

First Year Annual Report for the Period 3/15/2006 – 1/15/2007

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

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Web page: <http://space.mit.edu/hydra>

1 Introduction

This is the first annual report for the 3-year AISRP project HYDRA, covering the 10 month period from 15 March 2006 through 15 January 2007. In this time we have made tangible progress in several areas as described below and in more detail on the HYDRA web pages. We briefly describe how our plans for the second year build upon our current accomplishments.

2 Year One 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. To this end, we have prototyped and developed two alternative approaches to computing the incident spatial-spectral photon distribution produced by a 3D emitting region.

The first approach consists of a simple yet widely applicable set of “volumetric 3D” S-Lang routines to define the source geometry. The range of simple 3D shapes and distributions currently treated in the library has been extended beyond that developed in an earlier exploratory effort. Using these routines, it is possible to define a 3D source geometry and generate Monte-Carlo photons including Doppler velocity effects. As an example of the ability to easily combine modules implemented in S-Lang, the `v3d` routines were easily interfaced to serve as input to the MARX ray-trace code through a S-Lang user module.

The second approach involves computing the incident source flux by direct numerical integration along a line of sight (`los`) through an emitting region at selected points on the sky. The user defines the structure of the emitting region by providing a subroutine to compute the emissivity and opacity as a function of position within the emitting volume. In the absence of scattering processes, each line of sight is computationally independent and the line of sight integrals may be computed in parallel. This method complements the `v3d` approach, providing a more efficient alternative in certain applications. As a first application, we are using the `los` module to fit models to published observations of the radio and X-ray profiles of the forward shock supernova remnant SN1006. These computations were distributed over a heterogeneous network of desktop computers using PVM. Examples and a more detailed description of these HYDRA source modeling methods are available on the HYDRA web pages¹.

¹<http://space.mit.edu/hydra/sources.html>

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.

2.3 Visualization

We have refined our visualization requirements by experimenting with a wide range of software, from relatively small packages such as `volpack` to enormous, industrial strength systems like `ParaView` and `VisIT`². This strengthened our conviction that a productive low-end niche exists for lightweight visualization tools, such as our `volview` and `imdisplay` guilets; these are now routinely used to view our `v3d` generated source models, in both 3D as well as 2D sky projections, and are available for public download. We have continued to utilize and enhance `VWHERE`³ for visual correlation of multidimensional data. For example, with collaborators we have published papers which simultaneously examine features across scores of event list datasets from multiple missions. `VWHERE` has also been employed to mine for subtle interdependencies within abstract data, such as the model fitting parameters for hundreds of astronomical observations.

2.4 Fitting and Statistics

The fitting process involves adjusting model parameters and constructs to achieve an 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. 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.

Because `ISIS` was developed for X-ray spectroscopy, its fitting infrastructure historically supported the analysis of only 1D histogram data. We have begun generalizing the `ISIS` implementation so that it can be used to model more general, e.g. higher dimensional, forms of data. The internal `ISIS` fitting code has been re-structured so that the model data is accessed via an abstract software object, instead of pointers to histograms. This abstract object is defined by a small set of functions which govern how it may be manipulated, as well as associated private metadata. A particular implementation of this abstract object can then be provided by a software *plugin* that that is imported at run-time and that may be user-defined. Under this scheme the entire histogram modeling capability of `ISIS` is effectively transformed into a single 1D `HYDRA` plugin, and it should be possible for anyone to develop new plugins to allow the `HYDRA` fitting engine to be applied to different kinds of data. This generalized modeling capability gives `HYDRA` relevance beyond the domain of X-ray analysis, and we are aiming to stimulate interest within broader, e.g. particle physics, communities.

²<http://space.mit.edu/hydra/visualize.html>

³<http://arxiv.org/abs/astro-ph/0412003>

2.5 Implementation and Infrastructure

We are implementing HYDRA by developing a number of stand-alone S-Lang modules that, together, can be scripted to perform complex modeling and analysis tasks. These components are intended to be used in a generalized fitting application derived from the ISIS code base. Although HYDRA is still a young project, and as a whole is not available to the public, virtually all of its existing constituent modules are already available for public download and independent use.

Toward the specific goal of identifying ways to make parallel computation more accessible to scientists we have used the `los` infrastructure described in §2.1 to construct 3D source models that can be evaluated either on a single CPU or on multiple CPUs (via PVM) using the same S-Lang script. We have also enhanced the SLIRP module generator⁴ so that vectorized wrappers may be created which take advantage of the powerful array capabilities of S-Lang; in our development version these vectorized modules can even be parallelized to run on multiple cpus with OpenMP. We are aware of no other wrapper generator in the world with this combination of features.

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 site⁵, enhanced versions of ISIS, SLIRP, and VWHERE, brand new modules for volume visualization and the HDF5 file format and library, as well as the `v3d` geometric modeling routines.

We also have an internal development version of the HYDRA application itself, which is conceptually just the generalized ISIS with the various HYDRA modules⁶ 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 Two

Brief plans in these areas are described in the following sections as a list of simple bullets. Items in italics represent clear milestones we intend to accomplish in year two.

3.1 Source Models

- *finalize and document source modeling routines*
- create opaque objects
- design structures to specify complete 3D models
- optimize source modeling for distributed computation over networks, focus on computations which are inherently parallel such as Monte-Carlo simulations
- continue expanding model methods including from AMR hydro snapshots
- investigate useful and efficient radiation transfer

⁴<http://space.mit.edu/cxc/software/slang/modules/slirp>

⁵<http://space.mit.edu/hydra/docs.html>

⁶<http://space.mit.edu/hydra/implement.html>

3.2 Missions and Instruments

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

3.3 Visualization

- *improve the interactive controls for manipulating and probing volumes and images*
- *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*

3.4 Fitting and Statistics

- *replicate standard spectral fitting as a limiting case*
- define a set of standard plugins that can be used individually or in combination, e.g. extracted spectrum; surface brightness profile; light curve
- *perform joint fits of Chandra, XMM-Newton, and Suzaku data*
- optimize for distributed networks
- investigate flexible multi-dimensional filtering
- optimize fitting for both binned and event-based models

3.5 Implementation and Infrastructure

- *Publicly release PVM-aware error analysis and LOS routines*
- *Evaluate HYDRA on our 16 node Beowulf cluster*
- Implement a simple graphical interface for specifying models
- *Publicly release OpenMP-aware version of SLIRP & author paper*
- Establish bridge from S-Lang to Tcl (for DS9 and XSPEC user base) and potentially IDL(tm)

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 plan to submit the resulting paper in spring of 2007. In addition, external groups pursuing research agendas which complement HYDRA ⁷ are a natural source of collaboration.

⁷<http://space.mit.edu/hydra/related.html>