Archiving Computational Research in Virtual Machines

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Applied Mathematics Perspectives
Reproducible Research Workshop
Vancouver, BC
July 15, 2011

UNCvm

UNCvm

Implementing Godunov method

- fweb Literate programming
- LaTeX documentation
- C, Fortran code
- Matlab mex facility

```
[mitran-ThinkPad-W520:godunov1996]$pwd
/home/mitran/talks/2011/ICIAM/ReproducibleResearch/god
[mitran-ThinkPad-W520:godunov1996]$ls -al
total 92
drwxr-xr-x 2 mitran mitran  4096 2000-01-05 13:42 .
drwxr-xr-x 7 mitran mitran  4096 2011-07-14 18:17 ..
-rw-r----- 1 mitran mitran   715 1996-07-01 20:31 inde
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-rw-r----- 1 mitran mitran  1202 1996-07-14 20:59 inte
-rw-r----- 1 mitran mitran  1279 1996-07-01 20:30 make
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- ... or am I?
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- f2c, fweb, TeX - no problem
- Matlab 4.0 - now where's Cleve's phone number?

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#
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#       prog.tex
#       prog.dvi
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#   fweb system
#   TeX system
#   Matlab 4.0
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CC = wcc386
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LNK = laplace.lnk
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OBJS = prog.obj,interfac.obj

#  Implicit rules
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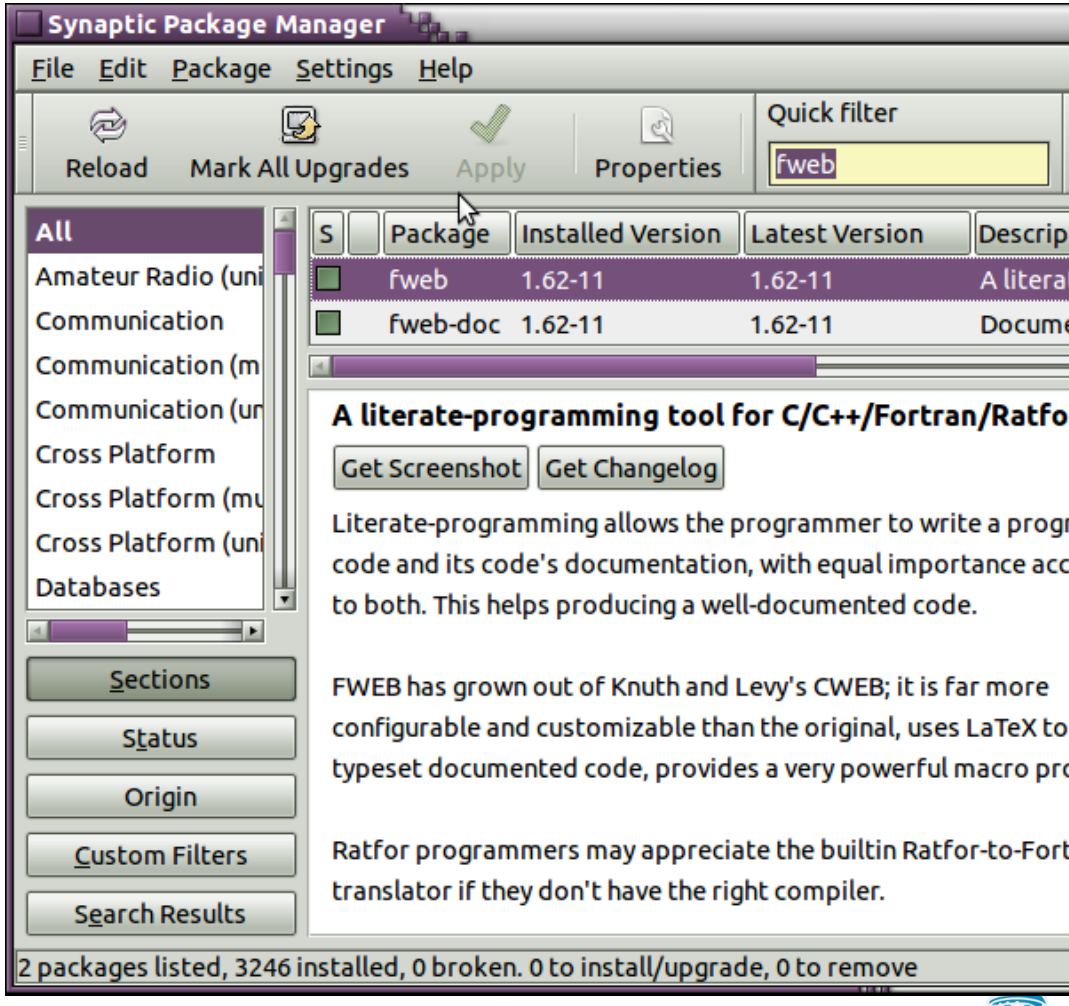
Some tools stick around, some don't

- Public domain tools are a bit more stable
- Proprietary tools are not
- Enough story-telling, get to work!
