The Initiative in Innovative Computing at Harvard

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> Scholar-in-Residence, WGBH Boston



Ideas worth spreading

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TEDGlobal 2009

Bio

Michelle Borkin works on creating new approa interdisciplinary scientific imaging, data exploimage analysis with a focus on 3D visualizatio wrote her undergraduate junior and senior the the application of medical imaging programs t astronomical data and has continued this rese part of the "Astronomical Medicine" project at I Initiative in Innovative Computing. She works to developers of medical visualization tools to im

A Student's Story

Y IC journey began in a Cambridge Starbucks on IV Broadway on a cold, cloudy day in 2005. I was a Harvard undergraduate concentrating in astrophysics and looking for a junior thesis topic. I had been working on star formation research with Alyssa Goodman and expected to have a conversation about some small project within that research area-perhaps studying the mass distribution in a cloud, or how fast young stars move. But when Prof. Goodman arrived, the conversation-and my career-took a sharp turn. She had just returned from a joint NSF/NIH workshop on scientific visualization, where she had presented the leading challenges in astronomy visualization, including the unsolved problem of visualizing 3D radio data cubes. Another Harvard researcher, Michael Halle, had approached her with a possible solution. They bounced around the crazy idea that maybe 3D medical visualization software could be used with astronomy data. I didn't think twice before saying "I'll do it!"

Next thing I knew, I was riding the M2 shuttle bus from Cambridge to Longwood Medical District with pre-med friends, heading over to Brigham and Women's Hospital. Working with Dr. Halle and the Surgical Planning Lab, I learned about the difference between a CT and MRI image, what software is used, and how the surgeons use it in practice in the operating room. By the end of my junior year, I had managed to demonstrate that astronomy data could be read into medical imaging software, and that viewing these data cubes in 3D (which no astronomer had done previously) reveals features that are invisible or obscured in traditional 2D projections. Thus the IIC's Astronomical Medicine (AM) pilot project was born. I went on in my senior thesis to get important astronomical results using the 3D visualization techniques.

from the 2009 IIC Report...

Instead off dashing of to graduate school in astronomy, I was intrigued by this new world of interdisciplinary research and this field called "visualization." So I chose to work at the newly formed IIC to continue my senior thesis research with the AM project. The AM team grew to include a dedicated software engineer, Douglas Alan, and a full-time astronomy postdoc, Jens Kauffmann.

In the two years I worked full-time at the IIC, the AM team accomplished much in terms of creating software tools for scientific visualization and in applying these tools in both astronomy and medicine. I gained the real-life research experience one cannot obtain in a classroom. I learned how to work as part of a team and to write grant proposals and journal articles. I traveled to astronomy, computer science and visualization conferences to present papers, give talks, and at the same time run exhibit booths. I learned how to conduct myself in a radio or magazine interview, make videos for outreach purposes, and make videos for sharing my visualizations with other scientists. I've had the joy of seeing how the physics and math I studied as an undergraduate is applied to real research: One has to know statistical mechanics to understand thermal noise in MRI machines or radio telescopes, so the algorithms to reduce the images can be coded identically, and one needs to understand differential equations and line integrals to create surfaces and render a 3D model. I've learned that a scientist cannot just be an "experimentalist" or a "theorist." To truly understand data, a scientist must compare observations and simulations using the same analysis and visualization techniques. The IIC has been invaluable not only in helping me acquire skills and knowledge, but also in developing my perspective on how to do research and advance the state of the art.

Where did IIC come from, and go?

Short Version

Response to Harvard's "expansion" in Science, and into Allston.

See IIC <u>Whitepaper</u> (2004) & Task Force on Science & Technology <u>report</u> (2005) for more.

Long Version

(see the News on Allston & Harvard)

Current Status

Part of Harvard's New School of Engineering and Applied Science



IIC 2010: Part of Harvard's New Engineering School



ABOUT US Mission of the IIC

The Initiative in Innovative Computing (IIC), now a suite of projects and activities administered by the Harvard School of Engineering and Applied Sciences, was launched as an interdisciplinary research and development center at Harvard dedicated to using innovative computing tools to accelerate discovery across all of the scientific disciplines. The IIC's researchers work in close collaboration with scientists and engineers in other fields, fostering a two-way collaborative flow of ideas and inventions between basic science and computer science, academia and industry, professional staff and faculty, teachers and students. The IIC trains the next generation of creative and computationally capable scientists, and communicates with the public at large about the value of computing in science and the science it enables.

FEATURE

Scientists' Discovery Ro Lab

The Scientists' Discovery Room Lab is an exploration of the ways people can understand and do science using the senses of vision and

touch. SDR research staff are colla with scientists to design richly int visual tools that facilitate collabo and cooperative learning. This wo recently been featured in the Harvard Gazette.

