Parallel Programming & Cluster Computing
Grab Bag: Scientific Libraries, I/O Libraries, Visualization

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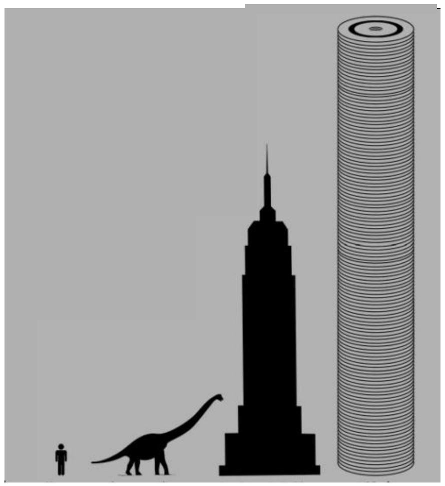
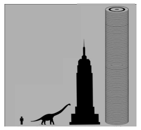


Outline

- 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

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

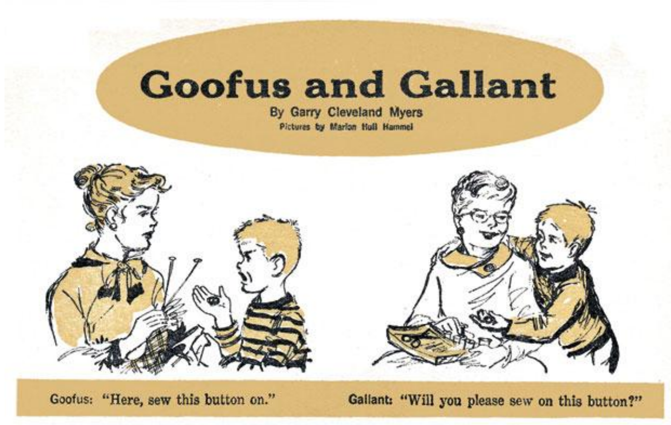
where **A** is a matrix of coefficients, **x** is a vector of unknowns, and **b** is a vector of knowns.

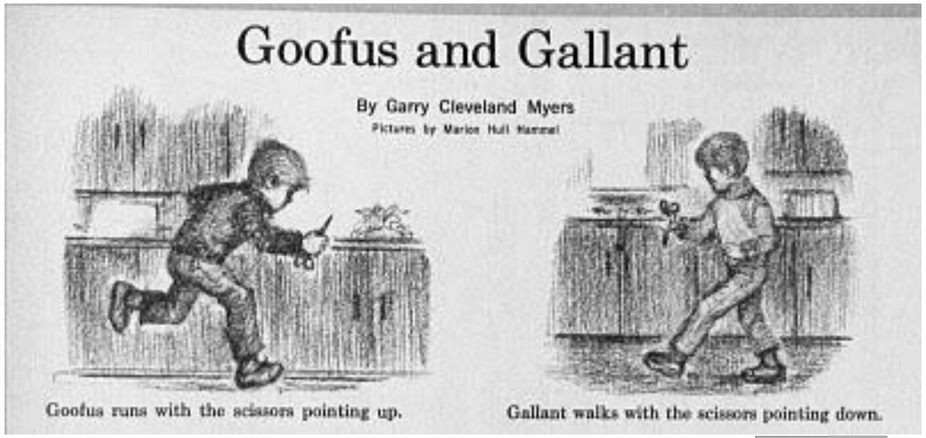
The goal is to solve for **x**.

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.

