

Scientific Software: Art, Engineering, or Science?

Robert Lupton, Princeton University

LSST Pipeline Scientist









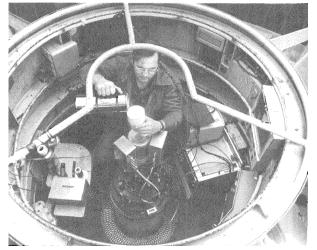


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 - Small cameras and small teams



Ed Danielson with Gunn and Westphal's PFUEI (Gustafson, 1983)





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 - But small computers



4*(32 + 7) 16 kbi chips; 256 kB





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- Simple Computers with Simple Operating Systems





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- Simple Computers with Simple Operating Systems ... but more than one of them (JCL v. VMS v. Unix v. DOS v. ...)





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Swæ clæne [lar] wæs oðfeallenu on Angelcynne ðæt swiðe feawa wæron behionan Humbre ðe hiora ðeninga cuðen understondan on Englisc, oððe furðum an ærendgewrit of Lædene on Englisc areccean; ond ic wene ðætte noht monige begiondan Humbre næren.

Ælfred se Cyning, c. 895 CE





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So general was [learning's] decay in England that there were very few on this side of the Humber who could understand their rituals in English, or translate a letter from Latin into English; and I believe that there were not many beyond the Humber.

Alfred the Great, c. 895 CE





I mixed up a lot of issues on that slide!









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Ever-larger instruments





- Ever-larger instruments
- Ever-more sophisticated algorithms





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Let's take a look at some of these issues.









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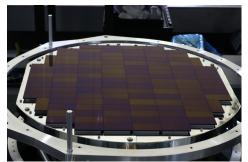


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Instruments



Why do you care that instruments are becoming larger?



Instruments



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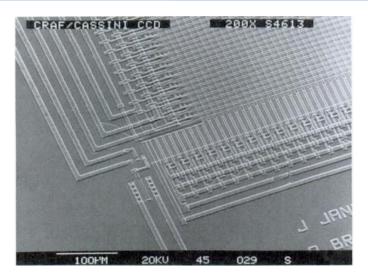
Instruments



Why do you care that instruments are becoming larger? Because someone has to understand them in detail, and it may be you.



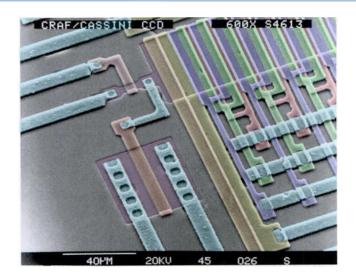
Real CCDs (a Tektronix CCD; Janesick



Corner of active area, parallel gates, serial register, and output capacitor



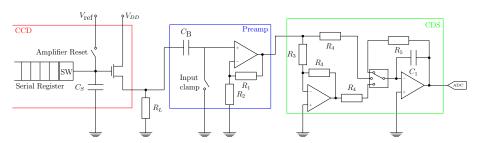
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Serial register, reset gate, and output capacitor

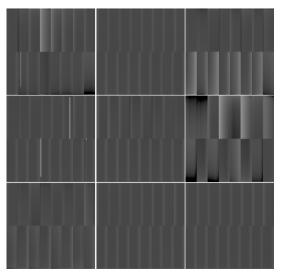


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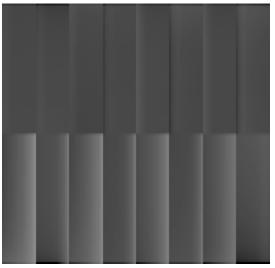




LSST Raft RTM5



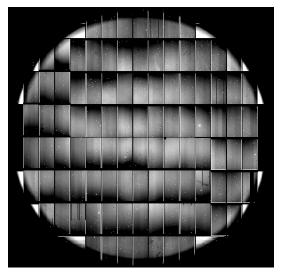




LSST Raft RTM5 S22







HSC g-band





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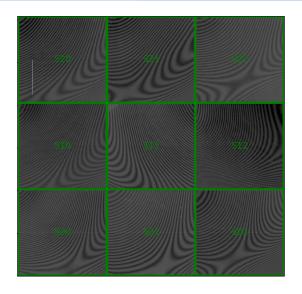
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LSST Raft RTM5 post-ISR







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We need large disks and large computer systems





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I am not convinced that this is true, even if we could compete financially with Google and Microsoft.



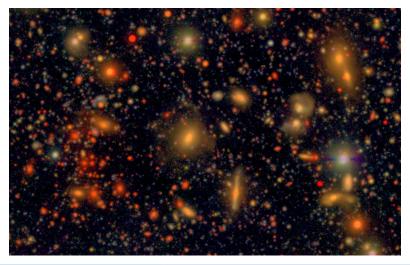


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If you were plowing a field, which would you rather use: Two strong oxen or 1024 chickens? Seymour Cray



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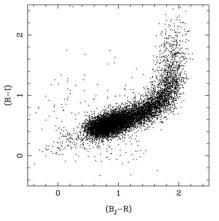
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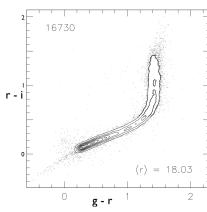


Better Data → Better Science





01)



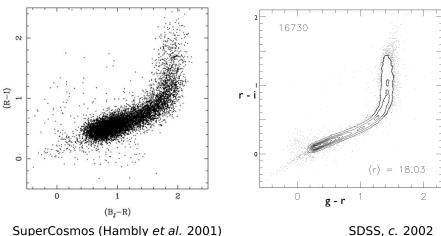
SuperCosmos (Hambly et al. 2001)

SDSS, c. 2002



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On the left, scanned Palomar plates; on the right SDSS CCD data.