  - copy the directory
  - make prog.tex
  - fweave prog.web
  - rm *.dvi; latex prog.tex
  - ftangle prog.web; f77 prog.f
  - vim prog.f; f77 prog.f; vim prog.web



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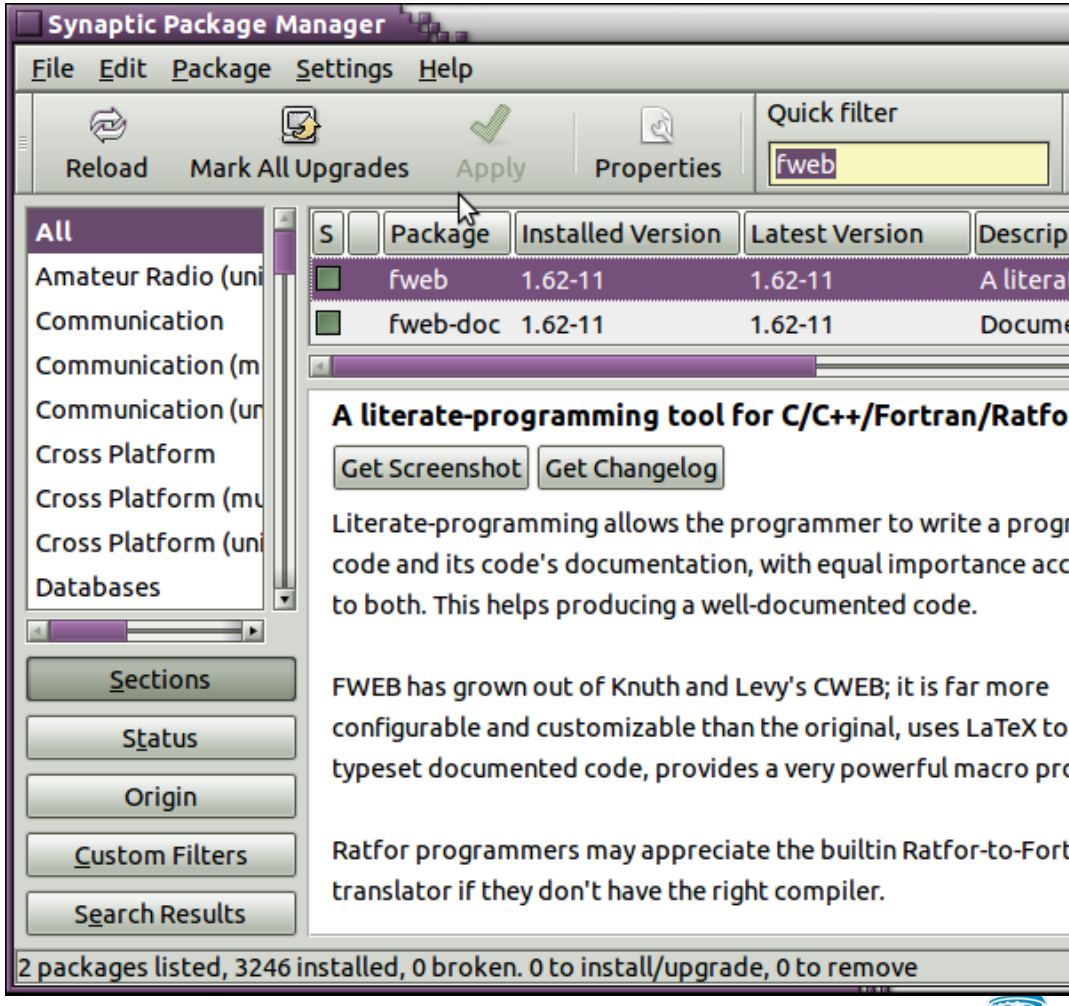

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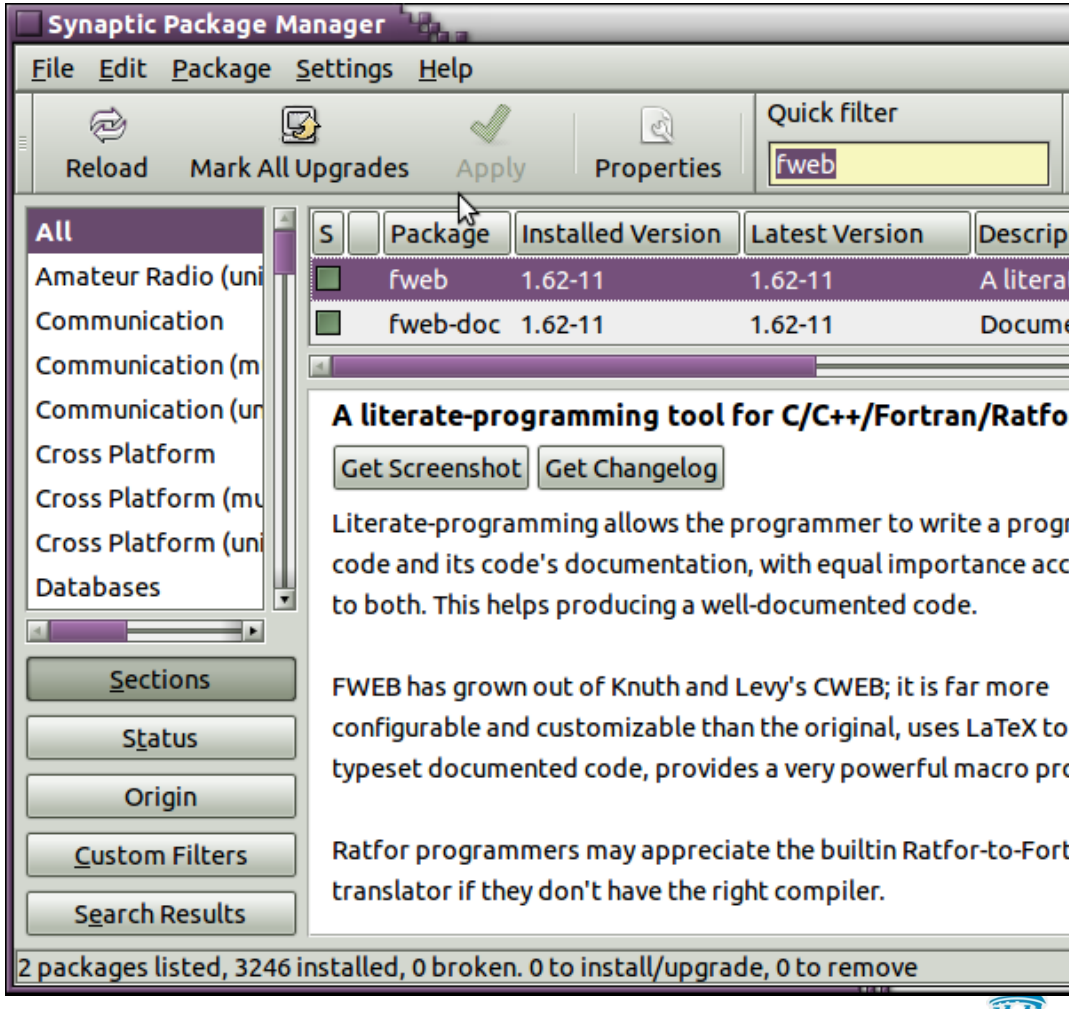

Lessons learned

- Panta rei, *Quingenti annus abhinc vos auditus mihi diversus*
- $p(x) = y_0 + [y_1, y_0](x - x_0) + [y_2, y_1, y_0](x - x_0)(x - x_1)$
- Science is a social endeavour ...