More on the SDR's work can be for

INNOVATIVE COMPUTING (IIC) Initiative in Inno NEWSLETTER

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seas to present distinguished lectures in computational science

SEAS to Present Distinguished Lectures in Computational Science

What are the algorithms DNA uses to "compute"? How can we understand the circuitry of the human brain? What new kinds of computation are needed to drive 21st century science? These and other important challenges at the forefront of science and computing will be explored as the Harvard School of Engineering and Applied Sciences (SEAS) sponsors a series of four Distinguished Lectures in Computational Science during February and March.

This series is a continuation of the joint IIC-Computer Science colloquia launched in 2008.

The seminars, open to the public, will take place in G-115 Maxwell Dworkin (33 Oxford Street, Cambridge, MA) on Wednesday and Thursday afternoons at 4 p.m. Confirmed speakers and dates are:

- February 3: David E. Shaw, Chief Scientist, D. E. Shaw Research, and Senior Research Fellow at the Center for Computational Biology and Bioinformatics. Shaw is developing new algorithms and machine architectures for high-speed molecular dynamics simulations for structural biology and biochemistry research and computer-aided drug design
- March 4: Erik Winfree, Associate Professor of Computer Science and lead investigator of the DNA and Natural Algorithms Group and the Molecular Programming Project at Caltech. Winfree was named a MacArthur Fellow in 2000.
- March 10: Michael Huerta, Associate Director of the National Institute of Mental Health. Huerta has directed NIH's efforts to map the human brain and is now leading development of the Human Connectome Project, a \$30 million initiative aimed at developing a whole-brain connectivity map for humans from brain images.
- March 24: Pat Hanrahan, CANON USA Professor at Stanford University. An established international leader in scientific visualization and computer graphics research, Hanrahan is now working in stream programming, browsing interfaces for multidimensional relational databases and the use of graphics processing units for scientific computing.

The new lecture series has been developed with help from the IIC and additional support from the Provost. The series is coordinated by Matt Welsh, Associate Professor of Computer Science and Thomas D. Cabot Associate Professor of Applied Science.

As the event dates approach, details will be available at seas.harvard.edu and iic.harvard.edu. For more information, contact gioia@pacific.harvard.edu.

Filling the "Gap" between Science and Computer Science



Increasingly, core problems in science require computational solution

Focused on finding elegant solutions to basic computer science challenges

Typically hire/"home grow" computationalists, but often lack the expertise or funding to go beyond the immediate pressing need

Often see specific, "applied" problems as outside their interests

Continuum

"Computational Science" Missing at Most Universities

"Pure" Discipline Science

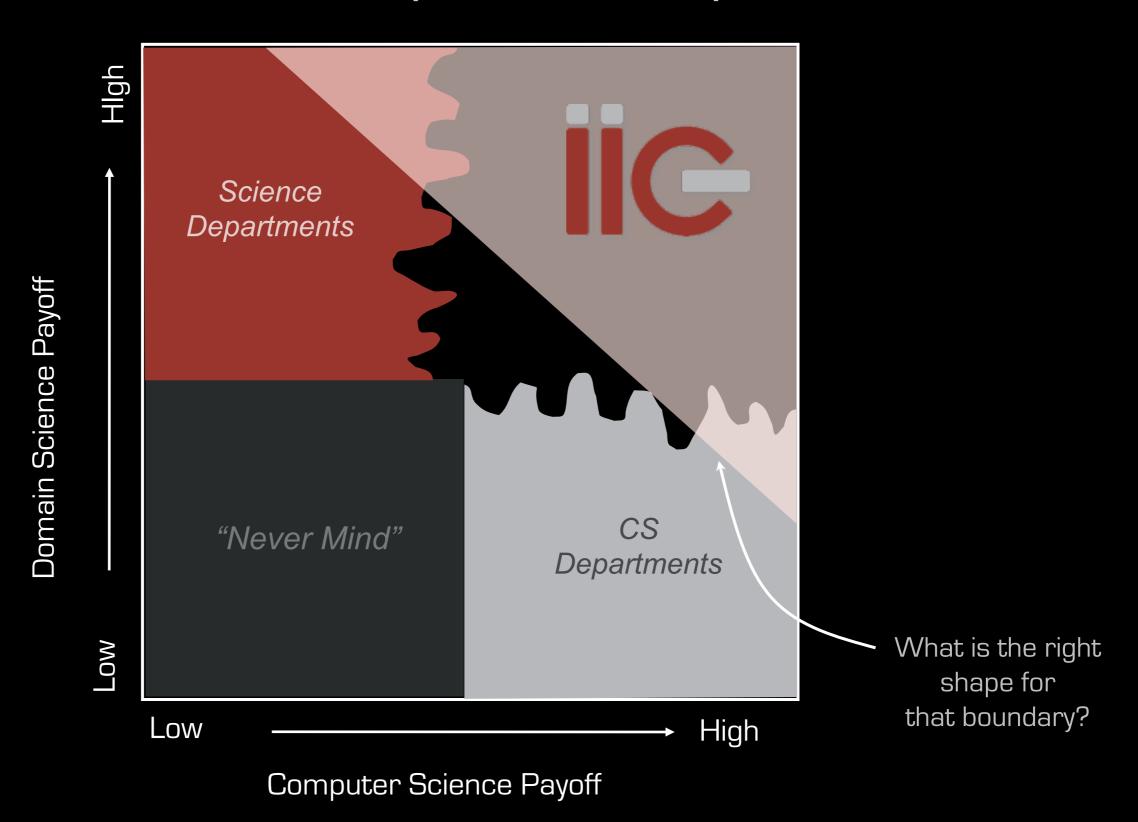
(e.g. Galileo)

