Supercomputing in Plain English

Grab Bag: Scientific Libraries, I/O Libraries, Visualizations

Henry Neeman, Director
OU Supercomputing Center for Education & Research (OSCER)
University of Oklahoma

Tuesday April 16 2013

This is an experiment!

It's the nature of these kinds of videoconferences that **FAILURES ARE GUARANTEED TO HAPPEN! NO PROMISES!**

So, please bear with us. Hopefully everything will work out well enough.

If you lose your connection, you can retry the same kind of connection, or try connecting another way.

Remember, if all else fails, you always have the toll free phone bridge to fall back on.

H.323 (Polycom etc) #1

If you want to use H.323 videoconferencing – for example, Polycom – then:

- If you AREN'T registered with the OneNet gatekeeper (which is probably the case), then:
  - Dial **164.58.250.47**
  - Bring up the virtual keypad.
    On some H.323 devices, you can bring up the virtual keypad by typing:
    #
    (You may want to try without first, then with; some devices won't work with the #, but give cryptic error messages about it.)
  - When asked for the conference ID, or if there's no response, enter:
    0409
  - On most but not all H.323 devices, you indicate the end of the ID with:
    #

H.323 (Polycom etc) #2

If you want to use H.323 videoconferencing – for example, Polycom – then:

- If you ARE already registered with the OneNet gatekeeper (most institutions aren't), dial:

  `2500409`

Many thanks to Skyler Donahue and Steven Haldeman of OneNet for providing this.

Wowza #1

You can watch from a Windows, MacOS or Linux laptop using Wowza from either of the following URLs:

http://www.onenet.net/technical-resources/video/sipe-stream/

OR

https://vcenter.njvid.net/videos/livestreams/page1/

Wowza behaves a lot like YouTube, except live.

Many thanks to Skyler Donahue and Steven Haldeman of OneNet and Bob Gerdes of Rutgers U for providing this.

Wowza #2

Wowza has been tested on multiple browsers on each of:

- Windows (7 and 8): IE, Firefox, Chrome, Opera, Safari
- MacOS X: Safari, Firefox
- Linux: Firefox, Opera

We've also successfully tested it on devices with:

- Android
- iOS

However, we make no representations on the likelihood of it working on your device, because we don't know which versions of Android or iOS it might or might not work with.

Wowza #3

If one of the Wowza URLs fails, try switching over to the other one.

If we lose our network connection between OU and OneNet, then there may be a slight delay while we set up a direct connection to Rutgers.

Toll Free Phone Bridge

IF ALL ELSE FAILS, you can use our toll free phone bridge:

800-832-0736

* 623 2847 #

Please mute yourself and use the phone to listen.

Don’t worry, we’ll call out slide numbers as we go.

Please use the phone bridge **ONLY** if you cannot connect any other way: the phone bridge can handle only 100 simultaneous connections, and we have over 350 participants.

Many thanks to OU CIO Loretta Early for providing the toll free phone bridge.

Please Mute Yourself

No matter how you connect, please mute yourself, so that we cannot hear you.

(For Wowza, you don't need to do that, because the information only goes from us to you, not from you to us.)

At OU, we will turn off the sound on all conferencing technologies.

That way, we won't have problems with echo cancellation.

Of course, that means we cannot hear questions.

So for questions, you'll need to send e-mail.

Questions via E-mail Only

Ask questions by sending e-mail to:

sipe2013@gmail.com

All questions will be read out loud and then answered out loud.

TENTATIVE Schedule

Tue Jan 22: Overview: What the Heck is Supercomputing?
Tue Jan 29: The Tyranny of the Storage Hierarchy
Tue Feb 5: Instruction Level Parallelism
Tue Feb 12: Stupid Compiler Tricks
Tue Feb 19: Shared Memory Multithreading
Tue Feb 26: Distributed Multiprocessing
Tue March 5: Applications and Types of Parallelism
Tue Apr 9: Grab Bag Madness
Tue March 19: NO SESSION (OU's Spring Break)
Tue Apr 9: High Throughput Computing
Tue Apr 9: Grab Bag: Number Crunching in Your Graphics Card
Tue Apr 9: Grab Bag: Scientific Libraries, I/O Libraries, Visualization

Supercomputing Exercises

Want to do the "Supercomputing in Plain English" exercises?

- The 3rd exercise will be posted soon at:

  http://www.oscer.ou.edu/education/

- If you don't yet have a supercomputer account, you can get a temporary account, just for the "Supercomputing in Plain English" exercises, by sending e-mail to:

  hneeman@ou.edu

Please note that this account is for doing the **exercises only**, and will be shut down at the end of the series. It's also available only to those at institutions in the USA.

- This week's Introductory exercise will teach you how to compile and run jobs on OU's big Linux cluster supercomputer, which is named Boomer.

Supercomputing Exercises #2

You'll be doing the exercises on your own (or you can work with others at your local institution if you like).

These aren't graded, but we're available for questions:

hneeman@ou.edu

Thanks for helping!

- OU IT
  - OSCER operations staff (Brandon George, Dave Akin, Brett Zimmerman, Josh Alexander, Patrick Calhoun)
  - Horst Severini, OSCER Associate Director for Remote & Heterogeneous Computing
  - Debi Gentis, OU Research IT coordinator
  - Kevin Blake, OU IT (videographer)
  - Chris Kobza, OU IT (learning technologies)
  - Mark McAvoy
- Kyle Keys, OU National Weather Center
- James Deaton, Skyler Donahue and Steven Haldeman, OneNet
- Bob Gerdes, Rutgers U
- Lisa Ison, U Kentucky
- Paul Dave, U Chicago

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Coming in 2013!