- ... hence a product of its time
- Historians can afford to decipher
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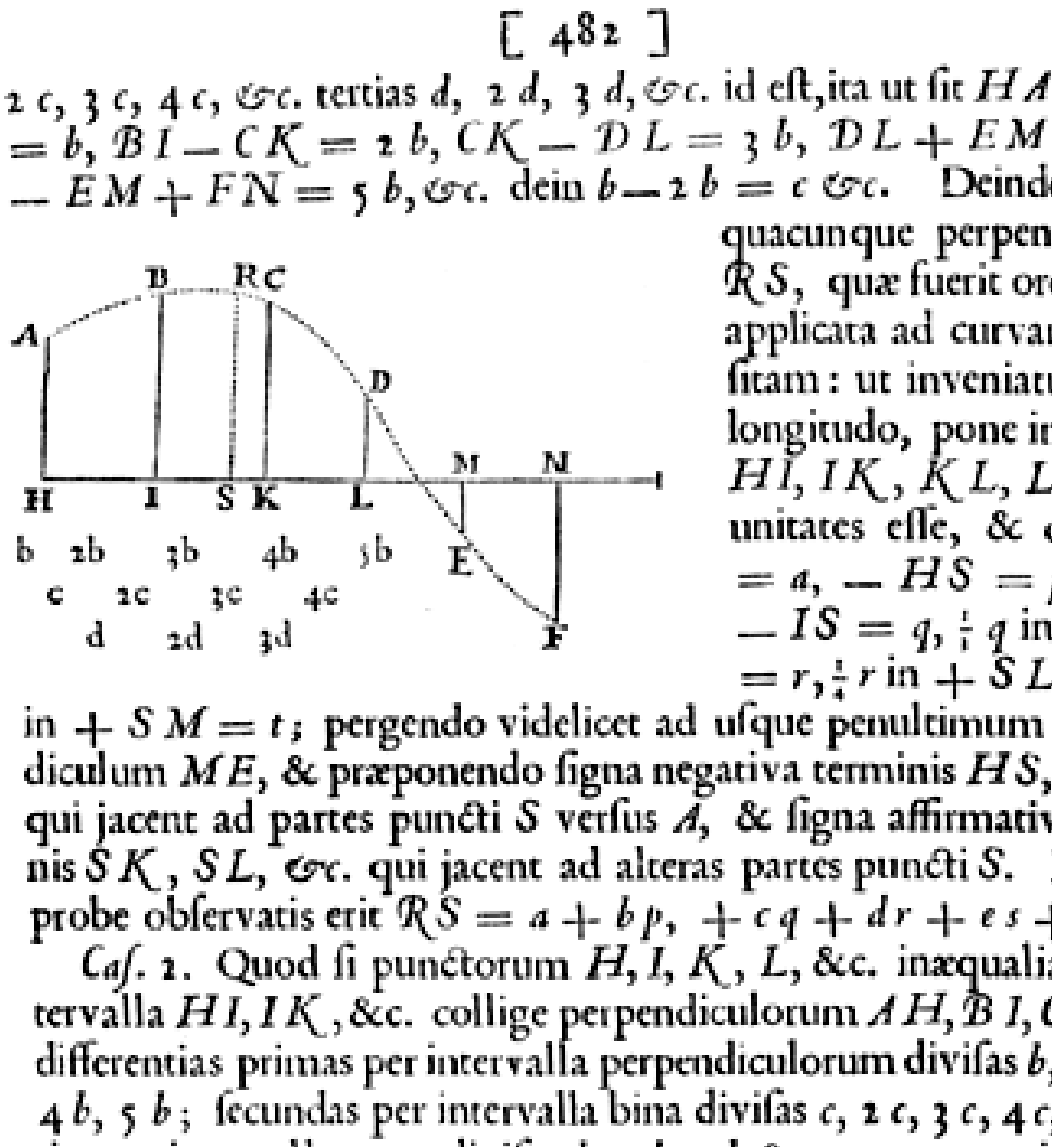

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2 c, 3 c, 4 c, &c. tertias d, 2 d, 3 d, &c. id eſt, ita ut ſit HA