"Pure" Computer Science

(e.g. Turing)



Where are the optimal "IIC" problems?



THE IIC REPORT

INITIATIVE IN INNOVATIVE COMPUTING AT HARVARD, 2006-09

lessons and results from an interfaculty initiative I HE HARVARD INSTITUTE FOR INNOVATIVE COMPUTING NOVEMBER 22, 2004

Principal Authors: Timothy Clark (HMS), Alyssa Goodman (FAS) & Christopher Stubbs (FAS)

Principal Editors: Felice Frankel (MIT), John Huth (FAS), Hanspeter Pfister (Mitsubishi Electric Research Laboratory), Joy Sircar (DEAS)1 Vhitepaper"

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IIC

INITIATIVE IN INNOVATIVE COMPUTING INAUGURAL SYMPOSIUM

ACCELERATING THE PACE OF SCIENCE

MARCH 21, 2007 HARVARD UNIVERSIT

IIC Symposium 2007





What does the wiring diagram of the human brain look like?

How do stars form in our Galaxy today?

How is science best communicated?

What's "Dark Energy"?

What are the earliest structures in the Universe? How should we model blood flow in the human body from atomic to physiological scales?

How should we use technology in teaching?



THE IIC REPORT C **Table of Contents** Table of Contents Timeline 0.2 Introduction: Harvard's Initiative in Innovative Computing 0.3 Efthimios Kaxiras, IIC Director 2008-09 **IIC Project Reports** Astronomical Medicine 1.1 Alyssa Goodman and Michael Halle A Student's Story 1.4 Michelle Borkin **Envisioning Science** 2.1 Felice Frankel IIC Report 2009: 2.7 A Student's Story Kelly Stecker 3.1 Science Collaboration Framework Tim Clark and Sudeshna Das A Student's Story 3.4 0+ pages Thomas Buckley **Time Series Center** 4.1 Pavlos Protopapas A Student's Story 4.7 available at this Alex Blocker Multiscale Hemodynamics 5.1 Effhimios Kaxiras Neuroinformatics Framework 6.1 Randy Buckner and Gabriele Fariello workshop's website 7.1 The Connectome Won-Ki Jeong, Hanspeter Pfister and Amelio Vázquez-Reina Visual Computing Group 8.1 Miriah Meyer GPU Computing for Science 9.1 Hanspeter Pfister Scientists' Discovery Room 10.1 Chat Shen Green Computing 11.1 Michael Halle Appendices

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MOTIVATION..... EXPECTED BENEFITS OF THE IIC...... AREAS OF IIC ENDEAVOR..... IIC STAFFING AND ORGANIZATIONAL (PLANNED STRUCTURE & EVOLUTION ... IIC LEADERSHIP: START-UP TASKS AND APPENDIX A: A REPRESENTATIVE SAMI APPENDIX A: A REPRESENTATIVE SAMI APPENDIX B: ONE-PAGE DESCRIPTIONS APPENDIX C: SAMPLE RESEARCH INSTI MEMBERS WOULD COLLABORATE WIT APPENDIX D: OUTSIDE EXPERTS WHO F EXTERNAL ADVISORY COMMITTEE...... APPENDIX E: FULL LIST OF LOCAL RES

PARSING, DISPLAYING, AND SERVING THE COMPLETE DATABASE ON THE WEB: A STEPPING STONE TO THE VIRTUAL OBSERVATORY

One example...