From Computational Biophysics to Systems Biology, May 19-21, Norman OK

Great Plains Network Annual Meeting, May 29-31, Kansas City

XSEDE2013, July 22-25, San Diego CA

IEEE Cluster 2013, Sep 23-27, Indianapolis IN

OKLAHOMA SUPERCOMPUTING SYMPOSIUM 2013, Oct 1-2, Norman OK

SC13, Nov 17-22, Denver CO

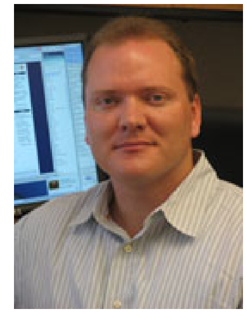
OK Supercomputing Symposium 2013

2003 Keynote:
Peter Freeman
NSF
Computer & Information Science & Engineering
Assistant Director

2004 Keynote:
Sangtae Kim
NSF Shared Cyberinfrastructure
Division Director

2005 Keynote:
Walt Brooks
NASA Advanced Supercomputing
Division Director

2006 Keynote:
Dan Atkins
Head of NSF's Office of Cyberinfrastructure

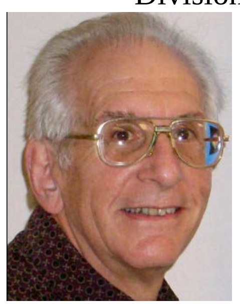


2007 Keynote:
Jay Boisseau
Director
Texas Advanced Computing Center
U. Texas Austin

2008 Keynote:
José Munoz
Deputy Office Director/ Senior Scientific Advisor
NSF Office of Cyberinfrastructure

2009 Keynote:
Douglass Post
Chief Scientist
US Dept of Defense HPC Modernization Program

2010 Keynote:
Horst Simon
Deputy Director
Lawrence Berkeley National Laboratory



2011 Keynote:
Barry Schneider
Program Manager
National Science Foundation

2012 Keynote:
Thom Dunning
Director
National Center for Supercomputing Applications

2013 Keynote to be announced!

FREE! Wed Oct 2 2013 @ OU

http://symposium2013.oscer.ou.edu/

Reception/Poster Session
Tue Oct 1 2013 @ OU
Symposium Wed Oct 2 2013 @ OU

Outline

- Scientific Computing Pipeline
- Scientific Libraries
- I/O Libraries
- Scientific Visualization

Scientific Computing Pipeline

Real World

Physics

Mathematical Representation (continuous)

Numerical Representation (discrete)

Algorithm

Implementation (program)

Port (to a specific platform)

Result (run)

Analysis

Verification

Thanks to Julia Mullen of MIT Lincoln Lab for this concept.

Five Rules of Scientific Computing

1. Know the physics.
2. Control the software.
3. Understand the numerics.
4. Achieve expected behavior.
5. Question unexpected behavior.

Thanks to Robert E. Peterkin for these.

Scientific Libraries

Preinvented Wheels

Many simulations perform fairly common tasks; for example, solving systems of equations:

$$\mathbf{Ax} = \mathbf{b}$$

where **A** is the matrix of coefficients, **x** is the vector of unknowns and **b** is the vector of knowns.

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,n} \\ a_{3,1} & a_{3,2} & a_{3,3} & \cdots & a_{3,n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{n,1} & a_{n,2} & a_{n,3} & \cdots & a_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

Scientific Libraries

Because some tasks are quite common across many science and engineering applications, groups of researchers have put a lot of effort into writing ***scientific libraries***: collections of routines for performing these commonly-used tasks (for example, linear algebra solvers).

The people who write these libraries know a lot more about these things than we do.

So, a good strategy is to use their libraries, rather than trying to write our own.

Solver Libraries

Probably the most common scientific computing task is solving a system of equations

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$

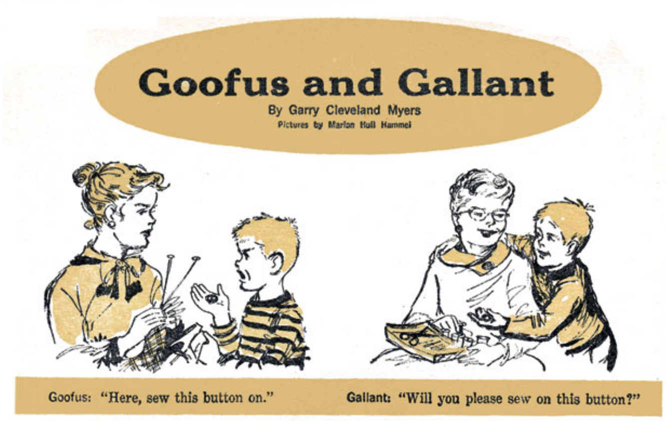
where **A** is a matrix of coefficients, **x** is a vector of unknowns, and **b** is a vector of knowns.

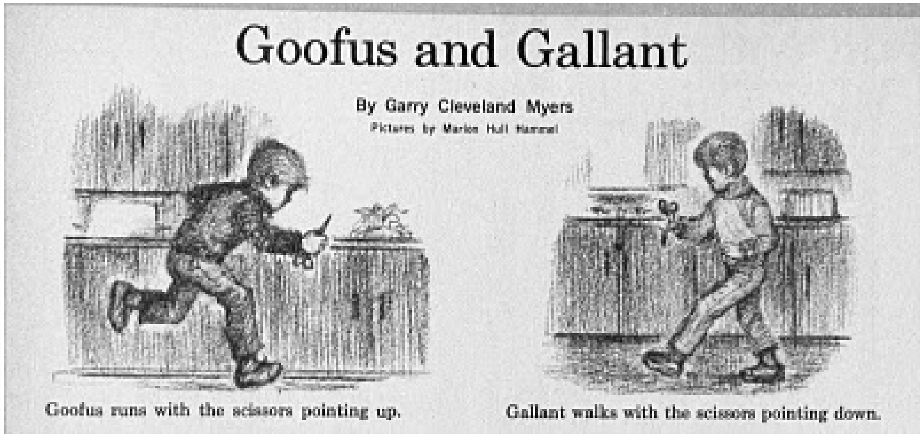
The goal is to solve for **x**.

Solving Systems of Equations

Don'ts:

- **Don't** invert the matrix ($\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$). That's much more costly than solving directly, and much more prone to numerical error.
- **Don't** write your own solver code. There are people who devote their whole careers to writing solvers. They know a lot more about writing solvers than we do.

