

Performance of Thyra Adapters in Anasazi

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1 Introduction

Anasazi is a Trilinos package for solving large-scale eigenvalue problems. In order to achieve as much flexibility as possible, the components of the package are templated according to scalar type and linear algebra objects (multivectors and operators). The functionality of these objects are accessed via traits classes, specialized on the template classes. Therefore, to make use of a particular linear algebra library for the underlying computation, the user needs only to implement specializations of these traits classes for the particular linear algebra objects. This creates a sort of wrapper around the functionality, without requiring the user to modify the inheritance hierarchy of the classes.

Thyra is a Trilinos package which defines a set of interfaces designed to ease interoperability of different numerical packages. Filling out specializations of the Anasazi traits classes allows any underlying linear algebra to be used with Anasazi. However, designing a linear algebra library in the Thyra framework allows this library to be used with any numerical software that recognizes Thyra.

With this in mind, Anasazi provides an adapter (via a traits class specialization) to the Thyra interfaces, to ease the interoperability of Anasazi with other packages. The goal of this report is to examine the performance overhead of using this adapter. The purpose of this is to document any such overhead, as users may be curious about the cost of using the adapter. Another goal is to discover inefficiencies in the adapter to allow their remedy.

2 Methodology

It is expected that there will be a small amount of overhead resulting from the use of the Anasazi adapters to Thyra. This overhead should be constant-time, and therefore should diminish in effect as the size of the problem increases. The study will be the solution of a general sparse eigenvalue problem. The overhead will be analyzed by three measures: total time to solve the problem, time spent manipulating multivectors, and time spent applying linear operators. Two eigensolvers will be analysed: LOBPCG and Block Davidson. Block Davidson performs much more multivector manipulation per operator application than

does LOBPCG, and therefore weights those computations heavier in the total time.

Recall that there are two major players in action during a call to Anasazi: the underlying linear algebra library and the adapter used to interface this linear algebra library. The analysis of overhead will be made by comparing two different linear algebra libraries and two different adapters. The tests will be performed for the following scenarios:

- Epetra_MultiVector, Epetra_Op via Epetra adapter
- Thyra_MultiVector, Epetra_Op via Thyra adapter
- Epetra_MultiVector, Epetra_Op via Thyra adapter and Epetra-Thyra wrappers

The input for each test was from the test class `ModelLaplace1DQ1`, available in the `anasazi/util` directory in the Trilinos source tree. This is a generalized eigenvalue problem. Both solvers were limited to a fixed number (50) of iterations. The results were checked to make sure that all three scenarios (Epetra, Thyra, and Thyra-Epetra) performed similarly.

The three scenarios will be tested in serial and in parallel, for problem sizes of $1e2$, $1e3$, $1e4$, $1e5$, and $1e6$. On paunchy and sophie, the reported times are the average of three tests. On qed, the reported times originate from a single run. The times will be computed on the following platforms:

- sophie: serial and mpi(2)
- paunchy: serial, mpi(2), and mpi(4)
- qed: mpi(2), mpi(4), mpi(8), mpi(16), mpi(32), mpi(64)

These platforms are described in the appendix.

3 Performance

3.1 Paunchy

Paunchy is an SMP Sun machine with 4 processors. We tested Paunchy in three scenarios: serial, 1 processor MPI and 2 processor MPI. Figure 1 shows the results of the testing. Each cluster of lines represent a choice of platform (serial or mpi), denoted by the x-axis label. The datapoints inside a cluster show problems of the following sizes (from left to right, in the cluster): $n = 1e2$, $n = 1e3$, $n = 1e4$, $n = 1e5$, $n = 1e6$.