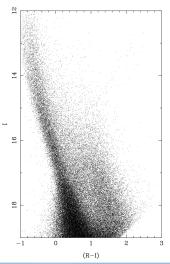


Getting something as good as that SuperCOSMOS colour-colour diagram took heroic efforts fighting photographic emulsions:





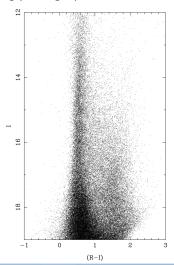
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Better Data → Better Analysis



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Once you think about even humble aperture photometry it's quite subtle

– How does the surface brightness vary across the pixel?





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- How about to Janskys?

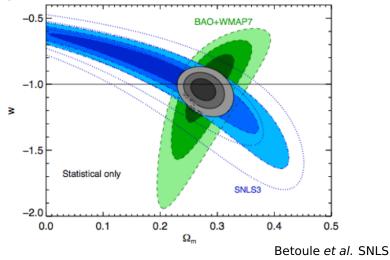






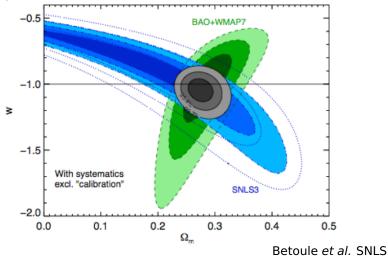
$\textbf{Large Data} \rightarrow \textbf{Systematics}$







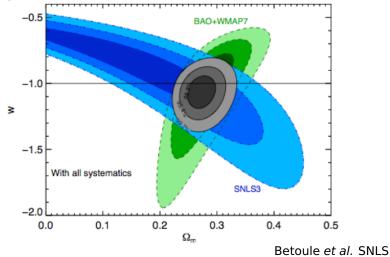






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- As statistical errors become smaller, systematic errors come to dominate.
 - Only about 50% of SNLS's variance in Ω_m based on c. 200 high-z SNe Ia is statistical.



$\mathsf{Large}\;\mathsf{Data}\to\mathsf{Systematics}$



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 - Only about 50% of SNLS's variance in Ω_m based on c. 200 high-z SNe Ia is statistical. LSST will detect c. 5×10^5 SNe Ia, of which maybe 20000 will be useful for cosmological analysis.



$\textbf{Large Data} \rightarrow \textbf{Systematics}$



Software can contribute to systematic errors.



$\textbf{Large Data} \rightarrow \textbf{Systematics}$



Software can contribute to systematic errors. Shhhhhh!



$\mathsf{Large}\;\mathsf{Data}\to\mathsf{Systematics}$



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$$I(\mathbf{x}) = A\phi(\mathbf{x} - \mathbf{x}_0) + \epsilon$$

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where I have subtracted the background level. If the noise ϵ has known variance σ^2 , and if I know the position, the (unbiased) optimal linear estimator for the flux A is

$$\hat{A} = \frac{\sum_{i} \phi(\mathbf{x}_{i} - \mathbf{x}_{0}) I(\mathbf{x}_{i}) / \sigma_{i}^{2}}{\sum_{i} \phi(\mathbf{x}_{i} - \mathbf{x}_{0})^{2} / \sigma_{i}^{2}}$$

and this is the MLE (and attains the Cramér-Rao bound) if the noise is Gaussian.





If the star is faint, the noise is the same in every pixel ($\sigma_i^2=\sigma_0^2$) and this reduces to

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I can in fact spurn my statistical friends and replace $\phi(\mathbf{x}_i - \mathbf{x}_0)/\sigma_i^2$ with any weight function w_i of my choice:

$$\hat{A} = \frac{\sum_{i} w_{i} l(\mathbf{x}_{i})}{\sum_{i} w_{i} \phi(\mathbf{x}_{i} - \mathbf{x}_{0})}$$

$$\equiv C \sum_{i} w_{i} l(\mathbf{x}_{i})$$

e.g.

$$w_i = \begin{cases} 1 & |\boldsymbol{x}_i - \boldsymbol{x}_0| < R \\ 0 & \text{otherwise} \end{cases}$$





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How should we choose w?





- If you want as small a *statistical* error as possible, $w_i = \phi(\mathbf{x}_i)/\sigma_i^2$
- If you want as small a *total* error as possible for *faint* sources, use $w_i = \phi(\mathbf{x}_i)$
- If you want as small a *total* error as possible for *bright* sources, use $w_i = (r < R?1:0)$ where R is large enough to include most of the photons and not too much background.





