Libraries

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What is a Library?

- Library - Wikipedia, the free encyclopedia.mht

Mathematical Software Libraries

- PETSc – Portable Extensible Toolkit for Scientific Computation
  PETSc Documentation.mht
- NetLib The Netlib.mht
- GSL - GNU Scientific Library - GNU Project - Free Software Foundation (FSF).mht

Must-Haves

- Linear Algebra: LAPACK
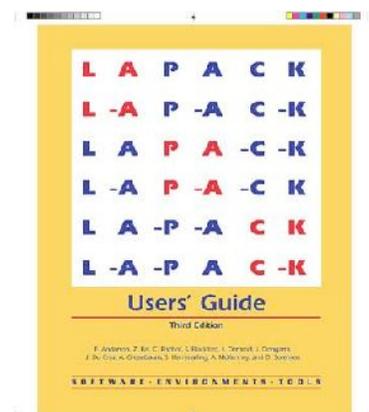
- LAPACK - Wikipedia, the free encyclopedia.mht

Why not write your own?
(or borrow from Numerical Recipes)

LAPACK

– Was written by a team of world experts in linear algebra

– Includes capabilities that you would be unlikely to incorporate into home-grown software

– Protects against common errors

– Does the best possible job of protecting against numerical instability

– Is built upon the BLAS
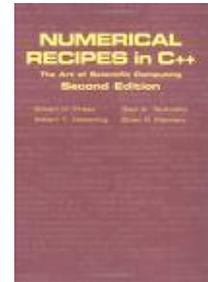
Basic Linear Algebra Subroutines (BLAS)

- BLAS
  Basic Linear Algebra Subprograms - Wikipedia, the free encyclopedia.mht

- A world-class resource
  Kazushige Goto Researcher Profile.mht

Production Code vs Your Own Software

- Classical 4th order Runge-Kutta method (from Numerical Recipes in C)
- RKF45 from Netlib rkf45_f.mht
  - Checks for errors and inconsistencies
  - Adaptive error control and stepsize selection
  - Diagnostics – tells you if the system is stiff, or if you have requested too much accuracy for the available precision on your computer
  - Can produce the solution value in between the mesh points
  - Fails gracefully

Beyond Libraries: Scientific Computing Environments

- Matlab
  MATLAB - Wikipedia, the free encyclopedia.mht
  - Fantastic for prototyping, graphics
  - May not be fast enough for your most demanding, large-scale applications

- COMSOL COMSOL Multiphysics®.mht

Coping with the Black Box

- Chances are, you will never understand everything that is going on inside your numerical black box

- So what! Since when did you understand everything that is going on in Windows XP or Mac OS X? Did it stop you from using it? Or would you prefer to write your own Operating System???!!!