3.2 Sophie

Sophie is a PowerMac G5 with 2 processors. We tested Sophie in two scenarios: serial and 2 processor MPI. Figure 2 shows the results of the testing. Each

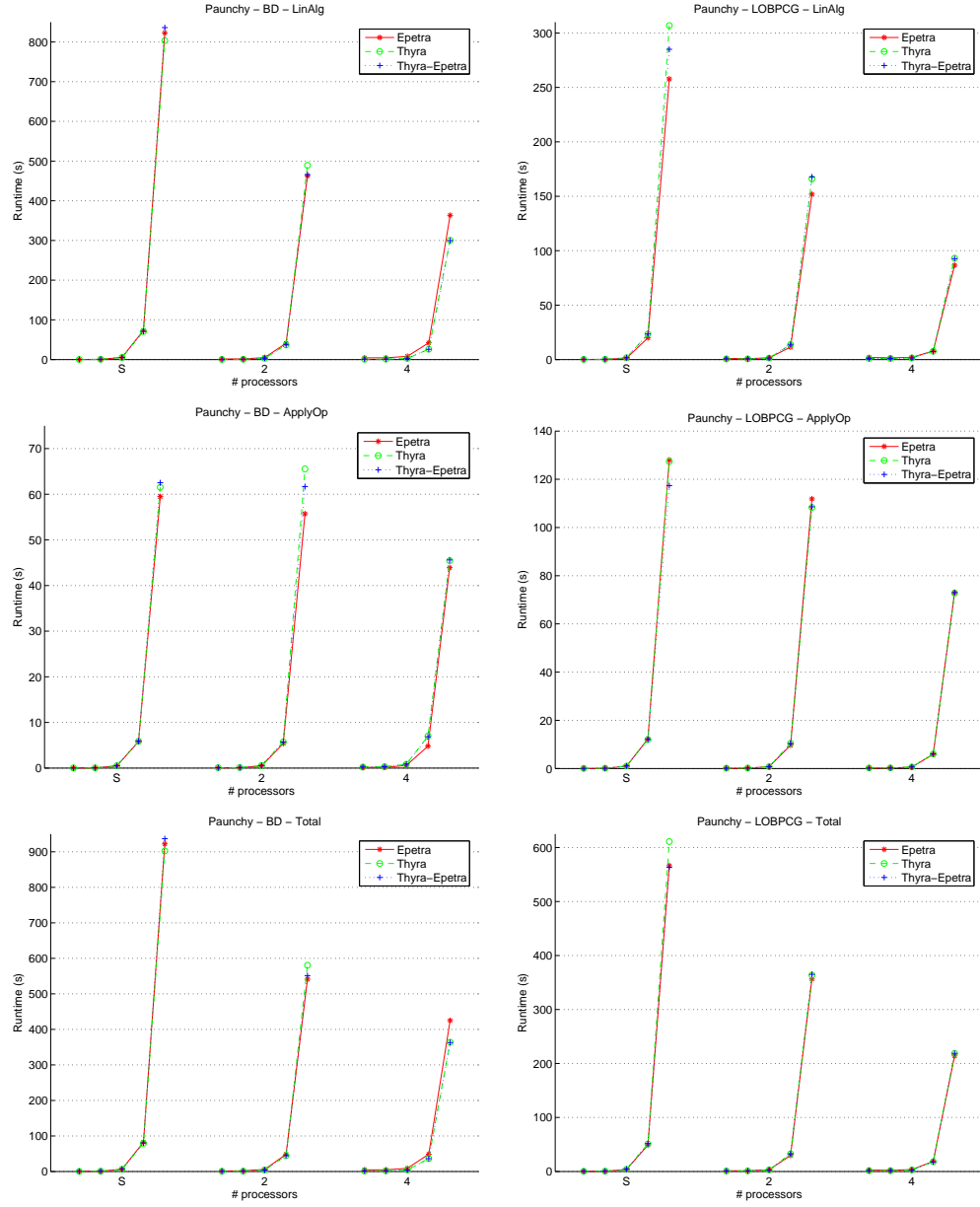


Figure 1: Performance of Block Davidson and LOBPCG on Paunchy.

cluster of lines represent a choice of platform (serial or mpi), denoted by the x-axis label. The datapoints inside a cluster show problems of the following sizes (from left to right, in the cluster): $n = 1e2$, $n = 1e3$, $n = 1e4$, $n = 1e5$, $n = 1e6$.