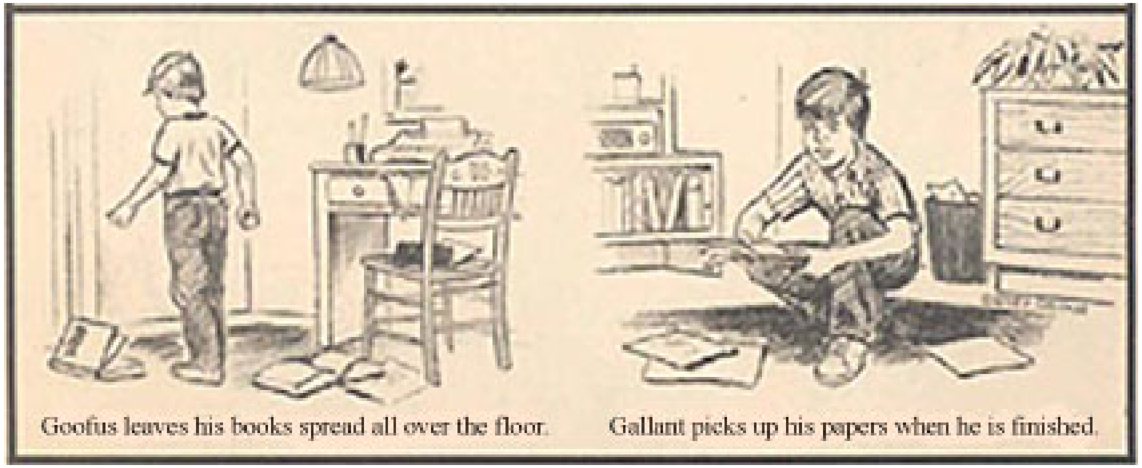


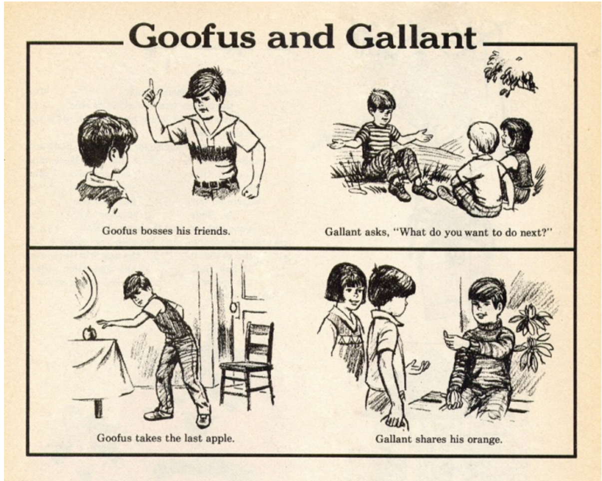


Solving Do's

Do's:

- **Do** use standard, portable solver libraries.
- **Do** use a version that's tuned for the platform you're running on, if available.
- **Do** use the information that you have about your system of equations to pick the most efficient solver.



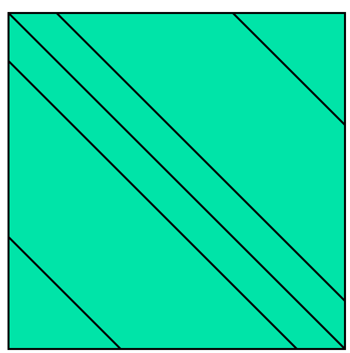


All About Your Matrix

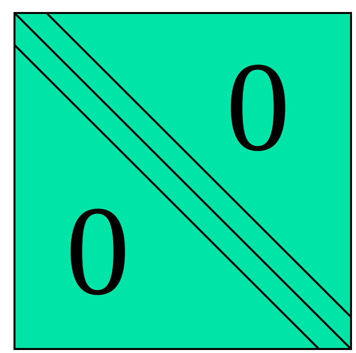
If you know things about your matrix, you maybe can use a more efficient solver.

- Symmetric: $a_{i,j} = a_{j,i}$
- Positive definite: $\mathbf{x}^T\mathbf{A}\mathbf{x} > 0$ for all $\mathbf{x} \neq 0$
  (for example, if all eigenvalues are positive)
- Banded:

zero except on the bands



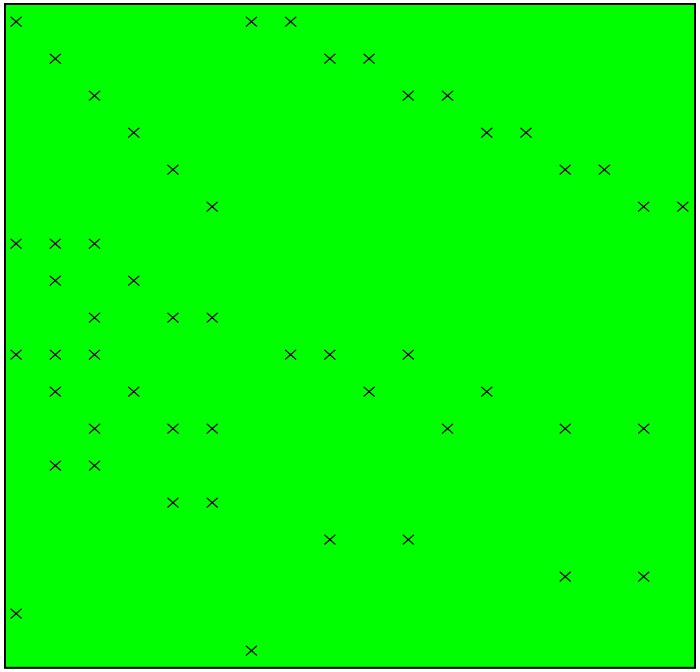
- Tridiagonal:



and …

Sparse Matrices

A ***sparse matrix*** is a matrix that has mostly zeros in it. "Mostly" is vaguely defined, but a good rule of thumb is that a matrix is sparse if more than, say, 90-95% of its entries are zero. (A non-sparse matrix is ***dense***.)