Alyssa A. Goodman Department of Astronomy, Faculty of Arts & Sciences, Harvard University

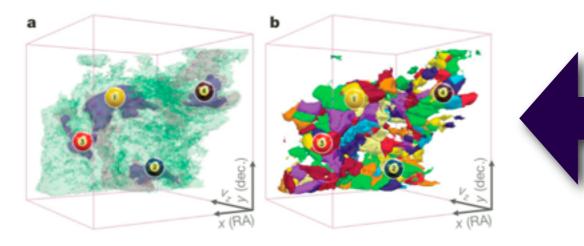
The COMPLETE Survey (cfa-www.harvard.edu/COMPLETE) currently underway is the largest, most diverse, systematic, multi-wavelength study of star-forming regions ever undertaken. Star formation, in spite of its central role in the evolution of the Universe, is currently very poorly understood, and the COMPLETE database will be used to answer a tremendous variety of physical questions, including ones like "How did the Sun form?". Without systematic surveys like COMPLETE, the data available are just too statistically sparse and poorly archived to make headway on these questions.

The COMPLETE data set includes maps made at wavelengths from optical through radio, some of which have an added "velocity" dimension beyond the three dimensions (position-position-intensity) astronomical images usually contain. Each of the mapping techniques employed produces a unique "kind" of data that is ordinarily dealt with almost exclusively by experts on that "type" of data, and very few researchers are expert in all the techniques. The tools for displaying and interpreting these kinds of data are, at this point in time, technique-specific. Trying to retrieve, use, and display COMPLETE and other similarly diverse astronomical data now is akin to trying to assemble a car from all of the one-thousand needed parts, but using directions partially in Chinese, partially in English, and partially in French, with some illustrations that can only be viewed on Windows PCs, others only on Macs, and some others only with the right brand of 3D glasses. Making all of COMPLETE's data readily searchable and accessible to astronomers worldwide, regardless of their expertise or computing platform, is an unprecedented—but definitely achievable—challenge in both database design and visualization.

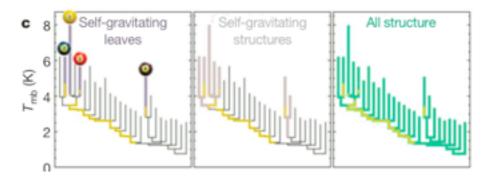
We envision two potential members of the IIC who would work together in making the COMPLETE dataset accessible to all on the Web. One IIC collaborator would be expert in the design and searching of large multi-dimensional databases, and the other would be more focused on designing tools to use existing and new visual interfaces to access and analyze the database. We expect that a total of four person-years (two years per participant, in parallel) would be needed to create a streamlined working system.

The result of this IIC work would be a new data retrieval/display system that would be the first to handle what is known as "velocity resolved" or "spectral line data cube" data sets that intrinsically have four dimensions. This system would be incorporated into all of the Virtual Observatory interfaces now being developed (see http://www.us-vo.org/) to provide this kind of access to multi-wavelength, multi-dimensional data sets across astronomy.

Astronomical Medicine/3D 2005-2009



Click to rotate



PARSING, DISPLAYING, AND SERVING THE COMPLETE DATABASE ON THE WEB: A STEPPING STONE TO THE VIRTUAL OBSERVATORY

Abssa A. Goodman Department of Astronomy, Faculty of Arts & Sciences, Harvard University

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Seamless Astronomy (2008-...)