$= b$, $BI - CK = 2b$, $CK - DL = 3b$, $DL + EM$
$- EM + FN = 5b$, &c. dein $b - 2b = c$ &c. Deinde

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tervalla HI, IK, &c. collige perpendiculorum AH, BI,
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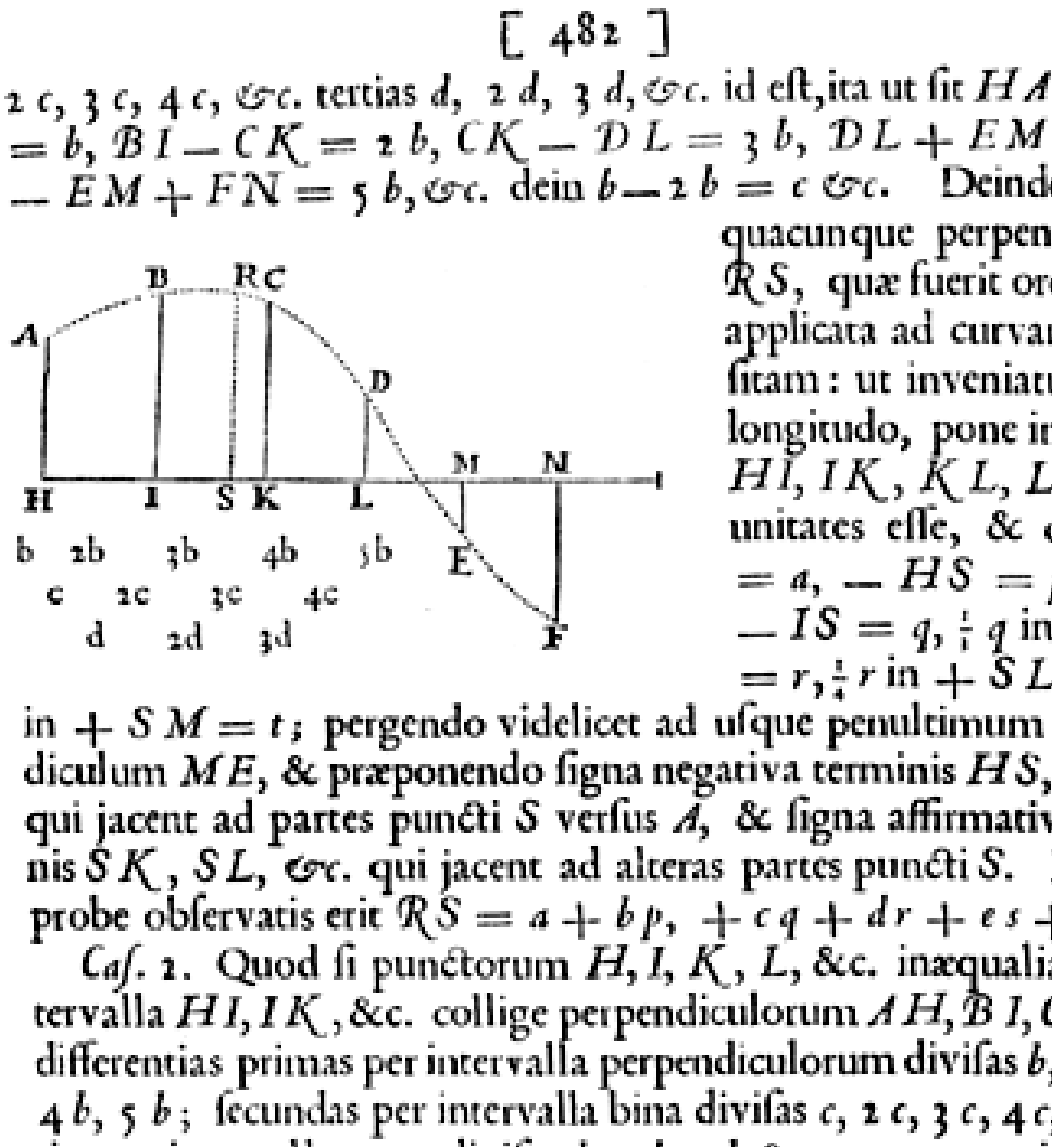

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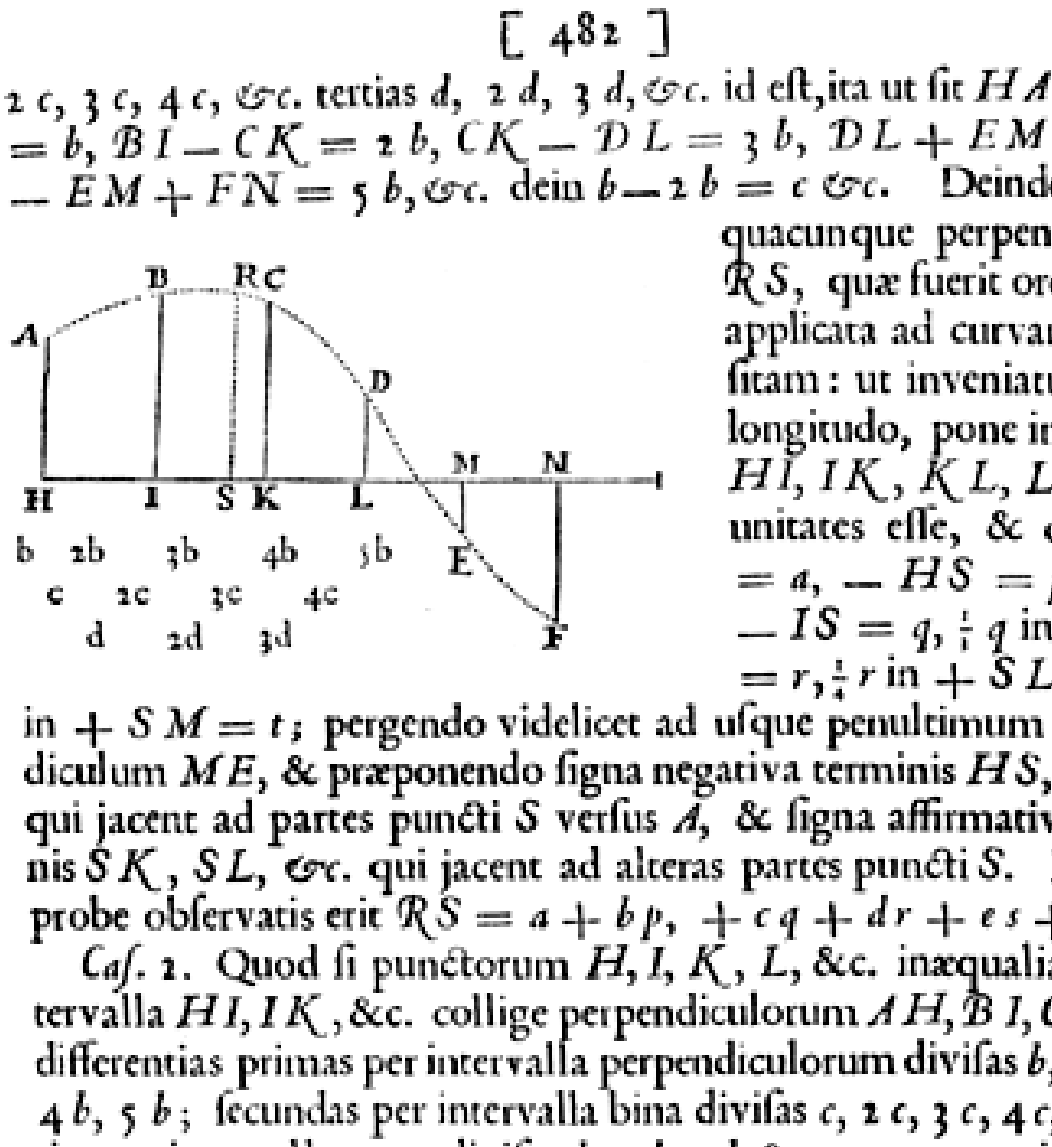

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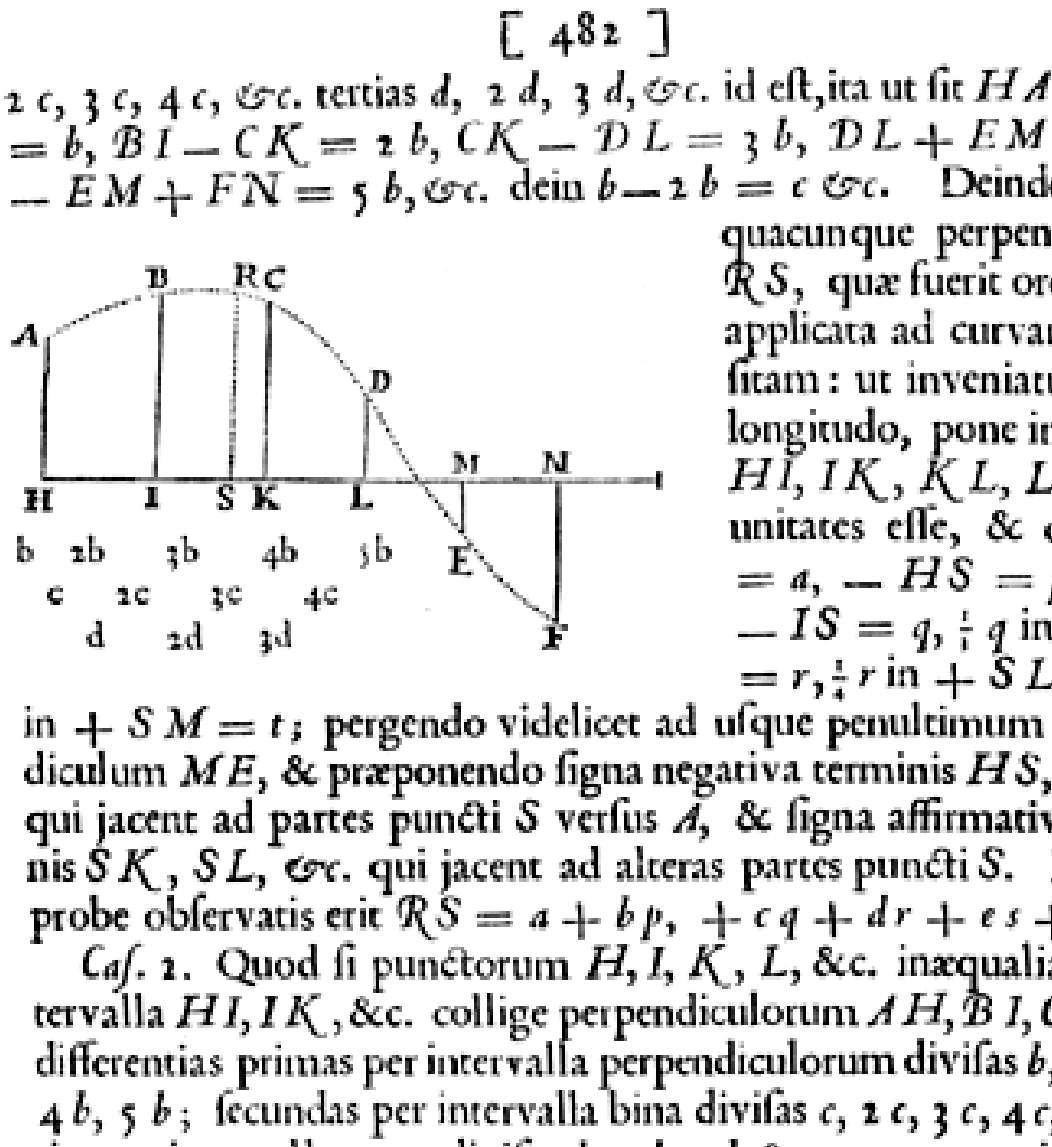