Linear Algebra Libraries

- BLAS [1],[2]
- ATLAS[3]
- LAPACK[4]
- ScaLAPACK[5]
- PETSc[6],[7],[8]

BLAS

The **Basic Linear Algebra Subprograms** (BLAS) are a set of low level linear algebra routines:

- Level 1: Vector-vector (for example, dot product)
- Level 2: Matrix-vector (for example, matrix-vector multiply)
- Level 3: Matrix-matrix (for example, matrix-matrix multiply)

Many linear algebra packages, including LAPACK, ScaLAPACK and PETSc, are built on top of BLAS.

Most supercomputer vendors have versions of BLAS that are highly tuned for their platforms.

ATLAS

The **Automatically Tuned Linear Algebra Software** package (ATLAS) is a self-tuned version of BLAS (it also includes a few LAPACK routines).

When it's installed, it tests and times a variety of approaches to each routine, and selects the version that runs the fastest.

ATLAS is substantially faster than the generic version of BLAS.

And, it's **FREE**!

Goto BLAS

Several years ago, a new version of BLAS was released, developed by Kazushige Goto (then at UT Austin, now at Intel).

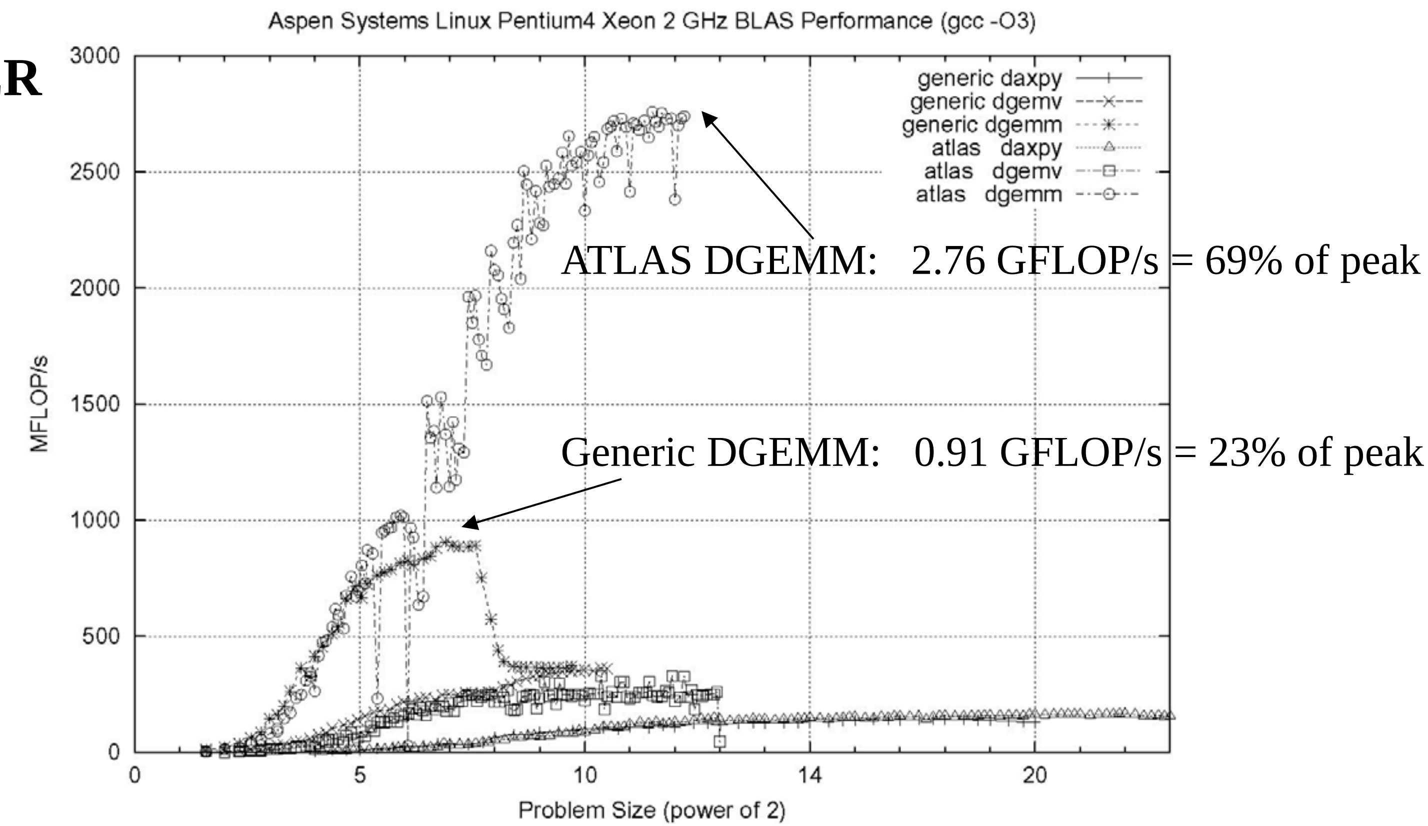
http://en.wikipedia.org/wiki/Kazushige_Goto

This version is unusual, because instead of optimizing for cache, it optimizes for the ***Translation Lookaside Buffer*** (TLB), which is a special little cache that often is ignored by software developers.

Goto realized that optimizing for the TLB would be more efficient than optimizing for cache.

ATLAS vs. Generic BLAS

BETTER



DGEMM: **D**ouble precision **GE**neral **M**atrix-**M**atrix multiply

DGEMV: **D**ouble precision **GE**neral **M**atrix-**V**ector multiply

LAPACK

LAPACK (Linear Algebra PACKage) solves dense or special-case sparse systems of equations depending on matrix properties such as:

- Precision: single, double
- Data type: real, complex
- Shape: diagonal, bidiagonal, tridiagonal, banded, triangular, trapezoidal, Hesenberg, general dense
- Properties: orthogonal, positive definite, Hermetian (complex), symmetric, general

LAPACK is built on top of BLAS, which means it can benefit from ATLAS.

