



# **Cray X1 Scientific Libraries**

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# LibSci for the Cray X1 System



## Topics

- What's in LibSci?
- What's new? What's changed?
- How does LibSci perform?
- Any hints for using LibSci?
- What's coming in future releases?



# What's in LibSci?

## Libraries Included



- FFTs
- BLAS
- LAPACK
- ScaLAPACK/BLACS
- Parallel FFTs (deferred until 12/03)
- Sparse direct solver (deferred until 12/03)



# What's in LibSci?

## Features



- Support for data types
  - 32 bit integers/32 bit reals, 64 bit double precision
  - 64 bit integers/64 bit reals
- Support for MSP and SSP modes
- Distributed memory parallel routines
  - ScaLAPACK and BLACS
  - FFTs (deferred until 12/2003)



# What's new? What's changed?

## New Features



- Updated routines:
  - LAPACK version 3.0 (+ updates)
  - ScaLAPACK version 1.7 (+ updates)
- Double precision routines provided (default LibSci only)



# What's new? What's changed?

## Data Type Support



- Default LibSci
  - 32 bits: **INTEGER, REAL**
  - 64 bits: **DOUBLE PRECISION, COMPLEX**
  - 128 bits: **DOUBLE COMPLEX**
- 64-bit LibSci (**-sdefault64**)
  - 64 bits: **INTEGER, REAL**
  - 128 bits: **COMPLEX**



# What's new? What's changed?

## Linking to LibSci



- To use default LibSci:
  - No need to specify library when linking
  - May use **-lsci** or **-lsci32**
- To link to 64-bit LibSci:
  - Use **-sdefault64** when linking (**ftn**)
  - Or, use **-lsci64**



## What's new? What's changed?



### Single Precision Support

- Single precision routines:
  - ‘S’ routines and ‘C’ routines
  - Example:  
**SCOPY(N, X, INCX, Y, INCY)**  
**CCOPY(N, X, INCX, Y, INCY)**
- Available in both default and 64-bit libraries
- 64-bit library supports Cray legacy codes
- Read FFT documentation for using default library (**TABLE** array is always 64-bit words)





# What's new? What's changed?

## Double Precision Support



- New to Cray X1 System
- Double precision routines provided
  - ‘D’ routines and ‘Z’ routines
  - Example:  
**DCOPY(N, X, INCX, Y, INCY)**  
**ZCOPY(N, X, INCX, Y, INCY)**
- Only available in default LibSci



## What's new? What's changed?

More info...



- For 64 bit integers, use 64-bit LibSci
- ScaLAPACK, BLACS only in default LibSci
- Providing Fortran module block interfaces is deferred until 2004



# What's new? What's changed?

## Unsupported Routines



- Non-standard BLAS routines
- Out-of-core solvers
- Sparse iterative solvers
- LINPACK, EISPACK



