Knowing Numbers: How Numerical Software Libraries Changed Scientific Practice

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Topic

- Why should historians of science/STS people should care about mathematical software libraries?
  - What are mathematical software libraries?
  - Why were they important
  - Relationship to well known concepts in STS
    - Black box
    - Immutable mobiles (Latour)
  - Questions raised for broader areas of science practice

Project

- History of mathematical software
- Consultant for Society for Industrial & Applied Mathematics on DOE supported project
  - 23 career oral history interviews
  - Several accompanying articles
- Materials at history.siam.org
  - Rather internalist
- Talk is initial attempt to explore issues of broader interest stemming from topic

Scientific Computing

- Original function of early machines
  - Harvard Mark I, ENIAC
  - Source of the term "computer"
- Many applications are concerned with modeling natural or man made systems
  - Hydrogen bomb physics
  - Fluid Dynamics of air for aerospace
  - Celestial mechanics for space navigation
- Require creating systems of equations and producing answers
  - Usually by numerical approximation methods

Mathematical Libraries

- Produced internally within computer centers
  - First example for EDSAC circa 1950
    - Invented along with subroutine
    - Discussed in 1951 programming text
    - Included Runge-Kutta differential equation routine
  - Routines stored on 5 track paper tape

Early Needs

- Initially: very basic assembly language subroutines
  - Multiplication, square root, binary to decimal, floating point simulation, etc.
- FORTRAN (1956) covers basics, but plenty of challenges left
  - Each computer center is likely to need routines for
    - Linear algebra and matrix manipulation
    - Ordinary and Partial Differential Equation solvers
    - Special and Elementary functions
    - Curve fitting and least squares
    - Fast Fourier Transformation

Argonne Case Study

- Argonne National Laboratory (Yood dissertation topic)
  - Computer building starts 1949
  - 2 ENIAC women hired for first library in 1951
- IBM 704 arrives in 1957
  - Standard hardware
  - Still rely on internally developed library
- Applied Mathematics Division formed 1956
  - Consolidation of 50 staff members
  - Monopoly on electronic computing
  - Division seeks ability to support computing research (vs. service)
  - Repeated reorganizations

Argonne Case II

- "Mathematical Algorithms Group" (20 people in late 1960s)
  - Distinct from "applied" and "systems" programming teams
  - Write, document new routines & improve old ones
  - Provide consulting to application programmers
  - Evaluate and modify externally produced routines
  - Argonne Code Center distributes routines
- 1970s: EISPACK (matrix routines) & LINPACK (linear algebra) projects
  - Collaboration with leading academic specialists
  - World class, portable packages in specialized areas

Packaging Expertise

- Craft knowledge of numerical methods formerly a part of carrying out computation
  - Held by generalist scientist/engineer, covered in textbooks
  - Intensive computation sometimes carried out by specialists
- Exchange of code spreads local practices beyond individual labs
  - Eventually leading to homogenization
- Code to solve specific equation types is now standardized and reused
  - Enables shift to newer, more complex mathematical methods
  - Traditional methods prove inefficient or highly inaccurate with high speed computers

Black Boxing Expertise?

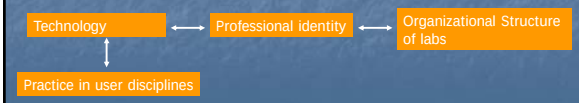
- In many ways, yes.
- But invocation of subroutines be dangerous without knowledge of methods used
  - May work very slowly or give meaningless results with specific equation
  - Library creators try to keep users aware of internal functioning – support role
- So is it a translucent box?

Division of Labor

- Author of application programs may not be computer specialist
  - Writes outline code for specific task
  - Most of the work accomplished by subroutine calls to standard routines written by experts
- Shift supports new groups of methods specialists
  - Expertise encapsulated in code
  - Some sharing of codes between labs
- By early 1970s, emerging as discipline
  - Conferences
  - Books
  - Journals
  - Interest groups
- Situated between applied mathematics & computer science

New Organizational Structures

- Computer departments provide new & secure location for expertise in applied mathematics
  - Library teams created in all(?) national labs
- Limitations of this position
  - Struggle to justify research agenda
  - Tend to collapse as computing is decentralized in 1980s
- Interplay between



Immutable Mobile?

- Latour, Science in Action
  - Artifacts issued by “centers of calculation” to “act at a distance”
    - Associated with adoption of printing
  - Mobile (within & between labs)
  - Immutable (sometimes)
  - Presentable (yes)
  - Readable (yes – open source)
  - Combinable with each other (that’s the point)
- Software seems to fit the description better than anything else!

Broader Implications for Science Practice

- Computers play ever more important role in scientific disciplines
  - So historians of science will have to get to grips with them
- Software packages/libraries allow computer use by non-specialists
  - Story of numerical routines parallels adoption of statistical software, modeling software, etc.
- Libraries & packages allow new division of labor
  - Embody split between experts and users
  - Separation of knowledge of internal functioning of routine from knowledge of how & when to use it