LAPACK Example

```
REAL,DIMENSION(numrows,numcols) :: A
REAL,DIMENSION(numrows)         :: B
REAL,DIMENSION(numcols)         :: X
INTEGER,DIMENSION(numrows)      :: pivot
INTEGER :: row, col, info, numrhs = 1
DO row = 1, numrows
  B(row) = …
END DO
DO col = 1, numcols
  DO row = 1, numrows
    A(row,col) = …
  END DO
END DO
CALL sgesv(numrows, numrhs, A, numrows, pivot, &
&          B, numrows, info)
DO col = 1, numcols
  X(col) = B(col)
END DO
```

LAPACK: A Library and an API

LAPACK is a library that you can download for free from the Web:

`www.netlib.org`

But, it's also an Application Programming Interface (API): a definition of a set of routines, their arguments, and their behaviors.

So, anyone can write an implementation of LAPACK.

It’s Good to Be Popular

LAPACK is a good choice for non-parallelized solving, because its popularity has convinced many supercomputer vendors to write their own, highly tuned versions.

The API for the LAPACK routines is the same as the portable version from NetLib, but the performance can be much better, via either ATLAS or proprietary vendor-tuned versions.

Also, some vendors have shared memory parallel versions of LAPACK.

LAPACK Performance

Because LAPACK uses BLAS, it's about as fast as BLAS.

For example, DGESV (Double precision General SolVer) on a 2 GHz Pentium4 using ATLAS gets 65% of peak, compared to 69% of peak for Matrix-Matrix multiply.

In fact, an older version of LAPACK, called LINPACK, is used to determine the top 500 supercomputers in the world.

ScaLAPACK

ScaLAPACK is the distributed parallel (MPI) version of LAPACK. It actually contains only a subset of the LAPACK routines, and has a somewhat awkward Application Programming Interface (API).

Like LAPACK, ScaLAPACK is also available from

`www.netlib.org`.

PETSc

PETSc (Portable, Extensible Toolkit for Scientific Computation) is a solver library for sparse matrices that uses distributed parallelism (MPI).

PETSc is designed for general sparse matrices with no special properties, but it also works well for sparse matrices with simple properties like banding and symmetry.

It has a simpler, more intuitive Application Programming Interface than ScaLAPACK.

Pick Your Solver Package

- Dense Matrix
  - Serial: LAPACK
  - Shared Memory Parallel: threaded LAPACK
  - Distributed Parallel: ScaLAPACK
- Sparse Matrix: PETSc

I/O Libraries

I/O Challenges

I/O presents two important challenges to scientific computing:

- Performance
- Portability

The performance issue arises because I/O is much more time-consuming than computation, as we saw in the "Storage Hierarchy" session.

The portability issue arises because different kinds of computers can have different ways of representing real (floating point) numbers.

Storage Formats

When you use a **`PRINT`** statement in Fortran or a **`printf`** in C or output to **`cout`** in C++, you are asking the program to output data in human-readable form:

```
x = 5
PRINT *, x
```

But what if the value that you want to output is a real number with lots of significant digits?

```
1.3456789E+23
```

Data Output as Text

`1.3456789E+23`

When you output data as text, each character takes 1 byte.

So if you output a number with lots of digits, then you're outputting lots of bytes.

For example, the above number takes 13 bytes to output as text.

Jargon: Text is sometimes called **ASCII** (American Standard Code for Information Interchange).

Output Data in Binary

Inside the computer, a single precision real number (Fortran **`REAL`**, C/C++ **`float`**) typically requires 4 bytes, and a double precision number (**`DOUBLE PRECISION`** or **`double`**) typically requires 8.

That's less than 13.

Since I/O is very expensive, it's better to output 4 or 8 bytes than 13 or more.

Happily, Fortran, C and C++ allow you to output data as **binary** (internal representation) rather than as text.

Binary Output Problems

When you output data as **binary** rather than as text, you output substantially **fewer bytes**, so you save time (since I/O is very expensive) and you save disk space.

But, you pay two prices:

- **Readability**: Humans can't read binary.
- **Portability**: Different kinds of computers have different ways of internally representing numbers.

Binary Readability: No Problem

Readability of binary data **isn't a problem** in scientific computing, because:

- You can always write a little program to read in the binary data and display its text equivalent.
- If you have lots and lots of data (that is, MBs or GBs), you wouldn't want to look at all of it anyway.

Binary Portability: Big Problem

<u>Binary data portability</u> is a **<u>very big problem</u>** in scientific computing, because data that's output on one kind of computer may not be readable on another, and so:

- You can't output the data on one kind of computer and then use them (for example, visualize, analyze) on another kind.
- Some day the kind of computer that output the data will be obsolete, so there may be no computer in the world that can input it, and thus the data are lost.

Portable Binary Data

The HPC community noticed this problem some years ago, and so a number of portable binary data formats were developed.

The two most popular are:

- **HDF** (Hierarchical Data Format) from the National Center for Supercomputing Applications:
  http://www.hdfgroup.org/
- **NetCDF** (Network Common Data Form) from Unidata:

http://www.unidata.ucar.edu/software/netcdf

Advantages of Portable I/O

Portable binary I/O packages:

- give you portable binary I/O;
- have simple, clear APIs;
- are available for **free**;
- run on most platforms;
- allow you to **annotate** your data (for example, put into the file the variable names, units, experiment name, grid description, etc).

Also, both HDF and netCDF support distributed parallel I/O.