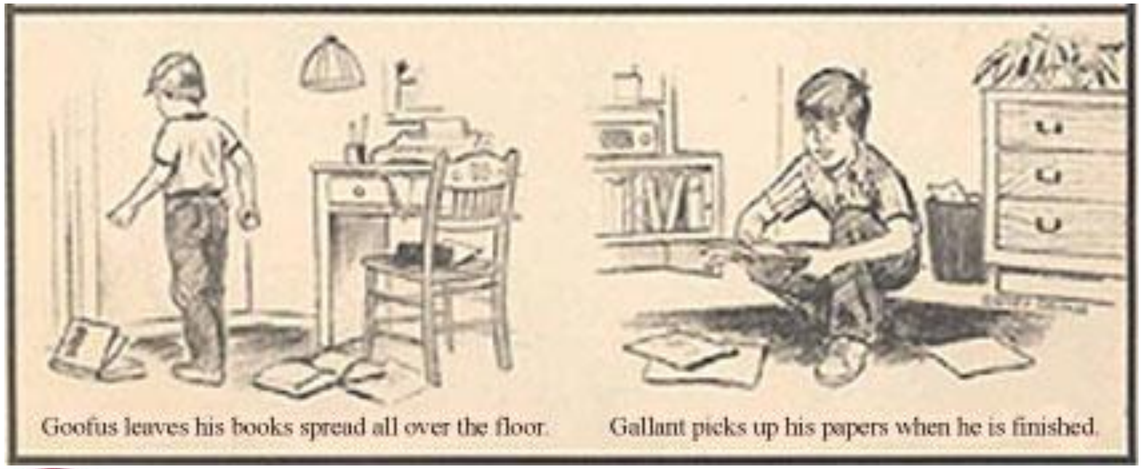

Goofus and Gallant
By Garry Cleveland Myers
Pictures by Marion Hull Hammel
Goofus: "Here, sew this button on."
Gallant: "Will you please sew on this button?"

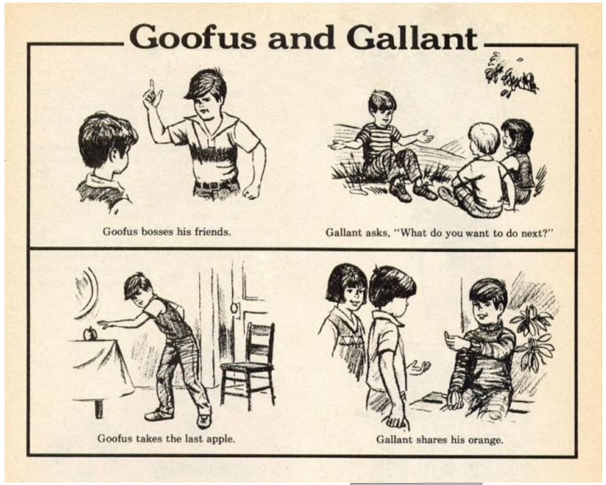

Goofus and Gallant
By Garry Cleveland Myers
Pictures by Marion Hull Hammel
Goofus runs with the scissors pointing up.
Gallant walks with the scissors pointing down.

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.


Goofus leaves his books spread all over the floor.
Gallant picks up his papers when he is finished.

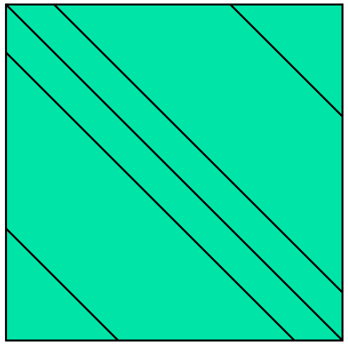

Goofus and Gallant
Goofus bosses his friends.
Gallant asks, "What do you want to do next?"
Goofus takes the last apple.
Gallant shares his orange.

All About Your Matrix

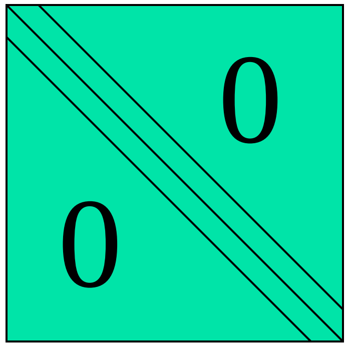
If you know things about your matrix, you maybe can use a more efficient solver.