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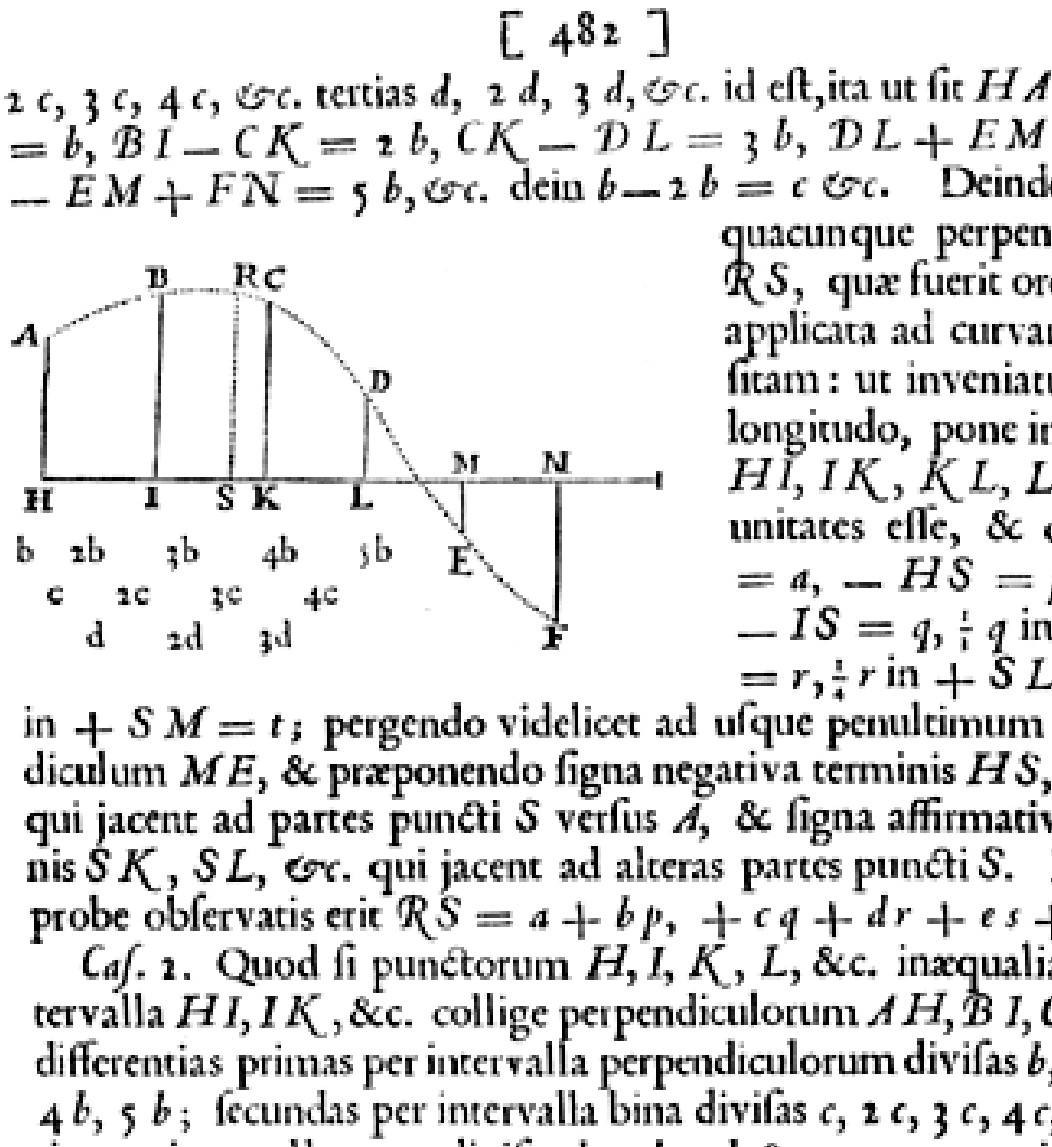

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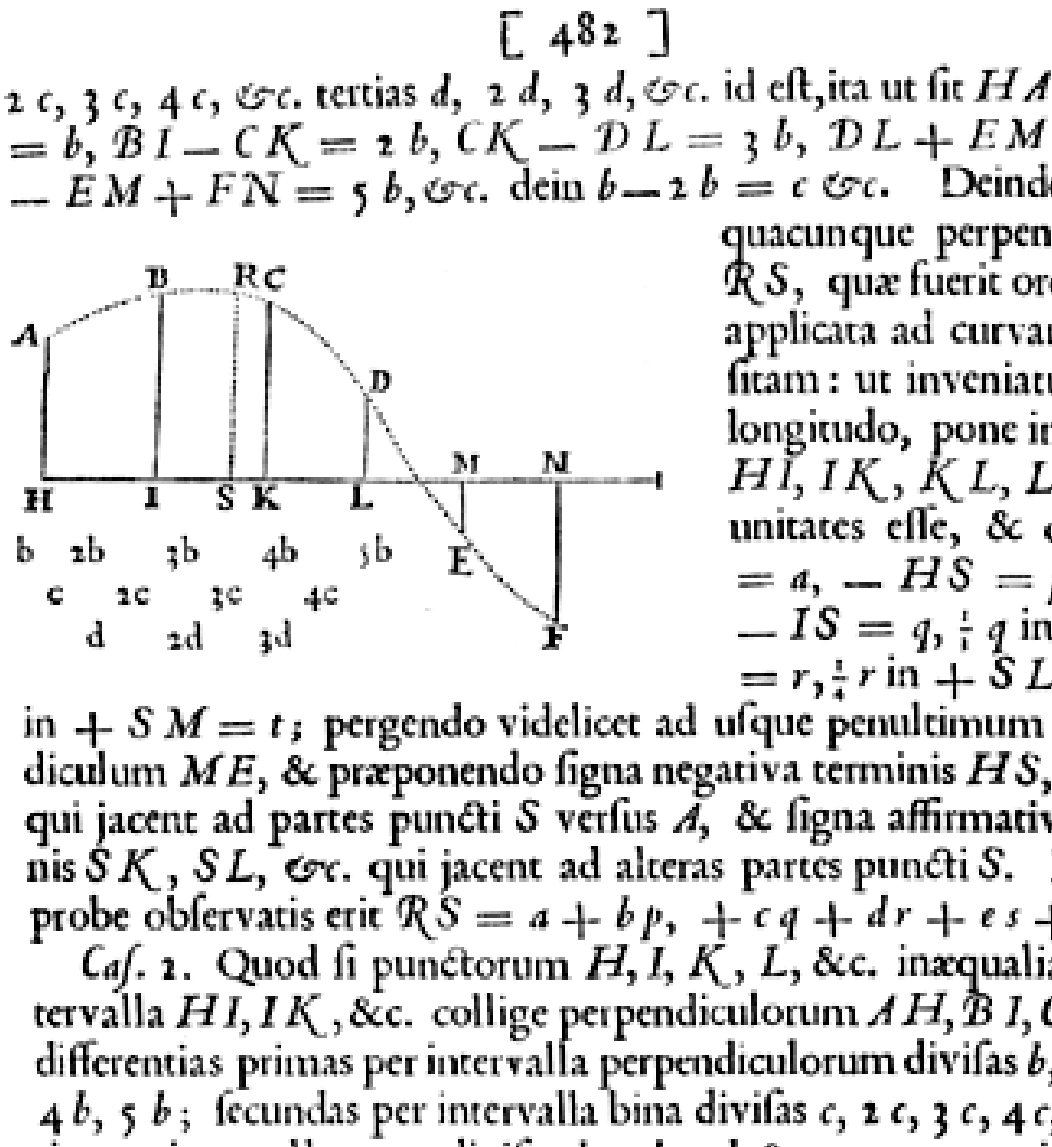

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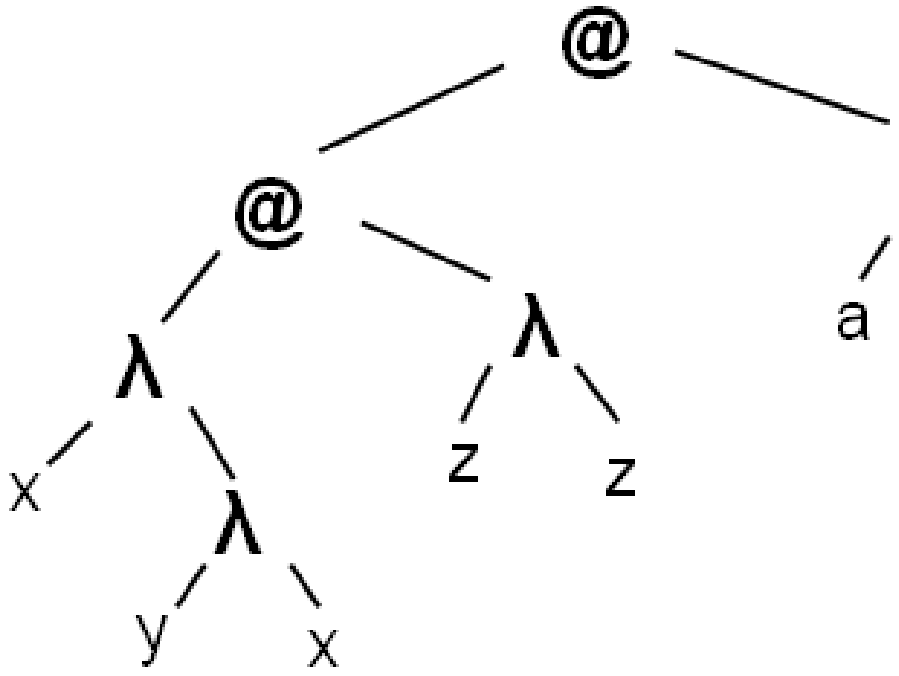
Live without side effects?