Scientific Visualization

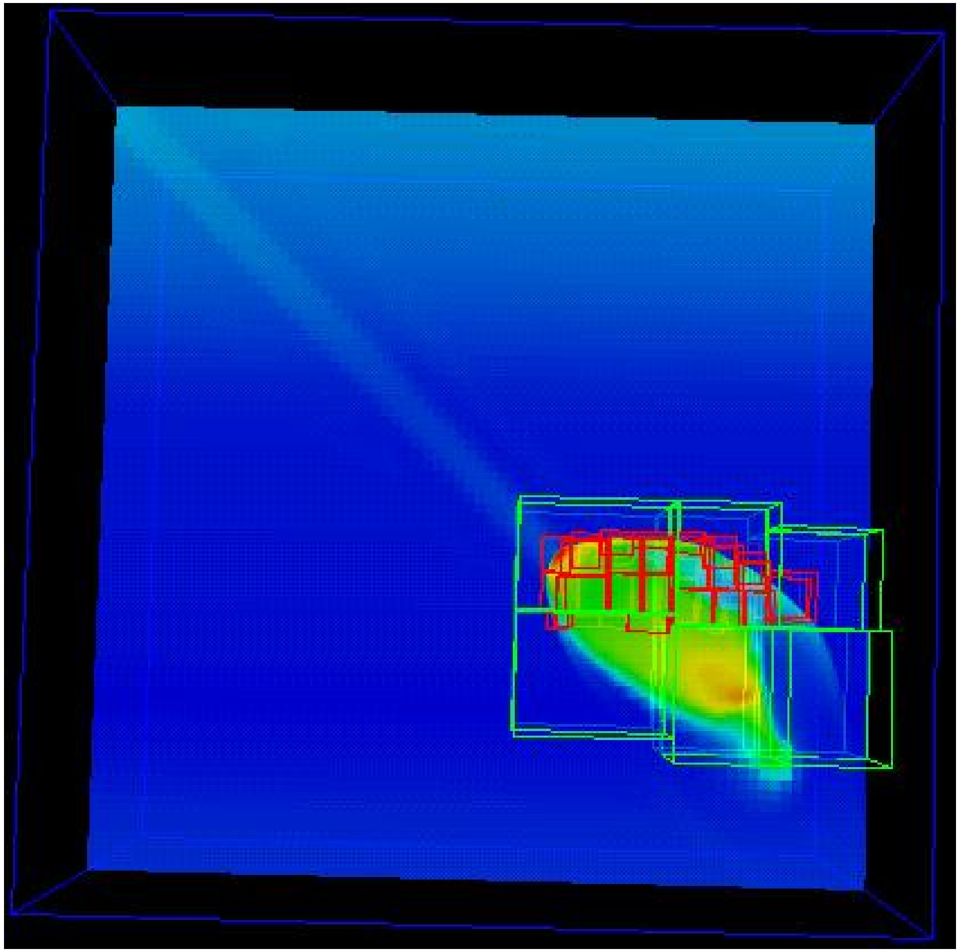
Too Many Numbers

A typical scientific code outputs lots and lots of data.

For example, the ARPS weather forecasting code, running a 5 day forecast over the continental U.S. with a resolution of 1 km horizontal and 0.25 km vertical outputting data for every hour would produce about **10 terabytes** (10^{13} bytes).

No one can look at that many numbers.

A Picture is Worth …



… millions of numbers.

This is Comet Shoemaker-Levy 9, which hit Jupiter in 1994; the image is from 35 seconds after hitting Jupiter's inner atmosphere.[9]

Types of Visualization

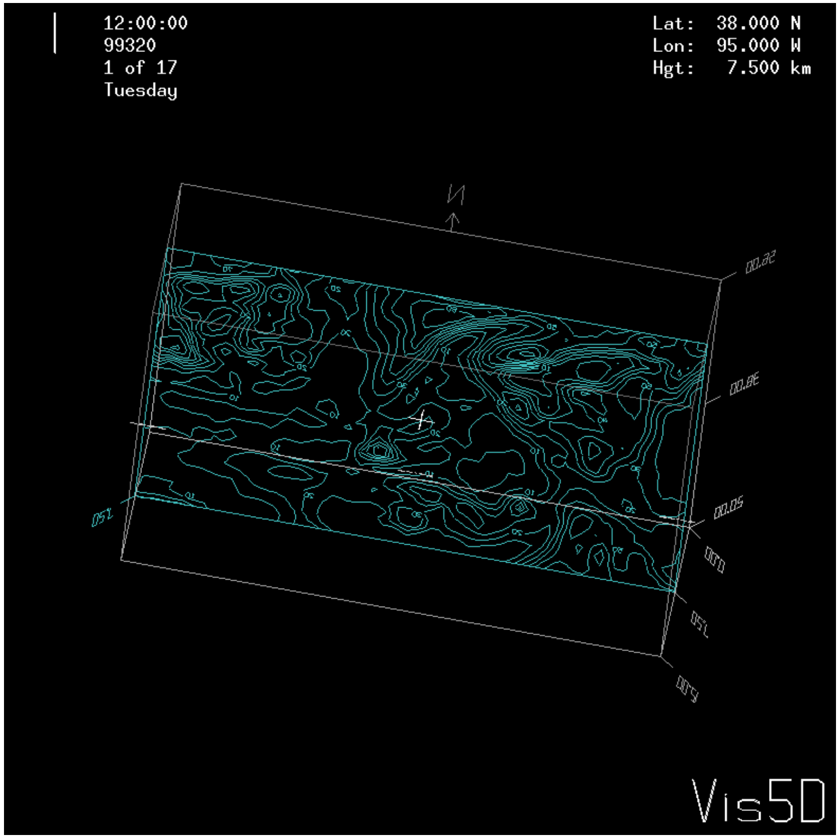
- Contour lines
- Slice planes
- Isosurfaces
- Streamlines
- Volume rendering

… and many others.

Note: except for the volume rendering, the following images were created by Vis5D,[10] which you can download for free.

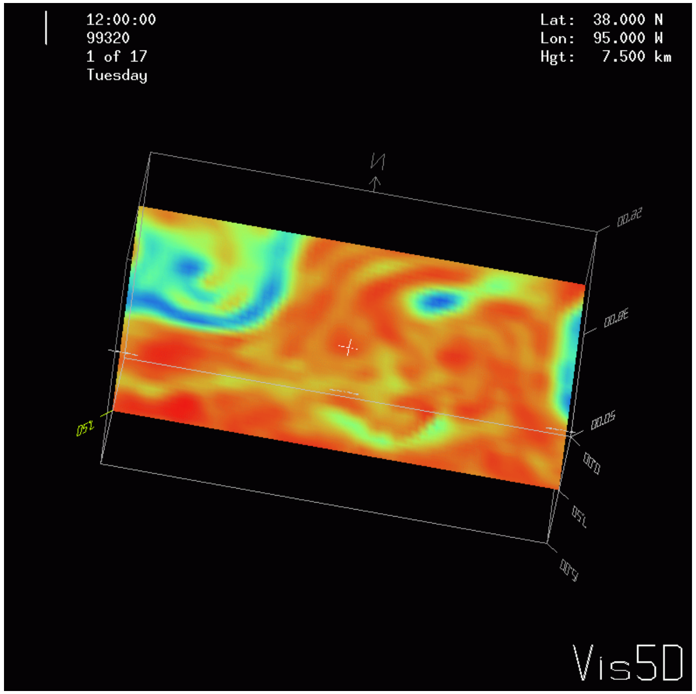
Contour Lines

This image shows ***contour lines*** of relative humidity. Each contour line represents a single humidity value.