3.3 QED

QED is a linux cluster with 32 nodes of 2 processors each. We tested QED in five scenarios: 2 processors, 4 processors, 8 processors, 16 processors, 32 processors and 64 processors. Figure 3 shows the results of the testing. Each cluster of lines represent a choice of platform (serial or mpi), denoted by the x-axis label. The datapoints inside a cluster show problems of the following sizes (from left to right, in the cluster): $n = 1e2$, $n = 1e3$, $n = 1e4$, $n = 1e5$, $n = 1e6$.

4 Conclusion

A quick glance at the figures shows that there are little penalties associated with the use of the Thyra adapters. In fact, because the Thyra adapters to Epetra multivectors are “fake” adapters (in the sense that they do not wrap the Epetra multivector functionality, but only the data), the performance of the Thyra implementation can surpass that of the Epetra implementation. This trend is noticeable as the number of processors increases.

In conclusion, we have documented the performance of three implementation of Anasazi. The results indicate that there is little penalty associated with choosing any particular implementation. Furthermore, the results do not indicate any obvious problems with the implementation of the adapters.

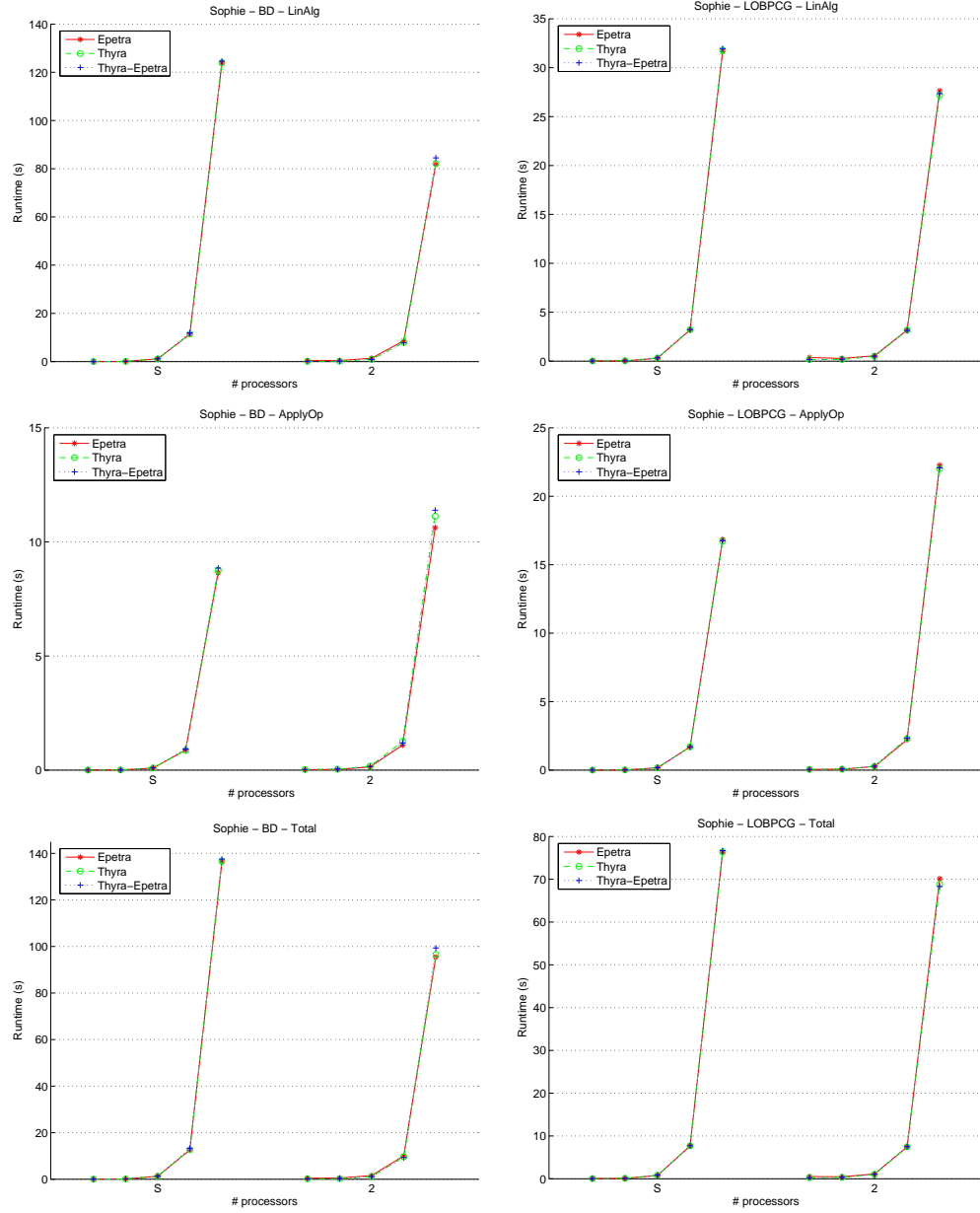


Figure 2: Performance of Block Davidson and LOBPCG on Sophie.

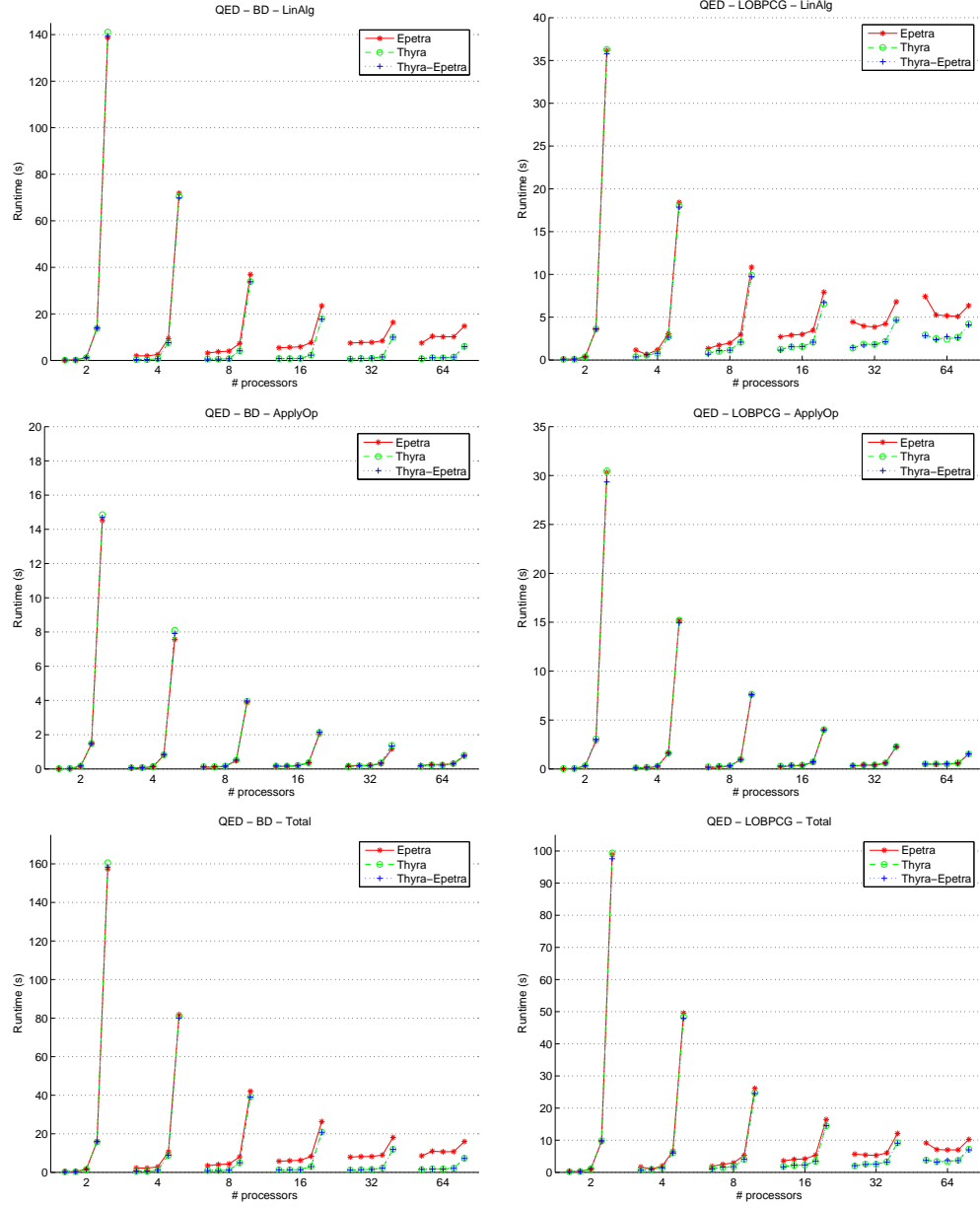


Figure 3: Performance of Block Davidson and LOBPCG on QED.