# How does LibSci Perform?

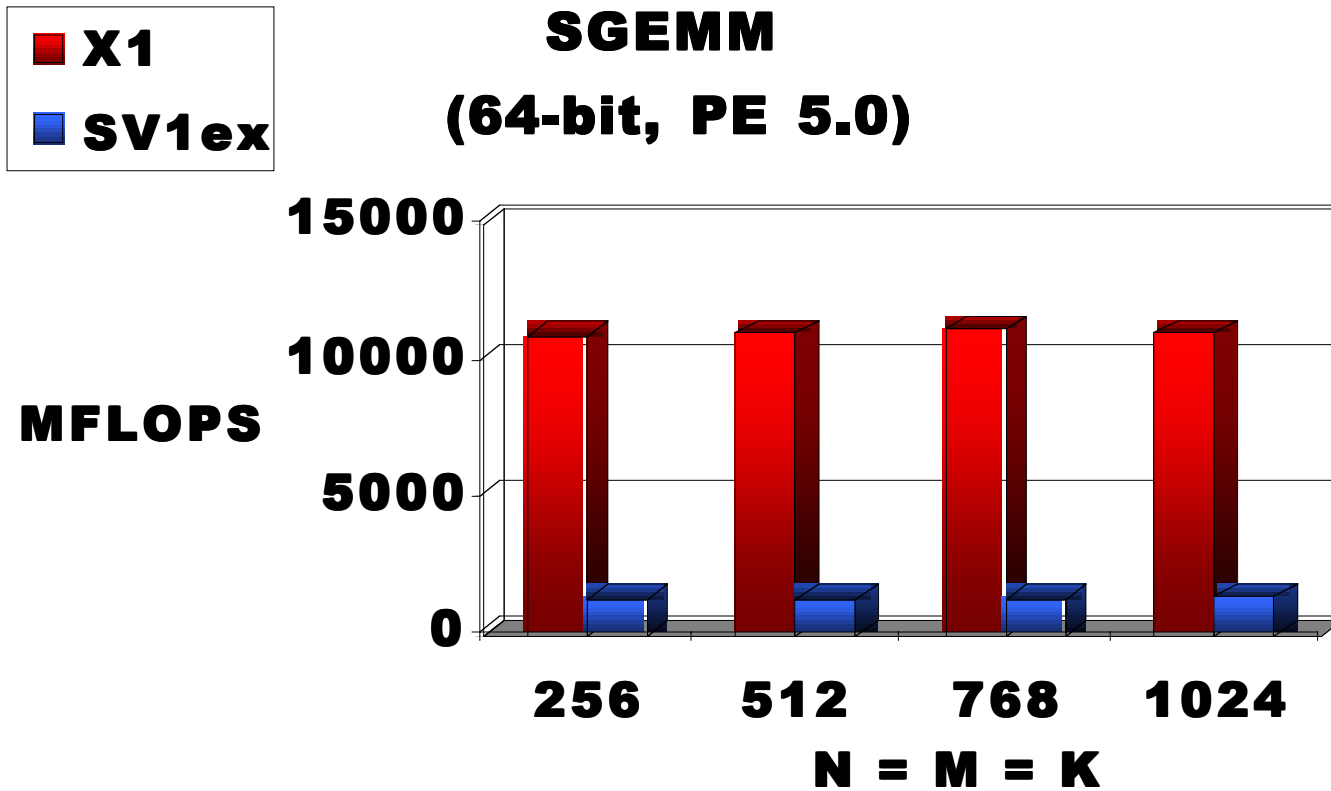
## Performance Status



- Performance is improving
- Tuning single processor case
  - BLAS level 2 and 3
  - FFTs
- Started LAPACK and ScaLAPACK
- Published LINPACK benchmark results