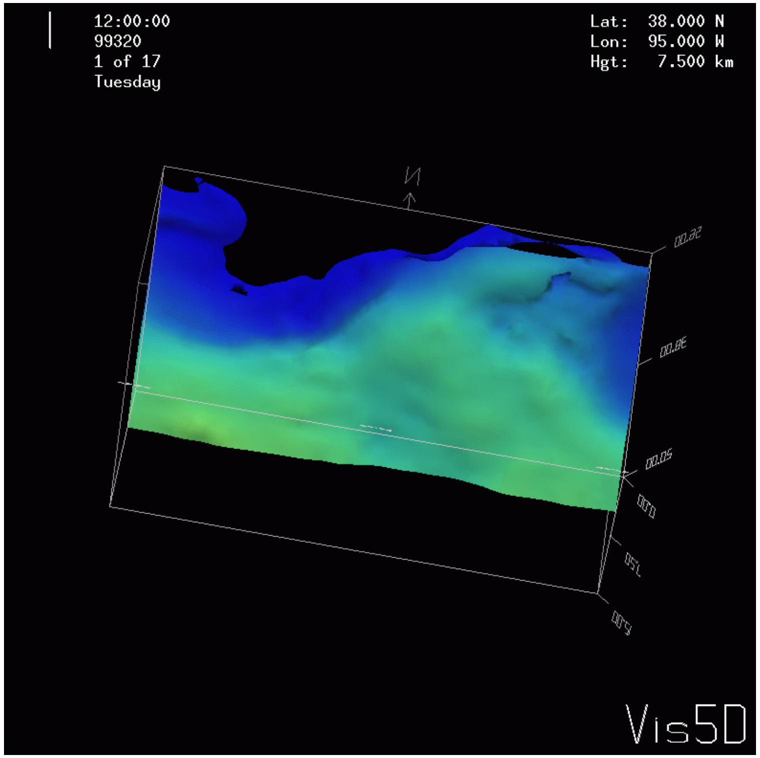
Slice Planes

A ***slice plane*** is a single plane passed through a 3D volume. Typically, it is color coded by mapping some scalar variable to color (for example, low vorticity to blue, high vorticity to red).



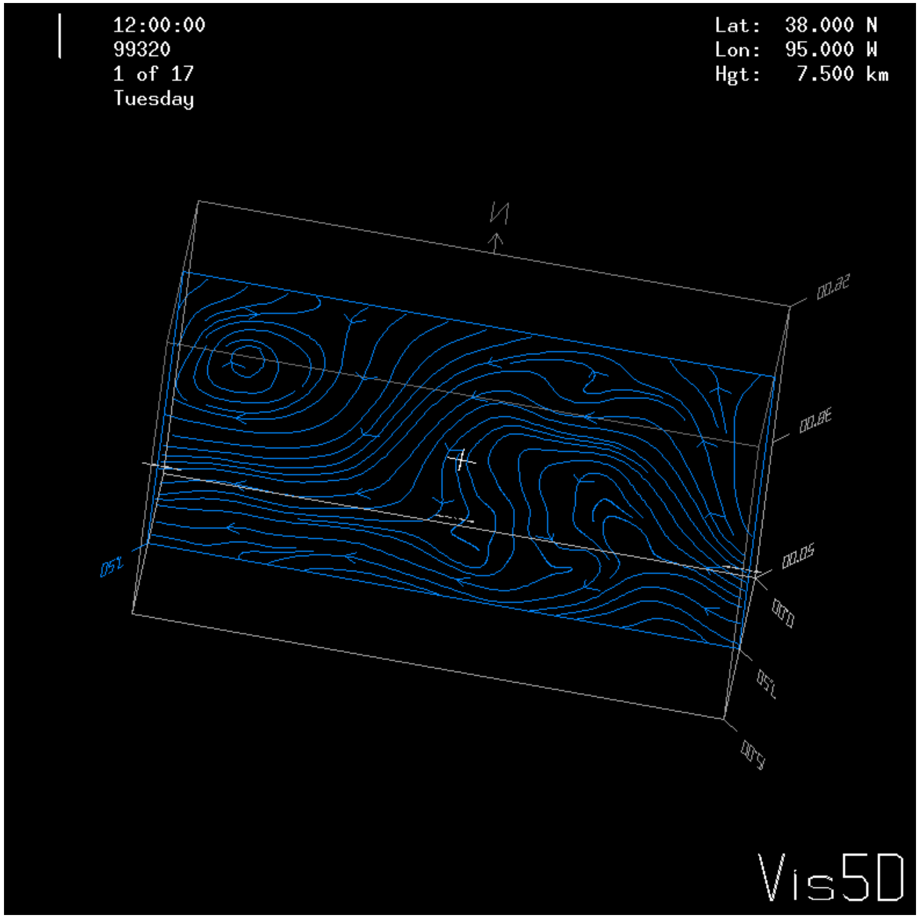
Isosurfaces

An ***isosurface*** is a surface that has a constant value for some scalar quantity. This image shows an isosurface of temperature at 0^o Celsius, colored with pressure.



