Second Year Annual Report
for the Period 1/15/2007 – 1/15/2008

Project Title: HYDRA: A New Paradigm for Astrophysical Modeling, Simulation, and Analysis

AISRP Grant Number: NNG06GE58G

PI: John C. Houck

Co-Is: John E. Davis, Dan Dewey, Michael S. Noble, Michael A. Nowak, Michael Wise

Web page: `http://space.mit.edu/hydra`

1 Introduction

This is the second annual report for the 3-year AISRP project HYDRA, covering the 12 month period from 15 January 2007 through 15 January 2008. During this period we have made progress in several areas as described below and in more detail on the HYDRA web pages. We also briefly summarize our plans for the final year of funding under the current grant.

2 Year Two Progress

2.1 Source Models

The goal of HYDRA source modeling is to support constructing source models that have realistic spatial structure and to use these models directly in the analysis of observational data.

During the past year, two sets of routines, `Source-3D` and `Event-2D`, were developed to do forward folding and comparison of 3D source models with 2D event-based data sets. These routines build on the volumetric 3D (`v3d`) routines developed during our first year of funding. One can define source models that include 3D spatial structure, including Doppler shifts in the observed spectra associated with internal bulk motions within the source. The two axes of the data/model can be chosen from the available event properties. Commonly useful 2D spaces include: X-Y sky images, wavelength–cross-dispersion grating images, or radius-energy "images". These 3D modeling capabilities are currently being used in the analysis of recent Chandra observations of SN1987A (Dewey et al., 2008), and other sources. Documentation for these routines and a number of detailed example applications are available on the HYDRA web pages[1].

2.2 Missions and Instruments

One goal is to couple the advanced source models of the previous section with simulations of a given observatory or instrument. A key ingredient in our thinking is the concept of simulating with appropriate fidelity, allowing a flexibility in the tradeoff of speed and accuracy. Especially in initial stages of 3D source modeling the model-data (dis)agreement is often very visible and not a subtle effect. Our exploratory prototyping to date has used crude approximations to the instrument response (*e.g.* simple PSFs, ARFs, and RMFs) and has shown that these are adequate to make modeling and science progress.

[1] `http://space.mit.edu/hydra/v3d.html`

2.3 Visualization

The visualization components reported on last year have been incrementally improved to support the development of the 3D modeling components and data analysis applications. New versions of the `SLgtk` module and the VWhere, Volview and Imdisplay visualization tools were released. A S-Lang interface for the `grace` plotting package was also developed.

2.4 Fitting and Statistics

The fitting process involves adjusting model parameters and constructs to optimize agreement between model and data. Our goals for HYDRA in this domain are to allow users nearly complete control over the analysis process and to let the user choose which characteristics of the data will drive the fitting engine.

We continue working to define a software interface that can be used to handle more general optimization problems. This generalized modeling capability would give HYDRA relevance beyond the domain of X-ray analysis in astronomy, and we hope to stimulate interest within the broader physics community.

2.5 Implementation and Infrastructure

Because an existing package, ISIS, provides a robust and well-tested analysis infrastructure, we have chosen it as the basis for the development of HYDRA capabilities. However, because it was developed for X-ray spectroscopy, important parts of the code base are somewhat application specific. Part of the ongoing effort to generalize ISIS involves separating the application specific components into modules that can be accessed through more generic interfaces.

This year, we used grant funds to purchase a 13-node Beowulf cluster (26 dual-core CPUs). Before making this equipment purchase, we did a considerable amount of research to educate ourselves about computer clusters available on the market and various options for cluster management software. This research included extensive discussions with cluster engineers from different vendors. Because the power and cooling infrastructure in our office building is inadequate for hosting a computer cluster, we arranged to have the cluster installed in MIT's Co-Location facility. We used free software to configure the cluster ourselves and, since delivery, have been using it to explore various methods for applying distributed computation to data analysis.