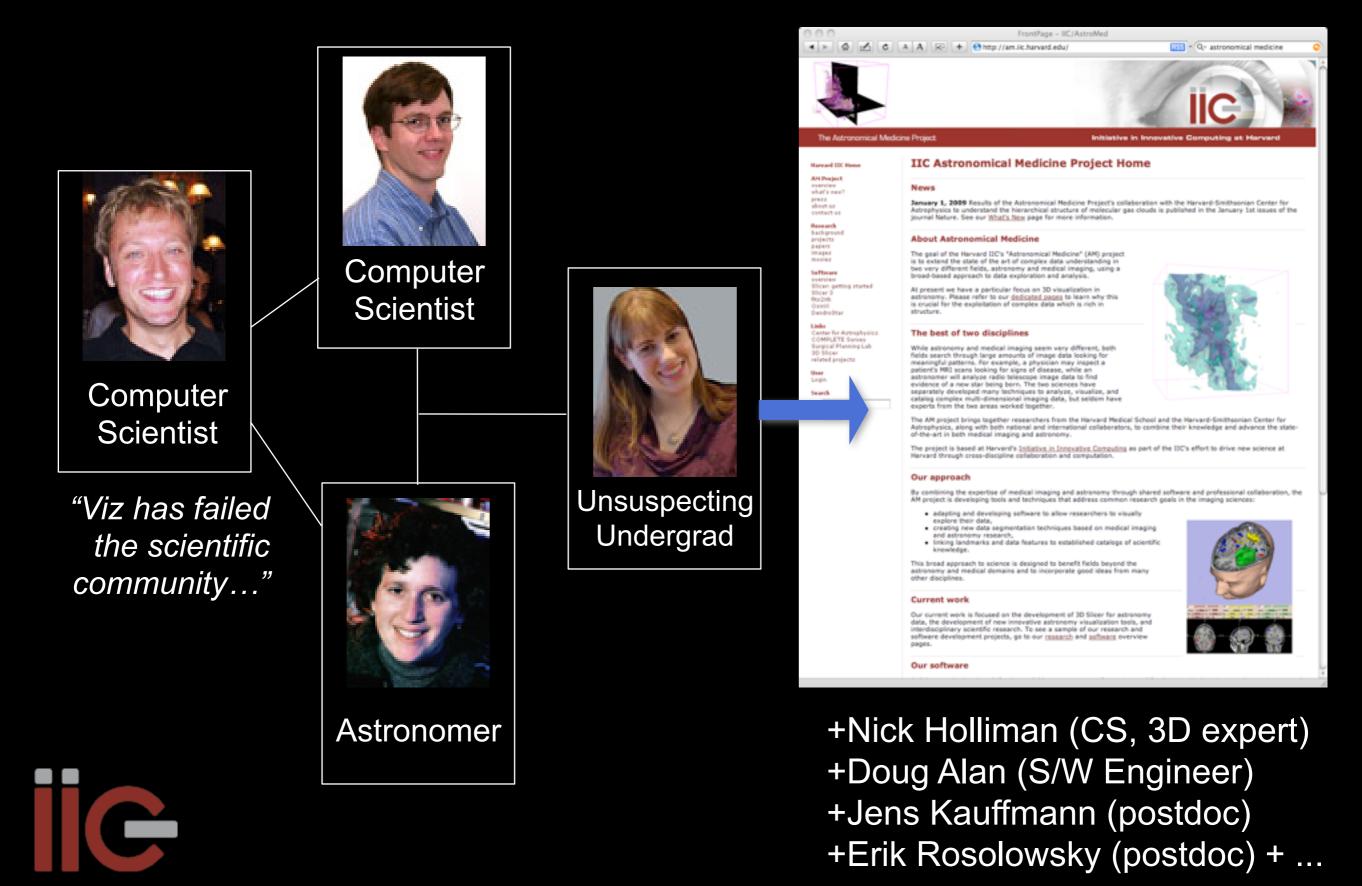


Astronomical Medicine

Alyssa Goodman (IIC/CfA/FAS) Michael Halle (IIC/SPL/HMS) Ron Kikinis (SPL/HMS) Douglas Alan (IIC) Michelle Borkin (FAS/IIC) Jens Kauffmann (CfA/IIC) Erik Rosolowsky (CfA/UBC Okanagan) Nick Holliman (U. Durham)



The Astronomical Medicine Story



Mage SE SEALETE = COordinated Molecular View stands of the Exinction Thermal Emission

mm peak (Enoch et al. 2006)

sub-mm peak (Hatchell et al. 2005, Kirk et al. 2006)

¹³CO (Ridge et al. 2006)

mid-IR IRAC composite from c2d data (Foster, Laakso, Ridge, et al. in prep.)

Optical image (Barnard 1927)



"Astronomical Medicine"

"KETH" "PERSEUS" Image: state stat

"z" is depth into head

"z" is line-of-sight velocity

Made In OsiriX

(This kind of "series of 2D slices view" is known in the Viz as "the grand tour")

Zoom: 227% Angle: 0

COMPLETE Perseus

/iew size: 1305 × 733 /L: 63 WW: 127

mm peak (Enoch et al. 2006)

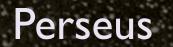
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mid-IR IRAC composite from c2d data (Foster, Laakso, Ridge, et al. in prep.)

Optical image (Barnard 1927)





