrightarrow{\beta} \\ C \\ \xrightarrow{\beta} \\ C \\ \xrightarrow{\beta} \\ \end{array} \xrightarrow{\beta} C \\ \xrightarrow{\beta} \\ C \\ \xrightarrow{\beta} \\ C \\ \xrightarrow{\beta} \\ \end{array} \xrightarrow{\beta} C \\ \xrightarrow{\beta} \\ C \\ \xrightarrow{\beta} \\ $	Standards for: Matrix-Vector & Matrix-Matrix operations	
LAPACK (1990's) (Blocking, cache friendly)		Rely on - Level-3 BLAS operations	
PVM and MPI		Standards for: Message passing	
ScaLAPACK (2000's) (Distributed Memory)		Rely on - PBLAS Mess Passing	
PLASMA / DPLASMA / MAGMA (2010's) (Many-core friendly & GPUs)		Rely on - DAG/scheduler - block data layout	
PaRSEC		Standards for: Scheduling	
SLATE (2020's) (DM and Heterogeneous arch)		Rely on C++ - Tasking DAG scheduling - Tiling, but tiles can come from anywhere - Heterogeneous HW, Batched dispatch	

Community Efforts

- BLAS
- MPI
- Top500
- International Exascale SW Project
- Big Data / Extreme Computing
- Collaborative Books
- Various National Reports





COMPUTING 2





Today's HPC Environment for Numerical Libraries

- Highly parallel
 - Distributed memory
 - MPI + Open-MP programming model
- Heterogeneous
 - Commodity processors + GPU accelerators
- Simple loop level parallelism too limiting in terms of performance
- Communication between parts very expensive compared to floating point ops
- Comparison of operation counts may not reflect time to solution
- Floating point hardware at 64, 32, and 16 bit levels





Parallel Region

half

single

double

quadruple

Serial Region

128 bits

Serial Region

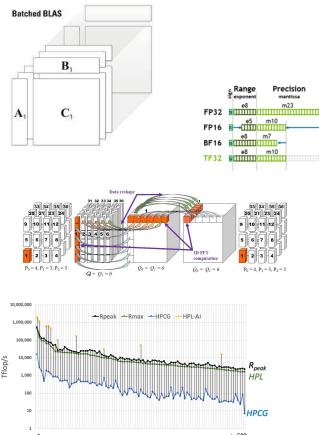




 $2^{-113} \simeq 9.6 \times 10^{-31}$

Today The Fun Continues at ICL ...

- SLATE, PLASMA, MAGMA, BALLISTIC
- Batched BLAS
- Mixed Precision Computations
- heFFTe
- PAPI
- PaRSEC
- TOP500/HPL, HPCG, HPL-AI
 - My hobby



Top500 Rank

Innovative Computing Laboratory, 2019



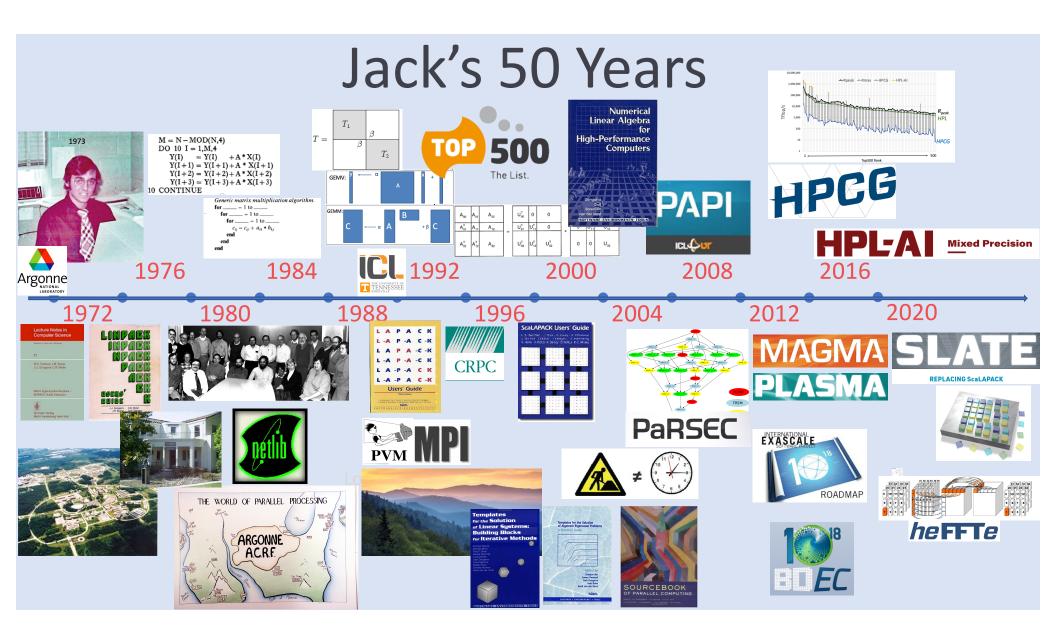
Stats from ICL: 33 PhD Graduates; 34 PostDocs; 135 Grad Students; 168 Staff



Mentors









Thanks to So Many People: Mentors, Colleagues Friends, Staff, and Students

Abdelfattah A Avala A **Beguelin** A Bouteiller A Cappello F Chow E Dong T Fagg G Garbow B Grodd B Heuveline V Kennedy K Lemarinier P Ma, T Meuer H Mrozek D Pool J Schreiber R Snir M Strohmaier E Vadhivar S Whaley R

Agullo E Baboulin M Berman F Boyle J Casanova H Cowell W Dongarra S Faverge M Gates M Guermouche A Higham N Keves D Ltaief H Manchek R Mohr B Mucci P Pozo R Schulthess T Solca R Sunderam V VandeGeign R Wilkinson J

Anderson E Barrett R Blackford S Browne S Chan T Danalis A Du P Finney J Geist A Haidar A Jagode H Kranzlmuller D Lumsdaine A Margues O Moler C Nath R Rafferty T Sevmour K Song F Tisseur F VanderVorst H Wolf F

Angskun T Beck M Blanchard P Buttari A Charara A Davis T Ducroz J Ford B Golub G Hammarling S Johnsson L Kurzak J Lusk R Matsuoka S Moore K Petitet A Reed D Shi Z Sorensen D Tomov S Walker D Wolski R



Ø **NVIDIA**.



Yamazaki I

Anzt H

Bland W

Chen Z

Duff I

Fox G

Canning A

Demmel J

Graham R

Herault T

Kabir K

Langou J

Luszczek P

Mawussi Z

Moore S

Robert Y

Simon H

Srikara P

Wang L

Tourancheau B

Beckman P



Bosilca G Cao C Choi J Desprez F Eiikhout V Gabriel E Grigori L Herrmann J Kagstrom B Langou J Lyness, J Messina P Moore T Piesivac-Grbovic J Plank J Roche K Smith. B Stewart P Tsai M Wasniewski J YarKhan A

Arnold D

Becker D



The MathWorks