- 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



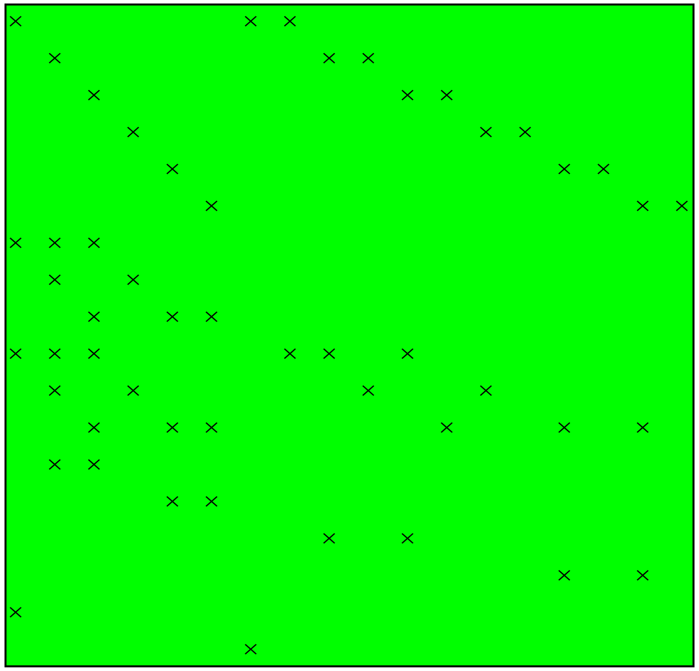
- Tridiagonal:



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

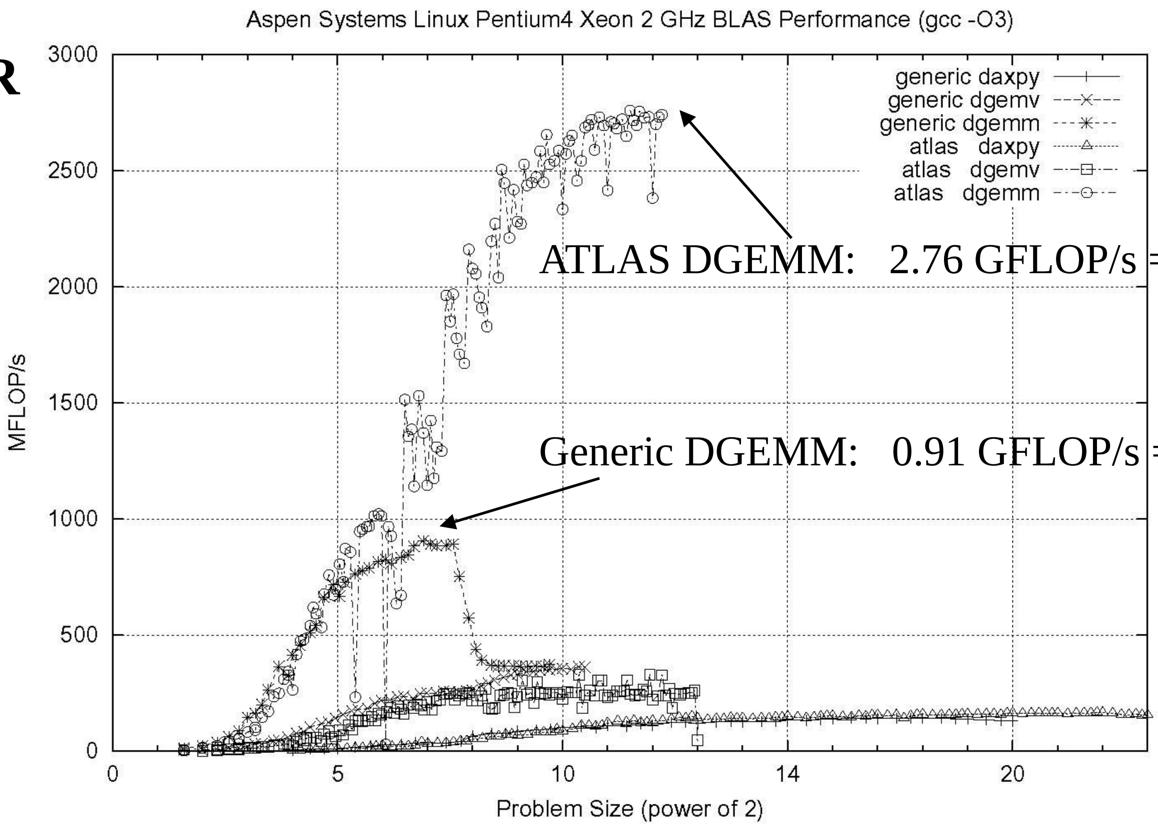
In the past several years, a new version of BLAS has been released, developed by Kazushige Goto (currently at UT Austin).