# How does LibSci perform?



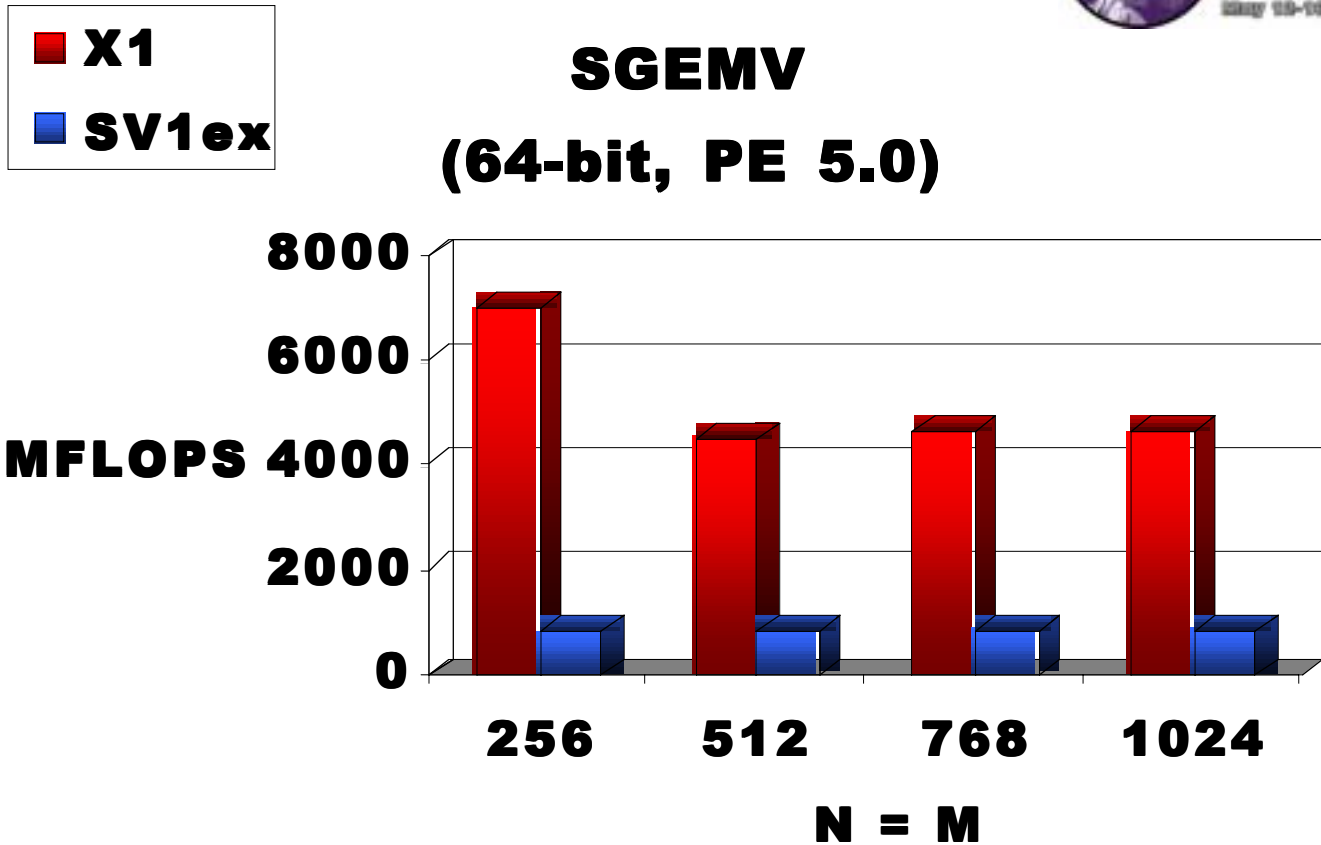
LDA = odd mult of 4

TRANS = 'N'