A Platforms

A.1 Paunchy

Paunchy is an SMP Solaris machine with the following statistics:

```
paunchy$ uname -a
SunOS paunchy 5.8 Generic_108528-29 sun4u sparc SUNW,Ultra-80
```

```
paunchy$ prtdiag
System Configuration: Sun Microsystems sun4u \
    Sun Enterprise 420R (4 X UltraSPARC-II 450MHz)
System clock frequency: 113 MHz
Memory size: 4096 Megabytes
```

===== CPUs =====

Brd	CPU	Module	Run MHz	Ecache MB	CPU Impl.	CPU Mask
---	---	-----	-----	-----	-----	-----
0	0	0	450	4.0	US-II	10.0
0	1	1	450	4.0	US-II	10.0
0	2	2	450	4.0	US-II	10.0
0	3	3	450	4.0	US-II	10.0

The compiler versions are as listed below:

```
version of "/opt/SUNWspro/bin/./prod/bin/./../bin/cc": Sun C 5.5 2003/03/12
version of "/opt/SUNWspro/bin/./prod/bin/./../bin/CC": Sun C++ 5.5 2003/03/12
version of "/opt/SUNWspro/bin/./prod/bin/./../bin/f90": Sun Fortran 95 7.1 200
```

The Trilinos serial build was configured as follows:

```
../configure -C \
LDLFLAGS="-xlic_lib=sunperf" \
CXXFLAGS="-O -pto" \
FFLAGS="-O" \
CFLAGS="-O" \
--with-gnumake \
--enable-export-makefiles \
--disable-default-packages \
--disable-examples \
--disable-tests \
--enable-anasazi \
--enable-thyra \
--enable-anasazi-thyra \
--enable-epetra-thyra \
--enable-anasazi-tests
```

The Trilinos MPI build was configured as follows:

```
../configure -C \  
LDFLAGS="-xlic_lib=sunperf" \  
CXXFLAGS="-O -pto" \  
FFLAGS="-O" \  
CFLAGS="-O" \  
CPPFLAGS="-I/local/arch/sun/sunos mpi/mpich/lib/sun4/ch_p4 \  
-I/local/arch/sun/sunos mpi/mpich/lib/sun4/ch_p4" \  
--with-gnumake \  
--enable-mpi \  
--with-mpi-libs="-lmpich -lnsl -lsocket -lrt" \  
--with-mpi-incdir=/local/arch/sun/sunos mpi/mpich/include \  
--with-mpi-libdir=/local/arch/sun/solaris mpi/build/solaris/ch_p4/lib \  
--enable-export-makefiles \  
--disable-default-packages \  
--disable-examples \  
--disable-tests \  
--enable-anasazi \  
--enable-thyra \  
--enable-anasazi-thyra \  
--enable-epetra-thyra \  
--enable-anasazi-tests
```

A.2 Sophie

Sophie is a dual-processor MacOSX machine with the following statistics:

```
[sophie] uname -a  
Darwin s863040.sandia.gov 7.8.0 Darwin Kernel Version 7.8.0: \  
Wed Dec 22 14:26:17 PST 2004; \  
root:xnu/xnu-517.11.1.obj~1/RELEASE_PPC \  
Power Macintosh powerpc
```

```
[s863040] sysctl -a hw  
hw.ncpu: 2  
hw.memsize: 8589934592  
hw.activecpu: 2  
hw.cputype: 18  
hw.cpusubtype: 100  
hw.pagesize: 4096  
hw.busfrequency: 1250000000  
hw.cpubfrequency: 2500000000  
hw.cachelinesize: 128  
hw.l1icachesize: 65536  
hw.l1dcachesize: 32768  
hw.l2cachesize: 524288
```



```

hw.tbfrequency: 33330001
hw.optional.floatingpoint: 1
hw.optional.altivec: 1
hw.optional.graphicsops: 1
hw.optional.64bitops: 1
hw.optional.fsqr: 1
hw.optional.stfiwx: 1
hw.optional.datastreams: 0
hw.optional.dcbtstreams: 1