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



ATLAS DGEMM: 2.76 GFLOP/s = 69% of peak

Generic DGEMM: 0.91 GFLOP/s = 23% of peak

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

<u>Readability</u> of binary data **<u>isn't a problem</u>** 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

Binary data portability is a **very big problem** 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

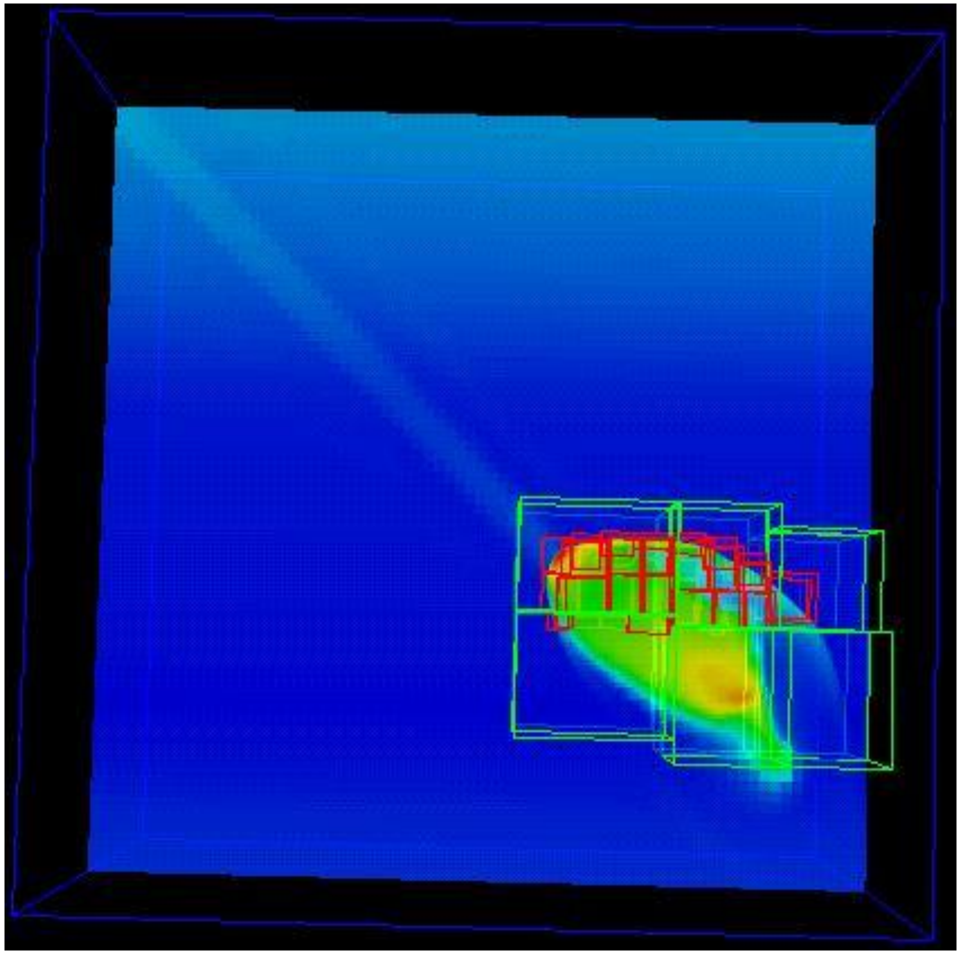
Too Many Numbers

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 **<u>10 terabytes</u>** (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