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There are similar discussions to be had about galaxy photometry, but they are harder as the uses of the fluxes are more complex (and non-linear); *e.g.* as inputs to photo-z codes used to estimate weak lensing kernels.



Better Analysis \rightarrow Complex Codes





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Finally something related to this school!



Better Analysis → Complex Codes



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 You can no longer rely on one person to hold the complete codebase and bug list in their head, exploit the catalogue, and write the papers.



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- You can no longer rely on one person to hold the complete codebase and bug list in their head, exploit the catalogue, and write the papers.
- Astronomers have to learn the tools of software engineering



SDSS and Hipparcos



This part of my presentation started out with a conversation with Michael Perryman (then P.I. of GAIA) about Hipparcos and SDSS.









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- Lesson 2: Don't join under-funded projects
- Lesson 3: Don't generate an inverted management structure
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I wrote these down in 2002; what have we learned in the last 16 years? Some of these are obvious, but were nevertheless ignored by SDSS. Many are being ignored by XXX and YYY too.



Disclaimer



The advice in this talk comes from a PCA analysis of my involvement in

- SDSS
- PanSTARRS
- ACT
- HSC
- LSST
- Euclid
- PFS
- WFIRST



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- Euclid
- PFS (Ask me about my job at http://web.astro.princeton.edu/jobs)
- WFIRST

Any resemblance to actual projects, living or dead, or actual events is largely coincidental.

No animals were harmed in the writing of this talk.





We've learned a lot about software engineering:





- C++
- python





- C++
- python
- git





- C++
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- jUnit





- C++
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- Jenkins, travis, ...





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- C++
- python
- git
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- Jenkins, travis, ...
- JIRA / github issues
- docker, conda, ...





Some of us have learned a lot about software engineering:

- C
- TCI
- cvs
- GNATS
- _

Actually SDSS didn't do too badly.

Douglas Adams (The Hitchhiker's Guide to the Galaxy. 1978)

Orbiting this at a distance of roughly ninety-two million miles is an utterly insignificant little blue green planet whose ape-descended life forms are so amazingly primitive that they still think fortran is a pretty neat idea.









Some of us have learned a lot about tools for software engineering. What have we learned about software design and practice?





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Unfortunately our new-found wisdom sometimes makes the job of managing software groups harder; some people love the journey more than the destination, others are Luddites who don't care about technical debt.



Project Managers



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You need a strong and impartial project manager. SDSS is a collaboration of a large number of institutions and we have never managed to take technical decisions unimpeded by politics.



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"Now we are only nice. One must specialise these days"

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I no longer innocently believe that all we need to do is to hire a project manager, as they mostly come from quite another world. We *do* need them, of course, but we need to choose them carefully.



Many project managers come from hardware backgrounds.



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So we have a recursive problem. How do we manage the DM Project Manager? Or, better, how should we find managers who don't need managing?





Tools don't write programs, people do.





Tools don't write programs, people do. Some of our problems are engineering ('How should we handle multiprocessing?'), some are algorithmic ('Please write me a weak-lensing-quality deblender'), and some are computational ('I'll give you 10ms per object to fit a galaxy model'), but most are about working together, making the best use of our varied skills.





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Neither Science nor Software can be run as a democracy. Not all participants are equal, and it's folly to pretend that they are. This is not to say that the most senior (or smartest) individual should simply lay down the law.





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A piece of good news:

Janel Garvin, Dr. Dobbs Journal (2015-10-01)

So, all told, developers are not the lonely, antisocial nerds that they are portrayed to be, nor are they free-wheeling socialites.









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The resolution is that the shortage is of the best engineers, not the median:

If the best software developer can do the work of 10, 20, or even 100 run-of-the-mill employees, a single-person company that attracts such a superstar can compete effectively against a much larger enterprise

[...]

In some cases, software developers who fall at the low end of the productivity curve may be essentially nonproductive or even counterproductive



Single point failures



Robert Lupton "Lesson 9: Avoid single points of failure"

OK, so this is totally obvious, but there are subtler aspects:

- If one person is allowed to become essential it implies that it's proved impossible to find someone else who could fill their rôle
 In consequence, if they are on the critical path, and problems arise, it's hard to add resources to solve the problem.
- If someone with an essential job isn't very good, then an essential component of your system isn't going to work very well.



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My only update would be:

Hire as many people as you can who have with the ability to become single points of failure; then try to manage the project so that they don't.



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Robert's Corollary

Roberts' paradox implies that we'll almost always have single points of failure





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 dreaming about CRTP and inventing cunning new deblending algorithms that enable us to characterise high-z Luminous Red Galaxies

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is of intrinsically higher worth? And which is a more valuable skill to teach our students?



LSST Status this Week







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- Our instruments generate big complicated data





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Scientific Software: Art, Engineering, or Science?





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Scientific Software: Art, Engineering, or Science?

and now we know the answer:

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Scientific Software: Art, Engineering, or Science? and now we know the answer:

Scientific Software: Art, Engineering, and Science. And Fun.



LSST Status this Week





A Condor over Cerro Pachón



LSST Status this Week





A Condor over Cerro Pachón