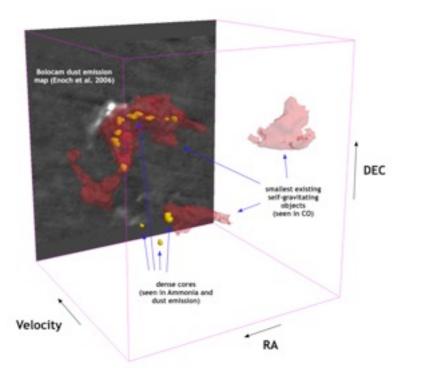
3D Viz made with VolView

AstronomicalMedicine@

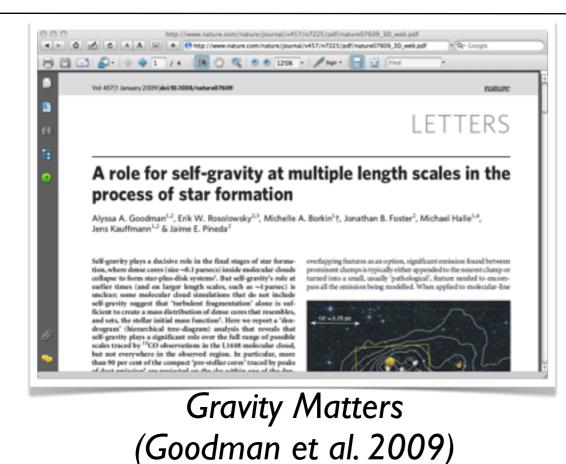


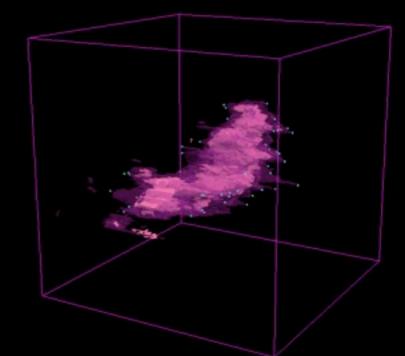
Some of What We've Learned...

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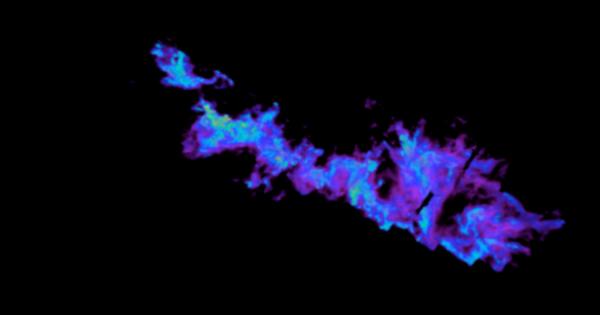


Cores nest in coccoons (Kauffmann et al. 2009)





Tripled Outflows (Borkin et al. 2008,9)



Shells Rule (Arce et al. 2009)

New ways to share insight "3D PDF"

LETTERS

NATURE Vol 457 1 January 2009

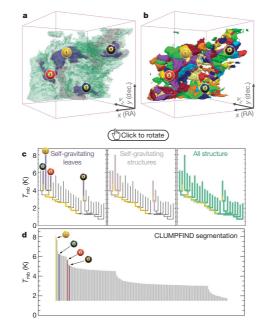


Figure 2 Comparison of the 'dendrogram' and 'CLUMPFIND' feature identification algorithms as applied to ¹³CO emission from the L1448 region of Perseus. a, 3D visualization of the surfaces indicated by colours in the dendrogram shown in c. Purple illustrates the smallest scale selfgravitating structures in the region corresponding to the leaves of the dendrogram; pink shows the smallest surfaces that contain distinct self gravitating leaves within them; and green corresponds to the surface in the data cube containing all the significant emission. Dendrogram branches corresponding to self-gravitating objects have been highlighted in yellow over the range of Tmb (main-beam temperature) test-level values for which the virial parameter is less than 2. The x-y locations of the four 'selfgravitating' leaves labelled with billiard balls are the same as those shown in Fig. 1. The 3D visualizations show position-position-velocity (p-p-v) space. RA, right ascension; dec., declination. For comparison with the ability of dendrograms (c) to track hierarchical structure, d shows a pseudodendrogram of the CLUMPFIND segmentation (b), with the same four labels used in Fig. 1 and in a. As 'clumps' are not allowed to belong to larger structures, each pseudo-branch in d is simply a series of lines connecting the maximum emission value in each clump to the threshold value. A very large number of clumps appears in b because of the sensitivity of CLUMPFIND to noise and small-scale structure in the data. In the online PDF version, the 3D cubes (a and b) can be rotated to any orientation, and surfaces can be turned on and off (interaction requires Adobe Acrobat version 7.0.8 or higher). In the printed version, the front face of each 3D cube (the 'home' view in the interactive online version) corresponds exactly to the patch of sky shown in Fig. 1, and velocity with respect to the Local Standard of Rest increases from front (-0.5 km s^{-1}) to back (8 km s^{-1})

data, CLUMPFIND typically finds features on a limited range of scales, above but close to the physical resolution of the data, and its results can be overly dependent on input parameters. By tuning CLUMPFIND's two free parameters, the same molecular-line data set⁸ can be used to show either that the frequency distribution of clump mass is the same as the initial mass function of stars or that it follows the much shallower mass function associated with large-scale molecular clouds (Supplementary Fig. 1).