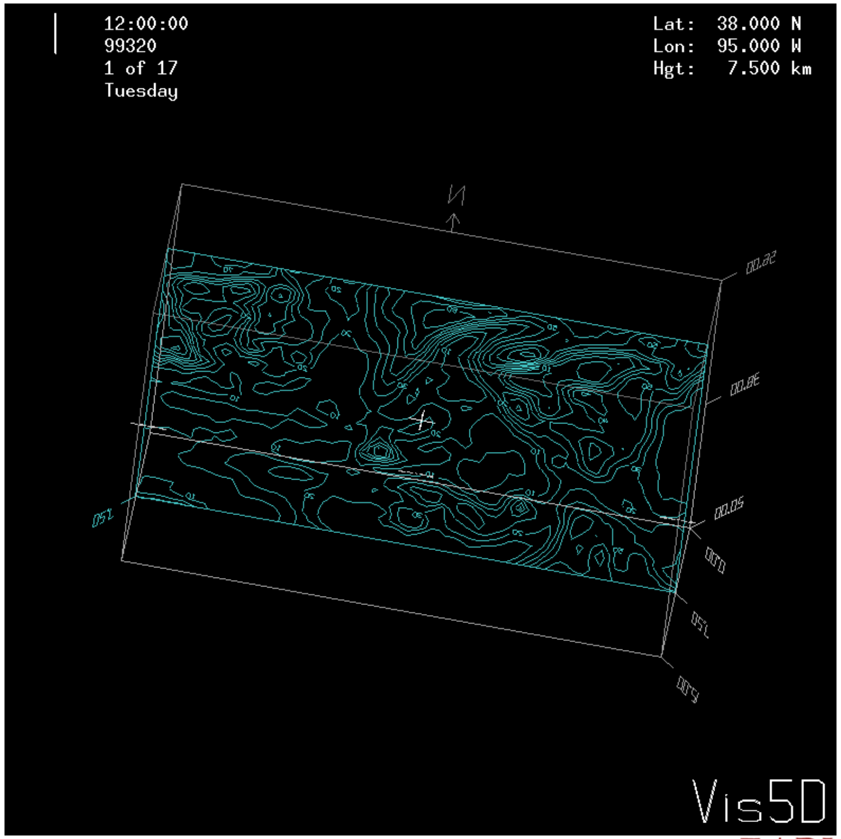
- Contour lines
- Slice planes
- Isosurfaces
- Streamlines
- Volume rendering

… and many others.