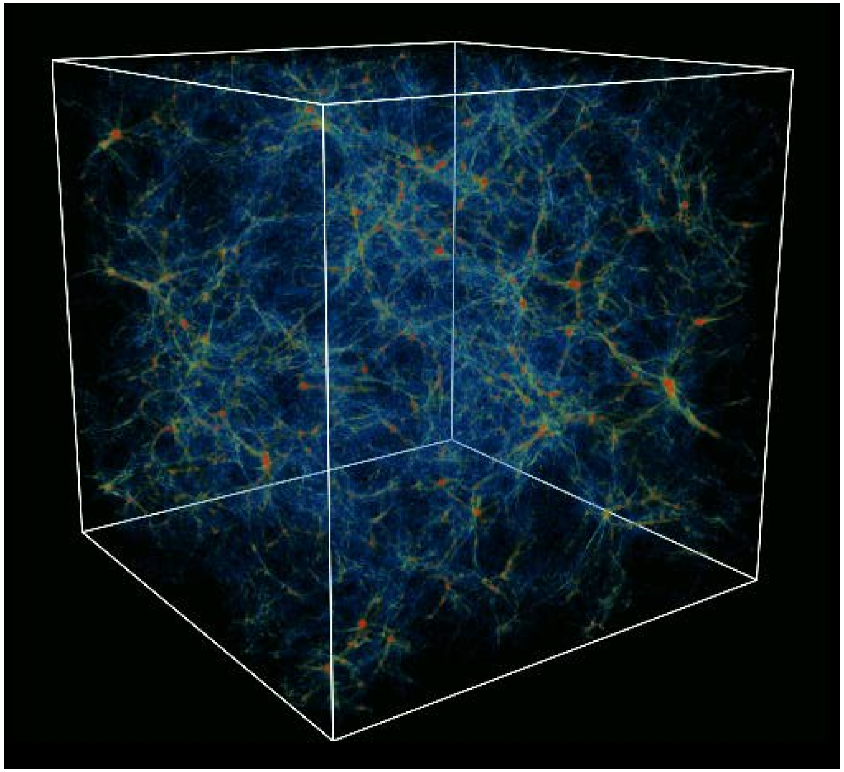
Streamlines

A ***streamline*** traces a vector quantity (for example, velocity).



Volume Rendering

A ***volume rendering*** is created by mapping some variable (for example, energy) to color and another variable (for example, density) to opacity.



This image shows the overall structure of the universe.[11]

Notice that the image looks like thick colored smoke.

References

[1] C. L. Lawson, R. J. Hanson, D. Kincaid, and F. T. Krogh, *Basic Linear Algebra Subprograms for FORTRAN Usage*, ACM Trans. Math. Soft., 5 (1979), pp. 308--323.

[2] http://www.netlib.org/blas/

[3] http://math-atlas.sourceforge.net/

[4] E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney, D. Sorensen, *LAPACK Users' Guide*, 3rd ed, 1999. http://www.netlib.org/lapack/

[5] L. S. Blackford, J. Choi, A. Cleary, E. D'Azevedo, J. Demmel, I. Dhillon, J. Dongarra, S. Hammarling, G. Henry, A. Petitet, K. Stanley, D. Walker, R. C. Whaley, *ScaLAPACK Users' Guide*, 1997. http://www.netlib.org/scalapack/

[6] S. Balay, K. Buschelman, W. D. Gropp, D. Kaushik, L. Curfman McInnes and B. F. Smith, PETSc home page, 2001. http://www.mcs.anl.gov/petsc

[7] S. Balay, W. D. Gropp. L. Curfman McInnes and B. Smith, *PETSc Users Manual*, ANL-95/11 - Revision 2.1.0, Argonne National Laboratory, 2001.

[8] S. Balay, W. D. Gropp, L. Curfman McInnes and B. F. Smith, "Efficient Management of Parallelism in Object Oriented Numerical Software Libraries", in *Modern Software Tools in Scientific Computing*, E. Arge, A. M. Bruaset and H. P. Langtangen, editors, Birkhauser Press, 1997, 163-202.

[9] http://hneeman.oscer.ou.edu/hamr.html

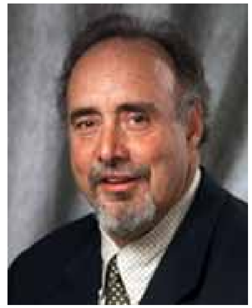
[10] http://www.ssec.wisc.edu/~billh/vis5d.html

[11] Image by Greg Bryan, MIT.

OK Supercomputing Symposium 2013

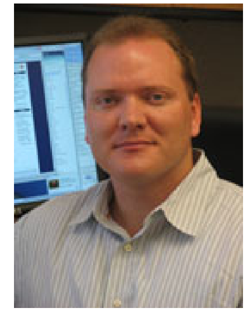
2003 Keynote:
Peter Freeman
NSF
Computer & Information Science & Engineering
Assistant Director

2004 Keynote:
Sangtae Kim
NSF Shared Cyberinfrastructure
Division Director



2005 Keynote:
Walt Brooks
NASA Advanced Supercomputing
Division Director

2006 Keynote:
Dan Atkins
Head of NSF's Office of Cyberinfrastructure

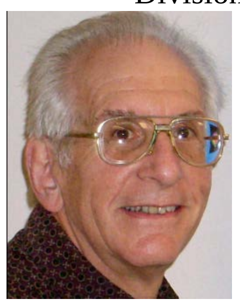


2007 Keynote:
Jay Boisseau
Director
Texas Advanced Computing Center
U. Texas Austin

2008 Keynote:
José Munoz
Deputy Office Director/ Senior Scientific Advisor
NSF Office of Cyberinfrastructure

2009 Keynote:
Douglass Post
Chief Scientist
US Dept of Defense
HPC Modernization Program

2010 Keynote:
Horst Simon
Deputy Director
Lawrence Berkeley National Laboratory



2011 Keynote:
Barry Schneider
Program Manager
National Science Foundation

2012 Keynote:
Thom Dunning
Director
National Center for Supercomputing Applications

2013 Keynote to be announced!

FREE! Wed Oct 2 2013 @ OU

http://symposium2013.oscer.ou.edu/

Reception/Poster Session
Tue Oct 1 2013 @ OU
Symposium Wed Oct 2 2013 @ OU

Thanks for your attention!

Questions?

www.oscer.ou.edu