```

The compiler version are as listed below:

```

[s863040:~] cgbaker% g++ --version
g++ (GCC) 3.3 20030304 (Apple Computer, Inc. build 1666)

```

```

[s863040:~] cgbaker% g77 --version
GNU Fortran (GCC) 3.4.3

```

The Trilinos serial build was configured as follows:

```

../configure -C \
CC=gcc \
CXX=g++ \
F77=/sw/bin/g77 \
FFLAGS="-O3" \
CFLAGS="-O3" \
CXXFLAGS="-O2" \
LDFLAGS="-framework vecLib" \
--with-gnu-make \
--enable-export-makefiles \
--disable-default-packages \
--disable-tests \
--disable-examples \
--enable-anasazi \
--enable-thyra \
--enable-anasazi-thyra \
--enable-epetra-thyra \
--enable-anasazi-tests

```

The Trilinos MPI build was configured as follows:

```

../configure -C \
CC=gcc \
CXX=g++ \
F77=/sw/bin/g77 \
FFLAGS="-O3" \
CFLAGS="-O3" \
CXXFLAGS="-O2" \

```

```

LDFLAGS="-framework vecLib" \
--enable-mpi \
--with-mpi-compilers \
--with-gnu-make \
--enable-export-makefiles \
--disable-default-packages \
--disable-tests \
--disable-examples \
--enable-anasazi \
--enable-thyra \
--enable-anasazi-thyra \
--enable-epetra-thyra \
--enable-anasazi-tests

```

A.3 QED

QED is a linux cluster. There are 33 nodes, each node having two cpus with the following statistics:

```

[cgbaker@node33 ~]$ uname -a
Linux node33 2.6.10-prep #1 SMP Tue Mar 8 13:42:20 EST 2005 \
i686 i686 i386 GNU/Linux

```

```

[cgbaker@node33 ~]$ cat /proc/cpuinfo
processor       : 0
vendor_id      : GenuineIntel
cpu family     : 15
model          : 2
model name     : Intel(R) Xeon(TM) CPU 2.80GHz
stepping       : 9
cpu MHz        : 2800.616
cache size     : 512 KB
bogomips       : 5521.40

```

```

processor       : 1
vendor_id      : GenuineIntel
cpu family     : 15
model          : 2
model name     : Intel(R) Xeon(TM) CPU 2.80GHz
stepping       : 9
cpu MHz        : 2800.616
cache size     : 512 KB
bogomips       : 5586.94

```

```

[cgbaker@node33 ~]$ cat /proc/meminfo
MemTotal:      2075764 kB

```

SwapTotal: 2096440 kB

The compilers versions are as follows:

```
[cgbaker@qed ~]$ mpicxx --version  
g++ (GCC) 3.4.2 20041017 (Red Hat 3.4.2-6.fc3)
```

```
[cgbaker@qed ~]$ mpif77 --version  
GNU Fortran (GCC) 3.4.2 20041017 (Red Hat 3.4.2-6.fc3)
```

The Trilinos MPI build was configured as follows:

```
../configure \  
--with-mpi="/usr/local/mpich-1.2.6-eth" \  
--with-mpi-libs=-lmpich \  
--with-mpi-compilers \  
--with-blas="/home/dmday/lib/libgoto_northwood32p-r1.00.so \  
-lpthread /home/dmday/lib/lapack_LINUX.a" \  
--with-lapack="/home/dmday/lib/lapack_LINUX.a" \  
--enable-export-makefiles \  
--cache-file=config.cache \  
--disable-default-packages \  
--disable-tests \  
--disable-examples \  
--enable-anasazi \  
--enable-anasazi-thyra \  
--enable-epetra-thyra \  
--enable-thyra
```