Four years before the advent of CLUMPFIND, 'structure trees'⁹ were proposed as a way to characterize clouds' hierarchical structure 64

using 2D maps of column density. With this early 2D work as inspiration, we have developed a structure-identification algorithm that abstracts the hierarchical structure of a 3D $(p-p-\nu)$ data cube into an easily visualized representation called a 'dendrogram'¹⁰. Although well developed in other data-intensive fields^{11,12}, it is curious that the application of tree methodologies so far in astrophysics has been rare, and almost exclusively within the area of galaxy evolution, where 'merger trees' are being used with increasing frequency¹³.

Figure 3 and its legend explain the construction of dendrograms schematically. The dendrogram quantifies how and where local maxima of emission merge with each other, and its implementation is explained in Supplementary Methods. Critically, the dendrogram is determined almost entirely by the data itself, and it has negligible sensitivity to algorithm parameters. To make graphical presentation possible on paper and 2D screens, we 'flatten' the dendrograms of 3D data (see Fig. 3 and its legend), by sorting their 'branches' to not cross, which eliminates dimensional information on the *x* axis while preserving all information about connectivity and hierarchy. Numbered 'billiard ball' labels in the figures let the reader match features between a 2D map (Fig. 1), an interactive 3D map (Fig. 2a online) and a sorted dendrogram (Fig. 2c).

A dendrogram of a spectral-line data cube allows for the estimation of key physical properties associated with volumes bounded by isosurfaces, such as radius (R), velocity dispersion (σ_v) and luminosity (L). The volumes can have any shape, and in other work14 we focus on the significance of the especially elongated features seen in L1448 (Fig. 2a). The luminosity is an approximate proxy for mass, such that $M_{\text{lum}} = X_{13\text{CO}}L_{13\text{CO}}$, where $X_{13\text{CO}} = 8.0 \times 10^{20} \text{ cm}^2 \text{ K}^{-1} \text{ km}^{-1} \text{ s}$ (ref. 15; see Supplementary Methods and Supplementary Fig. 2). The derived values for size, mass and velocity dispersion can then be used to estimate the role of self-gravity at each point in the hierarchy, via calculation of an 'observed' virial parameter, $\alpha_{obs} = 5\sigma_v^2 R/GM_{lum}$. In principle, extended portions of the tree (Fig. 2, yellow highlighting) where $\alpha_{obs} < 2$ (where gravitational energy is comparable to or larger than kinetic energy) correspond to regions of p-p-v space where selfgravity is significant. As α_{obs} only represents the ratio of kinetic energy to gravitational energy at one point in time, and does not explicitly capture external over-pressure and/or magnetic fields16, its measured value should only be used as a guide to the longevity (boundedness) of any particular feature.

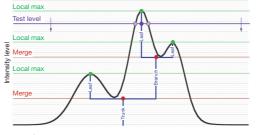
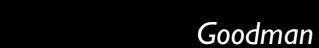


Figure 3 | Schematic illustration of the dendrogram process. Shown is the construction of a dendrogram from a hypothetical one-dimensional emission profile (black). The dendrogram (blue) can be constructed by 'dropping' a test constant emission level (purple) from above in tiny steps (exagerated in size here, light lines) until all the local maxima and mergers are found, and connected as shown. The intersection of a test level with the emission is a set of points (for example the light purple dots) in one dimensions. The dendrogram of 3D data shown in Fig. 2c is the direct analogue of the tree shown here, only constructed from 'isosurface' rather than 'point' intersections. It has been sorted and flattened for representation on a flat page, as fully representing dendrograms for 3D data cubes would require four dimensions.

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Goodman et al. Nature, 2009

Secret truths I learned from AstroMed at IIC

- I. The story about the hammer & the screw is a cliché, but it's true. Don't use "more" software than you must. (e.g. 3DSlicer/Osirix/VolView/AplPy/S2PLOT/custom apps)
- 2. Smart hackers rule. Software engineering is great when you have the money & time.
- 3. Distribution is key. There's too much great S/W no one knows about.

My advice re: IIC-like Enterprises

Alyssa Goodman's Advice to Tim Kaxiras and Ros Reid, about the IIC, May 2008

Key principles to be maintained, or established:

- Be firm about the expected life cycle of projects. Ramp-up and ramp-down periods, and re-evaluation
 of progress ~bi-annually is essential.
- Maintain the IIC "core" technical staff principles. Do not turn IIC into a "soft-money" institute. A good goal may be 50/50 internal/external funding. Solving the O/H problem could potentially bring some "internal" money into IIC as either "recovered" O/H or services received for O/H.
- 3. Maintain a strong Seminar series. Many "converts" have come to the IIC through the Seminar series.
- Maintain, and expand, student-centric programs. The Summer Internships are good, but there should be more term-time participation by students.
- Create a set of clear guidelines for what it means to be **faculty** with a partial appointment at IIC (salary from IIC).
- Create a clear definition of what affiliated faculty ("Core Members") should expect to give/take from IIC. (See Business Plan ideas.)
- Establish IIC as the "coordinator" for DISC. URGENT the IIC convene DISC meetings ASAP. Greenhill is IIC representative, and he and Cuff should host meetings.
- 8. Establish IIC as a center for experimentation through internal projects, e.g. SDR.
- 9. Establish rigorous proposal **review** process.
- 10. Form and make good use of external advisory committee(s).