The cluster has become a focal point for nurturing multiple collaborations in high-performance astrophysical computing. One result of these efforts is a parallelizing wrapper for XSTAR, which makes it feasible for us to probe thousands of photoionized gas physical scenarios in the time it has previously taken to compute only a handful of such models (Ji & et al., 2008). We have also developed scripts to simplify the parallel computation of statistical confidence limits, and applied them to a number of models such as jet phenomena in active galactic nuclei (Markoff & Maitra, 2008).

As an alternative approach to improving parallelism in data analysis applications, we have also explored the use of OpenMP-based parallelism in S-Lang scripting (Noble, 2008).

2.6 Hydra Products and Applications

While HYDRA as a whole is not yet available to the public, our work to date has nevertheless yielded a number of deliverables for public use. These include the papers and presentations listed on our site[2], enhanced versions of ISIS, SLIRP, and VWhere, modules for volume visualization, the HDF5

[2] http://space.mit.edu/hydra/docs.html

file format and library, the `v3d` geometric modeling routines, and the `Source-3D` and `Event-2D` routines for the analysis of event-based data sets.

A number of new scientific modules have also been created using the SLIRP automatic code generator. These provide access, directly in HYDRA memory at runtime, to internal functions and data structures (such as common blocks) from the XSTAR and XSPEC astrophysical modeling tools. Through these modules collaborators may reuse important legacy functionality in ways that are fundamentally distinct from their original design, and in more rapid, scriptable fashion (Ji & et al., 2008).

We also have an internal development version of the HYDRA application itself, which is conceptually just the generalized ISIS with the various HYDRA modules[3] preloaded. Most HYDRA components have been successfully installed and utilized by relatively inexperienced users, demonstrating their general robustness. Likewise we are beginning to apply HYDRA concepts and code in our published scientific work.

3 Plans for Year Three

Brief plans in these areas are described in the following sections:

3.1 Source Models

- optimize source modeling for distributed computation over networks, focus on computations which are inherently parallel such as Monte-Carlo simulations
- expand model methods to include models based on snapshots from AMR hydrodynamics computations
- investigate useful and efficient radiation transfer
- expand the library of geometric models available (*e.g.* disk model with variable thickness)
- survey other model specification methods

3.2 Missions and Instruments

- investigate / prototype non-X-ray instruments: *e.g.* is there overlap with LOFAR in some sources?
- implement a fully functioning multi-instrument X-ray module.

3.3 Visualization

- improve the interactive controls for manipulating and probing volumes and images
- implement color-coding in Volview
- VWhere: include analytic functions as filter constraints & support 1D inputs and 1D, 2D+1 cuts
- apply multi-dimensional data mining more widely to modeling and fitting
- evaluate X3D for model visualization

[3]http://space.mit.edu/hydra/implement.html

3.4 Fitting and Statistics

- Implement more general optimization interface that supports plugin components for specialized cases.
- Experiment with different ways to distribute computations associated with fitting and modeling computations.

3.5 Implementation and Infrastructure

- Evaluate HYDRA on our 13 node Beowulf cluster
- Implement a simple graphical interface for specifying models

3.6 Hydra Products and Application

- Create a nominal distribution for beta testing including documentation and examples
- Introduce HYDRA as part of some Education/Public Outreach activity

A Hydra Adopters and Related Activities

Our early adopters are primarily local collaborators not directly funded by the AISRP grant. However, as the project continues we've come to recognize a need to raise awareness in the X-ray community of the limitations inherent in traditional software approaches to spectral analysis, and how they can be mitigated in systems like HYDRA. Towards that end we've undertaken a comprehensive quantitative analysis of the defacto standard spectral modeling tool, XSPEC, and have submitted a paper on our findings (Noble & Nowak, 2007). In addition, external groups pursuing research agendas which complement HYDRA [4] are a natural source of collaboration.

References

Dewey, D., Zhekov, S. A., McCray, R., & Canizares, C. R., 2008, ApJ, 676, L131

Ji, L., & et al. 2008, ApJ, in prep

Markoff, S., & Maitra, D., 2008, ApJ, in prep

Noble, M. S., 2008, Concurrency and Computation: Practice and Experience, accepted

Noble, M. S., & Nowak, M. A., 2007, PASP, submitted

[4] `http://space.mit.edu/hydra/related.html`