LibSci 5.0.0.4



# How does LibSci perform?



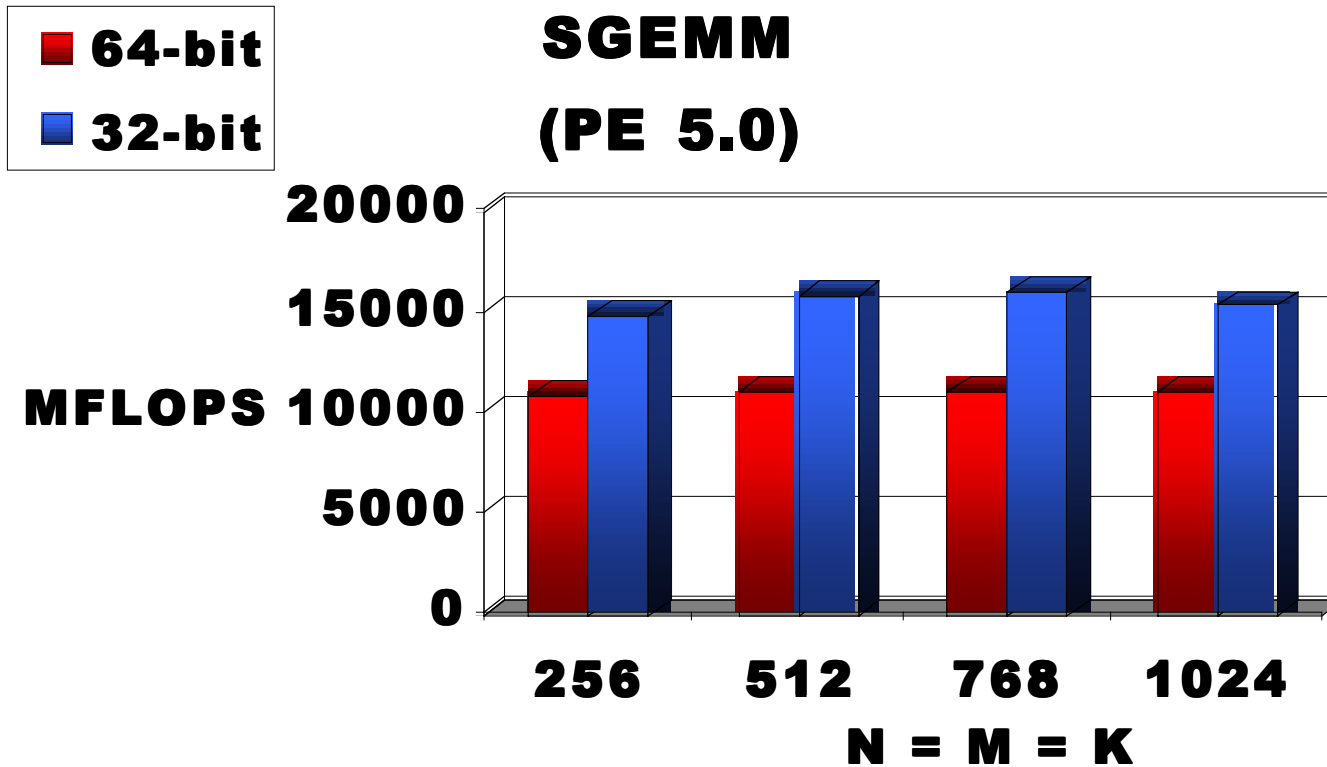
LDA = odd mult of 4

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LibSci 5.0.0.4