- Alonzo Church lambda calculus
  - no side effects
  - all expressions are calculable
- Imperative languages have side effects
- If we use imperative coding
  - store the context
  - store the state

Lambda expression:

((λ x . (λ y . x)) (λ z . z)) (λ a . a



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- Alonzo Church lambda calculus
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  - all expressions are calculable
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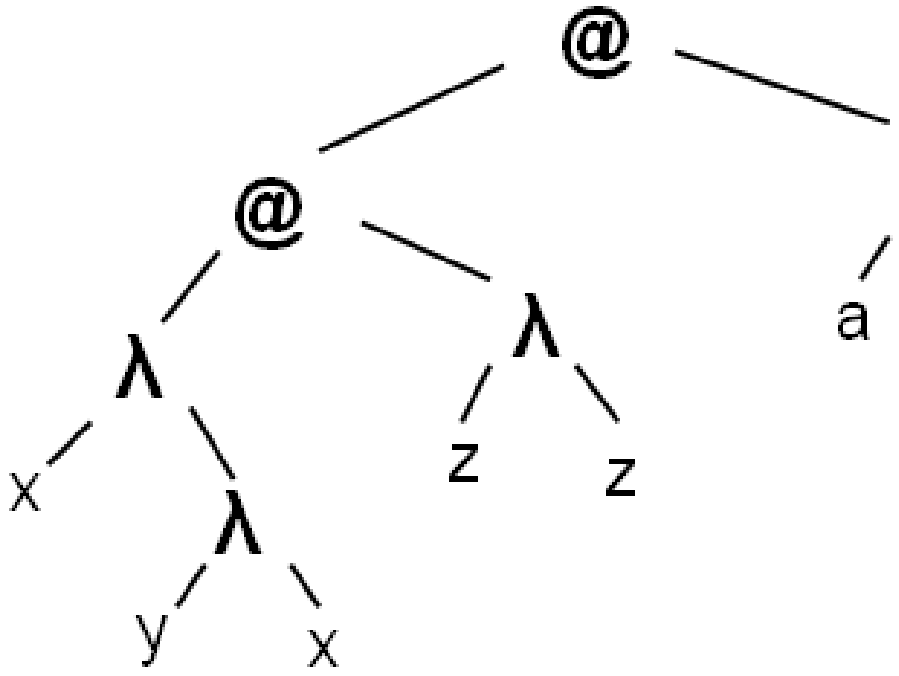

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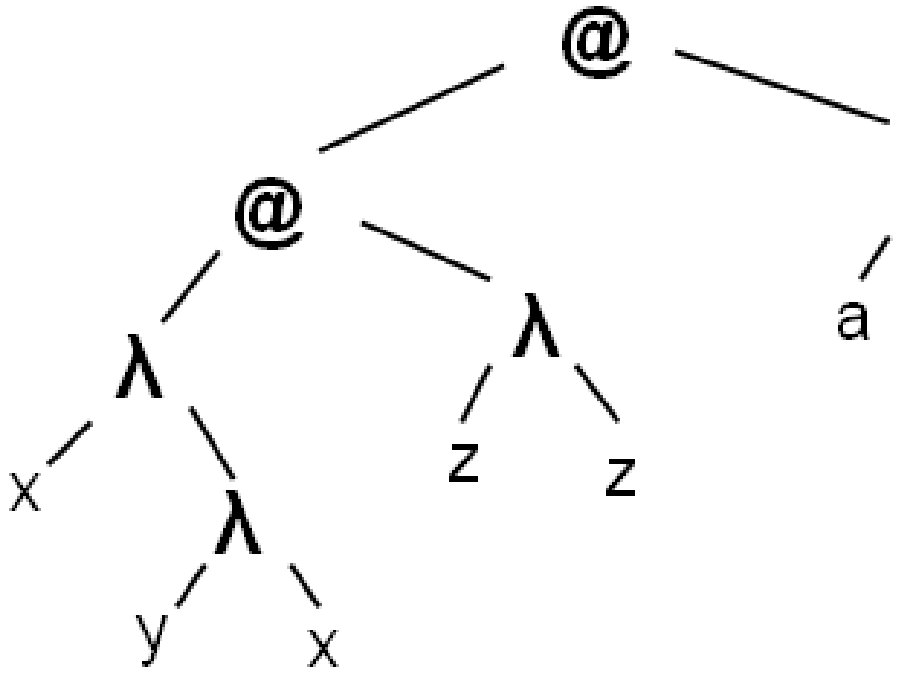

Virtual machines

- What should be stored?
  - Compiler, library versions
  - Tool versions
  - OS idiosyncracies
  - this might be a long list ...
- What should be restored, and how?
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Virtual machine pros and cons

- On the plus side
  - Hardware support (virtualization bit)
  - Saves entire context
    - Turbo Pascal 5.5 (1989)
    - Shock code from 1990 still runs (with graphics!)
- On the loss side
  - Large amount of data to store - the entire OS
  - What guarantees that the VM emulator will still run in 20 years?
  - What about hardware essential to code execution (multiple CPUs for MPI, GPUs)
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  - Storage is cheap and always getting cheaper
  - Current strong vendor support for VM emulators
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Virtual machines for all

- Whatever your workflow
  - store it
  - document it
- Use version management
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  - store forks
- Distribute your code
  - with preset environment
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Peculiarities of an academic environment

- Incoming students are required to have a laptop

Minimum Laptop Specifications for First Year Students/Freshman

Students in the class of 2015 are required to have a laptop that meets or exceeds
All CCI models meet or exceed the specifications below:

- **Processor:** Intel Core i5, Dual Core 2.3 GHz or better
- **Memory:** 4 GB Minimum
- **Operating System:** Microsoft Windows 7 Enterprise or Ultimate
  - Can be installed for UNC-Chapel Hill students at no extra cost. Visit
    for more details.
- **Hard Disk Drive:** 250 GB
- **Optical Drive:** DVD Read/Write
- **Display:** 12 inches or larger

Peculiarities of an academic environment

- As for research scientists ...

Research Computing: Getting Started

UNC Research Computing makes a number of computing resources available for researcher
these are a 4160-processor Dell Linux cluster (Topsail); a 480 processor Linux cluster (Kure);
cluster (Emerald); and four 16-processor IBM P575 machines (accessed through Emerald).

An Onyen is required to get an account on any of the Research Computing servers. If you alr
request access to these servers by visiting the Onyen Services page and selecting **Subscrib**
these servers are available to faculty, staff, and graduate students. Undergraduate students n
instructions in the Research Accounts section of the Onyen Policy document.

At this time, requests for accounts on the large Dell cluster (Topsail) or the HP cluster (Kure)
research@unc.edu. Note that these resources are intended for use for very large parallel jobs
information to provide in your request for an account on either of these clusters includes: onye
([onyen]@email.unc.edu format), your full name, your campus address, your campus or cell p
your faculty sponsor (PI) and your sponsor's onyen (if you are not a faculty member), and a d
be working on.

How to guide the transition?