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

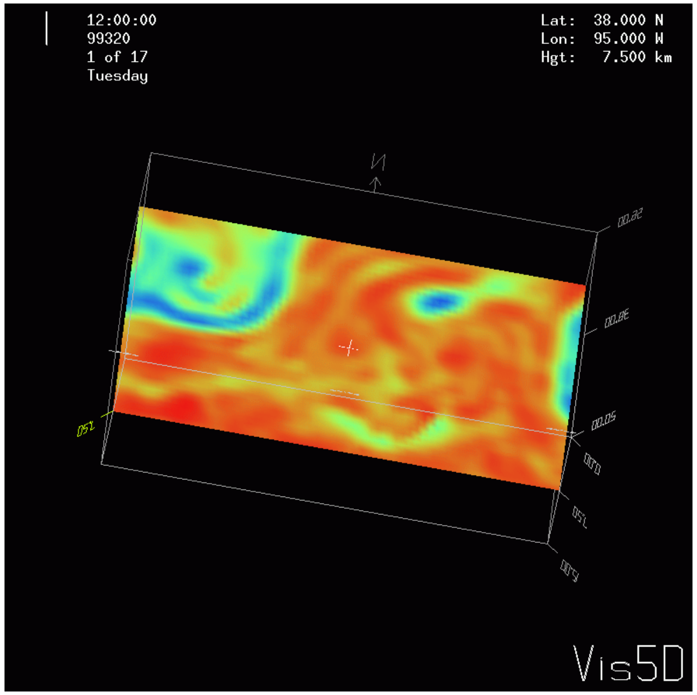
Contour Lines

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



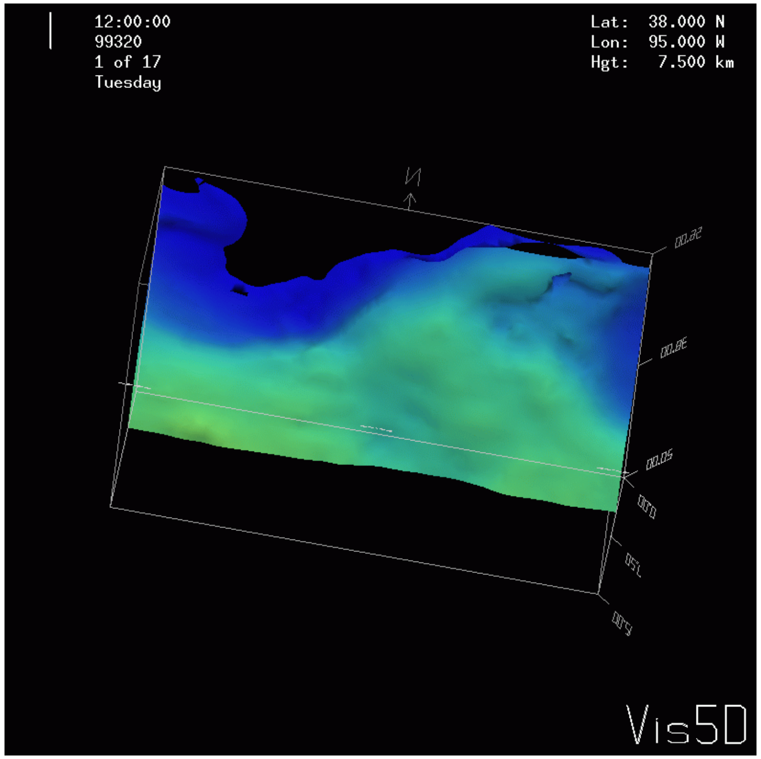
Slice Planes

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).