# How does LibSci perform?



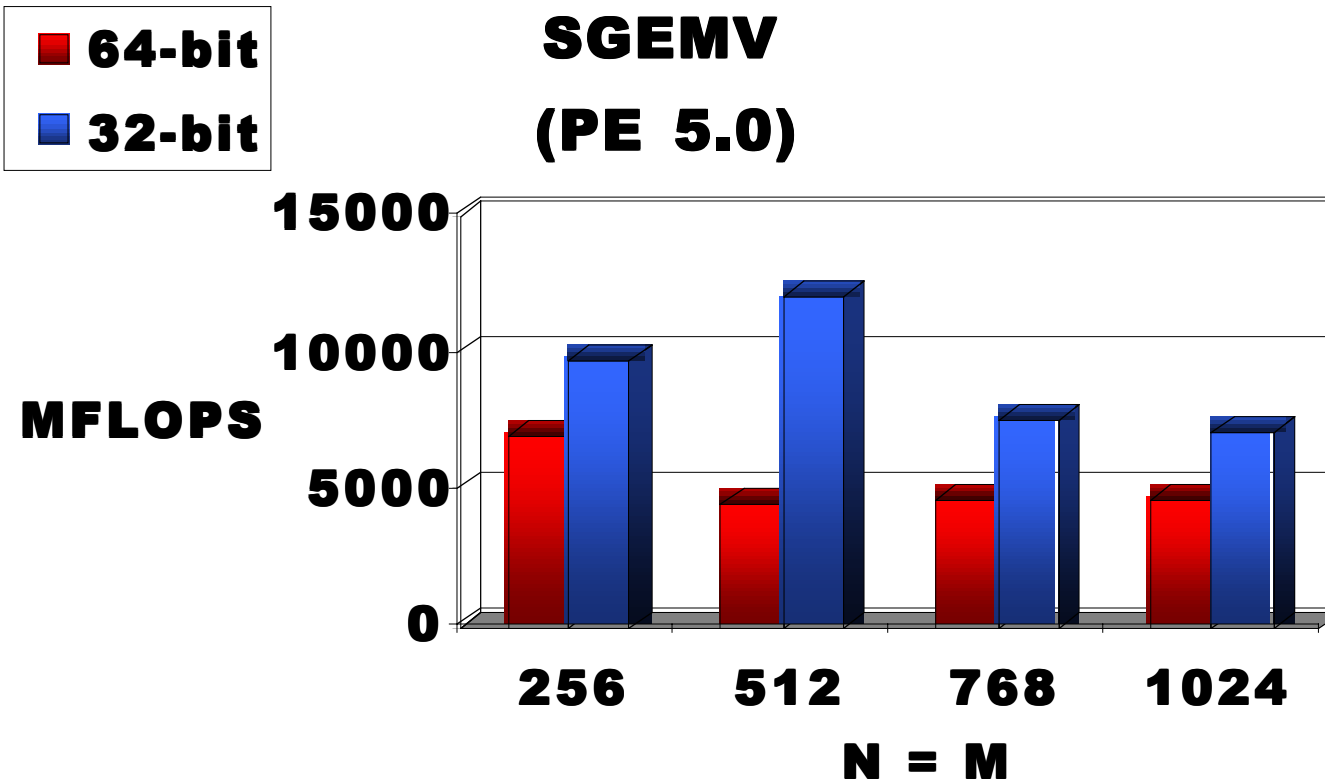
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# How does LibSci perform?



LDA = odd mult of 4

TRANS = 'N'