- Advocate for more research-friendly platforms
  - OS X (Carnegie-Mellon Mach kernel)
  - Ubuntu (Debian)
  - CentOS (Redhat)
- 1-click Linux install on Lenovo UNC-contract hardware

- Difficulties
  - The Linux environment still has to be configured
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UNCvm

- Lubuntu (Lightweight Ubuntu with LXDE)
- Contains free mathematical tools
  - Python, Octave, Gnuplot, Maxima
  - TeXmacs
- Supports via version forks
  - MPI, OpenMP (UNCvmMP)
  - rCUDA GPU (UNCvmGPU)
- Contains in-house code
  - BEARCLAW, Diapason
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Challenges

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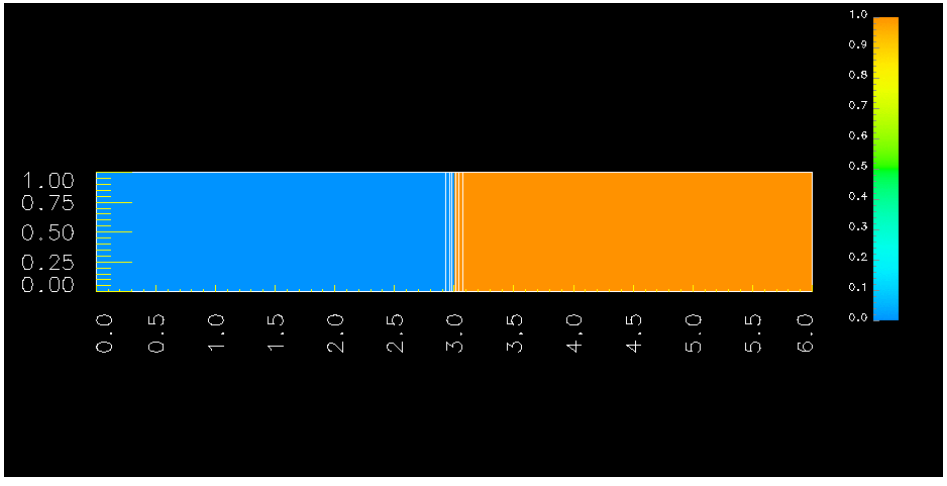
Software PDE solver package

- AMR
- MPI
- multiphysics
- mixed-mode CPU/GPU

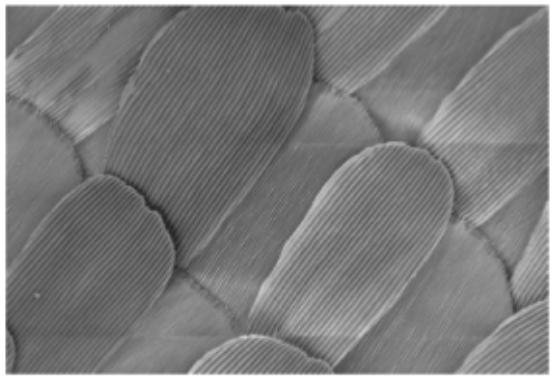


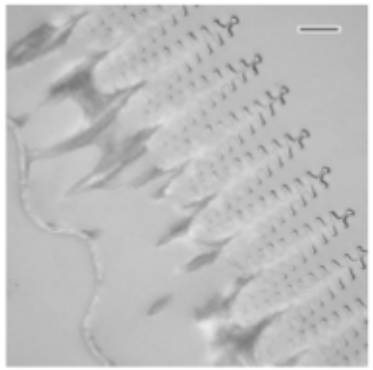
Patterned organic solar cells

- Mimic nature

Morpho Menelaus butterfly (Smentkowski et al., 2006)

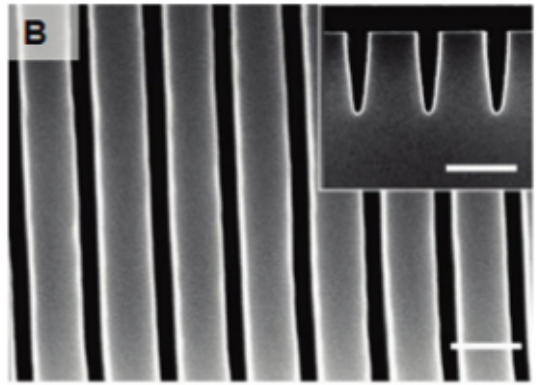
wing span $\sim 11.5\,\mathrm{cm}$



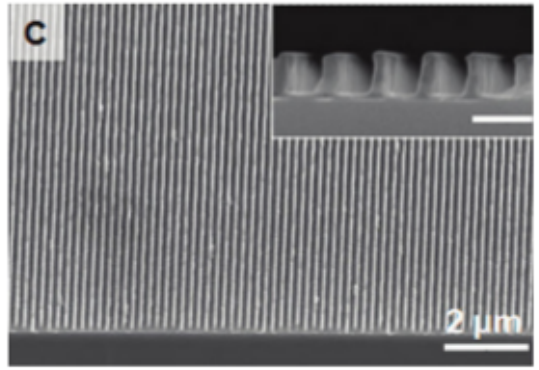


TEM, bar $500\,\mathrm{nm}$

Nanoimprint Lithography (Aryal et al., 20

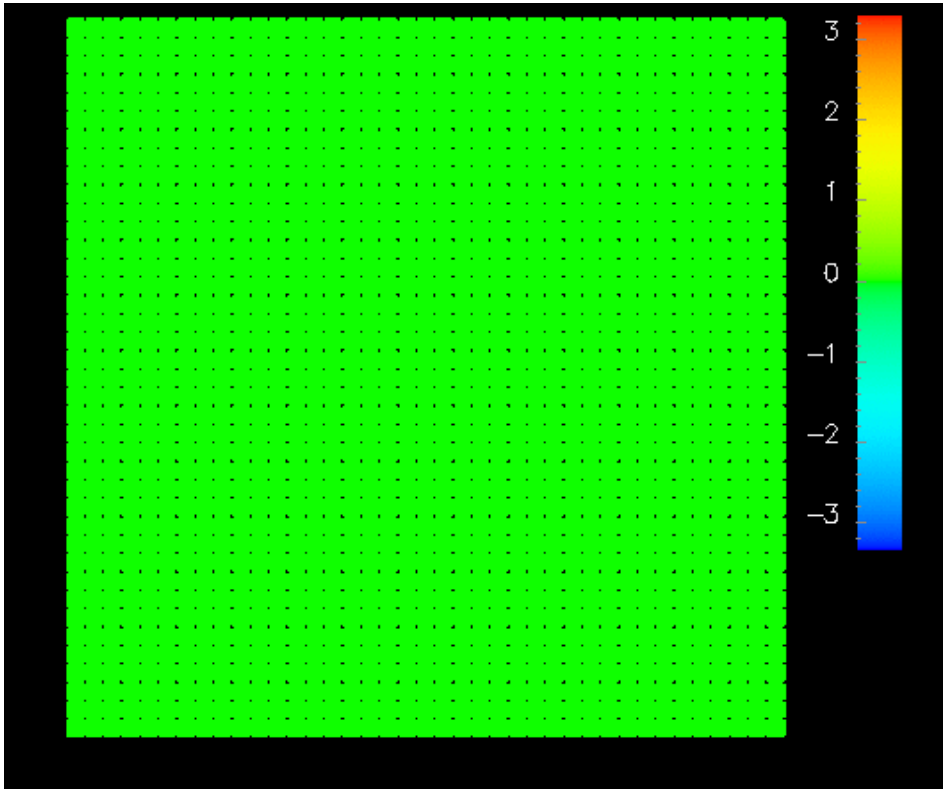


Si mold, bar $200\,\mathrm{nm}$



photonic Computational model

- Solve Maxwell equations
- Time domain
- Dispersive media
- Auxiliary equation



UNCvm

The whole thing

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- Reproduce your workflow
- Comment and write as you code

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