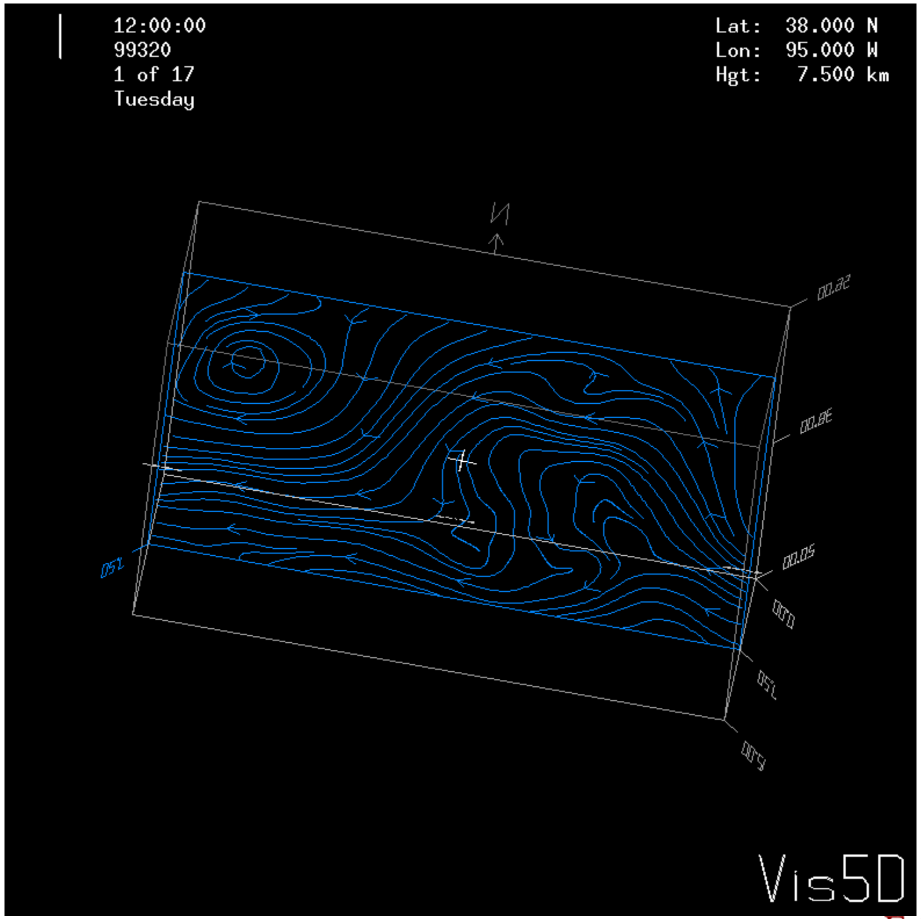
Isosurfaces

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

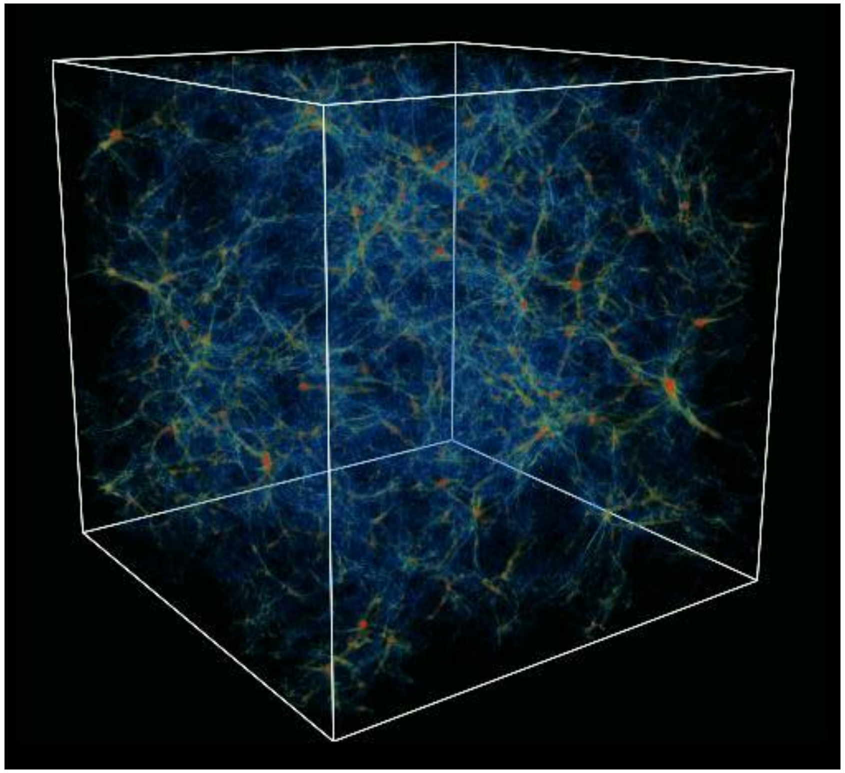
A ***streamline*** traces a vector quantity (for example, velocity).



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.



Thanks for your attention!

Questions?

www.oscer.ou.edu

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/

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[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

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[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.