LibSci 5.0.0.4





## How does LibSci perform?

### LINPACK Benchmark

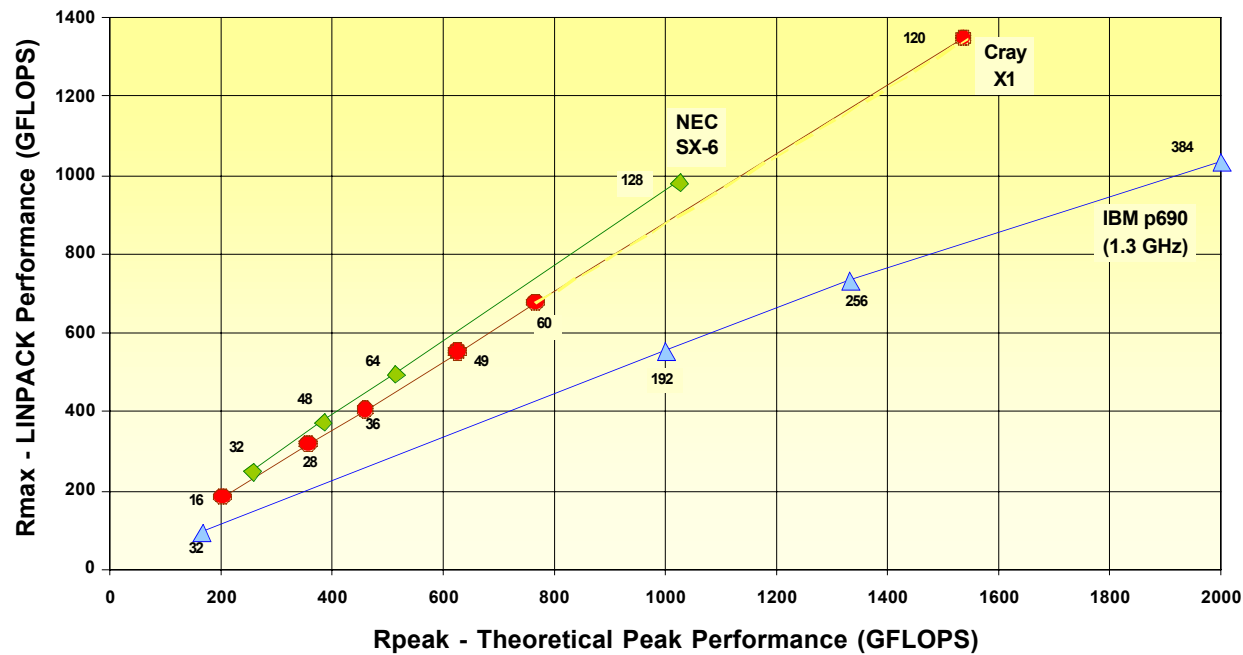


- Published first LINPACK results for Cray X1 systems
- Results for 4 – 60 MSPs
- Achieves about 90% of peak
  - Use highly tuned sgemm (12 Gflops)
  - Implemented with shmem



# How does LibSci perform?

## LINPACK Benchmark



Note: 120 MSP result for Cray X1 is estimated.



# LINPACK Benchmark



Computer	Processors (MSPs)	Rmax [GFLOPS]	Nmax	N 1/2	Rpeak
[GFLOPS]					
Cray X1	60	675.5	168960	20160	768.0
Cray X1	49	550.5	150528	16128	627.2
Cray X1	36	404.3	129024	13824	460.8
Cray X1	28	318.1	114688	11302	358.4
Cray X1	16	182.3	81920	8242	204.8
Cray X1	12	137.6	73728	6294	153.6
Cray X1	8	92.4	61440	4996	102.4
Cray X1	4	46.5	41984	3048	51.2



# Performance Comparison Of Cray X1 System with 8 MSPs

Computer		CPUs	Rmax [GFLOPS]	Rpeak [GFLOPS]	% of peak
<b>Cray X1</b>	<b>800 MHz</b>	<b>8</b>	<b>92.4</b>	<b>102.4</b>	<b>90%</b>
IBM P690 Turbo	1.3 GHz	32	91.3	166.4	55%
HP Superdome	552 MHz	64	86.4	141.3	61%
Cray T3E 1200E	600 MHz	112	90.4	134.0	67%
NEC SX-6	500 MHz	8	63.2	64.0	99%
SGI Origin 3000	600 MHz	128	125.5	154.0	81%



# Any hints for using LibSci?

## Documentation



- Currently available:
  - Man pages
    - intro\_libsci, intro\_fft,
    - intro\_blas1, intro\_blas2, intro\_blas3,
    - intro\_lapack, intro\_scalapack, intro\_blacs
  - Manuals
    - *Cray X1 User Environment Differences*
    - *Migrating Applications to Cray X1 Systems*



# Any hints for using LibSci?

## Documentation



- More coming:
  - *Optimizing Applications on the Cray X1 System*  
(adding chapter for using LibSci)
  - A Libsci reference manual



# Any hints for using LibSci?

## Hints



- Use odd strides for FFTs, odd multiples of 4 for BLAS
- Check data types carefully!
  - Try **-U CRAY** if stumped
- Use standard conventions if calling from C
- Check *Cray X1 User Environment Differences* manual for list of unsupported routines



# What's coming?

## Coming Features



- PE 5.0 release of LibSci:
  - Improved BLAS, FFTs, LAPACK
  - ScaLAPACK and BLACS
  - SSP mode available
- PE 5.1 release of LibSci:
  - Improved performance
- 12/2003: Parallel FFTs, Sparse direct solver





# Cray X1 Scientific Libraries

## Acknowledgements



- Scientific Libraries Group
  - Bracy Elton: FFTs
  - Chao Yang: BLAS, LINPACK, Sparse solvers
  - Rick Hangartner: BLAS
  - Neal Gaarder: BLAS
  - Wendy Thrash: FFTs
- Others:
  - Kitrick Sheets, Jim Hoekstra (ISU)