What I'm doing now...

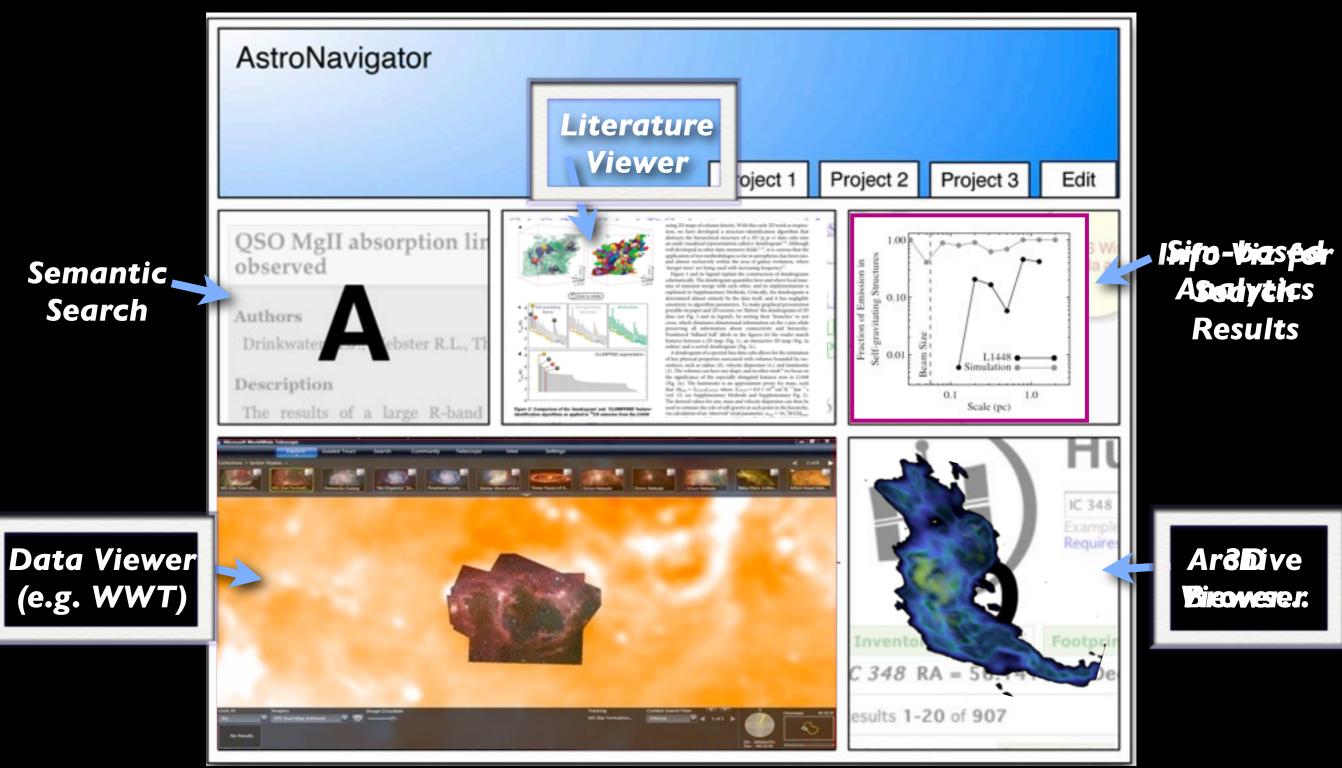
Seamless Astronomy

www.cfa.harvard.edu/~agoodman and worldwidetelescope.org



"Seamless Astronomy" is collaboration amongst many researchers at CfA, MSR, Princeton, STScI, NYU, RPI, and UCLA, and it is supported by NASA, NSF and Microsoft External Research.

Seamless Astronomy



Mockup based on work of Eli Bressert, excerpted from NASA AISRP proposal by Goodman, Muench, Christian, Conti, Kurtz, Burke, Accomazzi, McGuinness, Hendler & Wong, 2008

Touching Insight The Scientists' Discovery Room





movie courtesy Daniel Wigdor, equipment now in Chia Shen's SDR lab at SEAS