

Visions for an alliance: UW perspective

Jim Pfaendtner

Member, Hyak Governance Board

Chemical Engineering (primary)

Chemistry (affiliate)

UNIVERSITY *of* WASHINGTON



Two anecdotes

1. 2005 → 2007 → 2009
2. What else is happening in computational molecular science and engineering (around the country)

Framework for a vision of scientific computing...

Our vision is based on:

1. Our current **resources** and **strengths**:

- **Human** resources: world class domain scientists across all colleges, dozens of departments.
 - > This represents hundreds of people at all stages: trainees (beginning to advanced, research staff, support staff, and faculty)
- **Hardware** resources: a condominium model that works beautifully (almost flawlessly) at significant scale that meets the needs of our institution

*The resources and capabilities presented by UW combine to dramatically increase the speed of science. We are all doing more than we ever thought possible. **And we are doing it together.***

Framework for a vision of scientific computing...

Our vision is based on:

2. Our current needs and opportunities:

- Human resources: we see significant potential in two areas
 1. Top down: institutional/regional support for computational science in the form of code optimization, deployment, etc.
 2. Middle out: institutional/regional support for novel training (NSF IGERT/NRT, postdoctoral scholars program, conferences and short courses)
- Hardware resources: Domain scientists at UW are ready *today* to make use of a dramatic increase capacity computing (e.g., Hyak)

There is a huge potential (opportunity gap) to work together in the region to meet these needs

Examples of existing training programs: recent WRF investments



CLEAN ENERGY
INSTITUTE

JOIN OUR MAILING LIST

search here ...

Go

About

Research

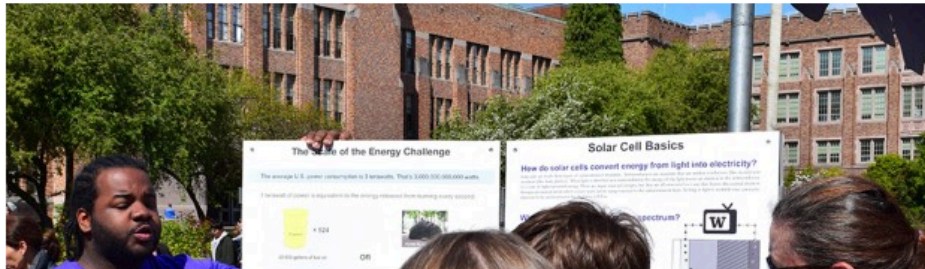
People

News & Events

Education

Partnerships

Opportunities



The CEI is a hub for schools and community. Ambassadors are solar, battery and through hands-on and presentations

Exploration Grant Program

Graduate Fellowships

Faculty Positions

Postdoc Program

CEI Student Activities

Travel Grant Program

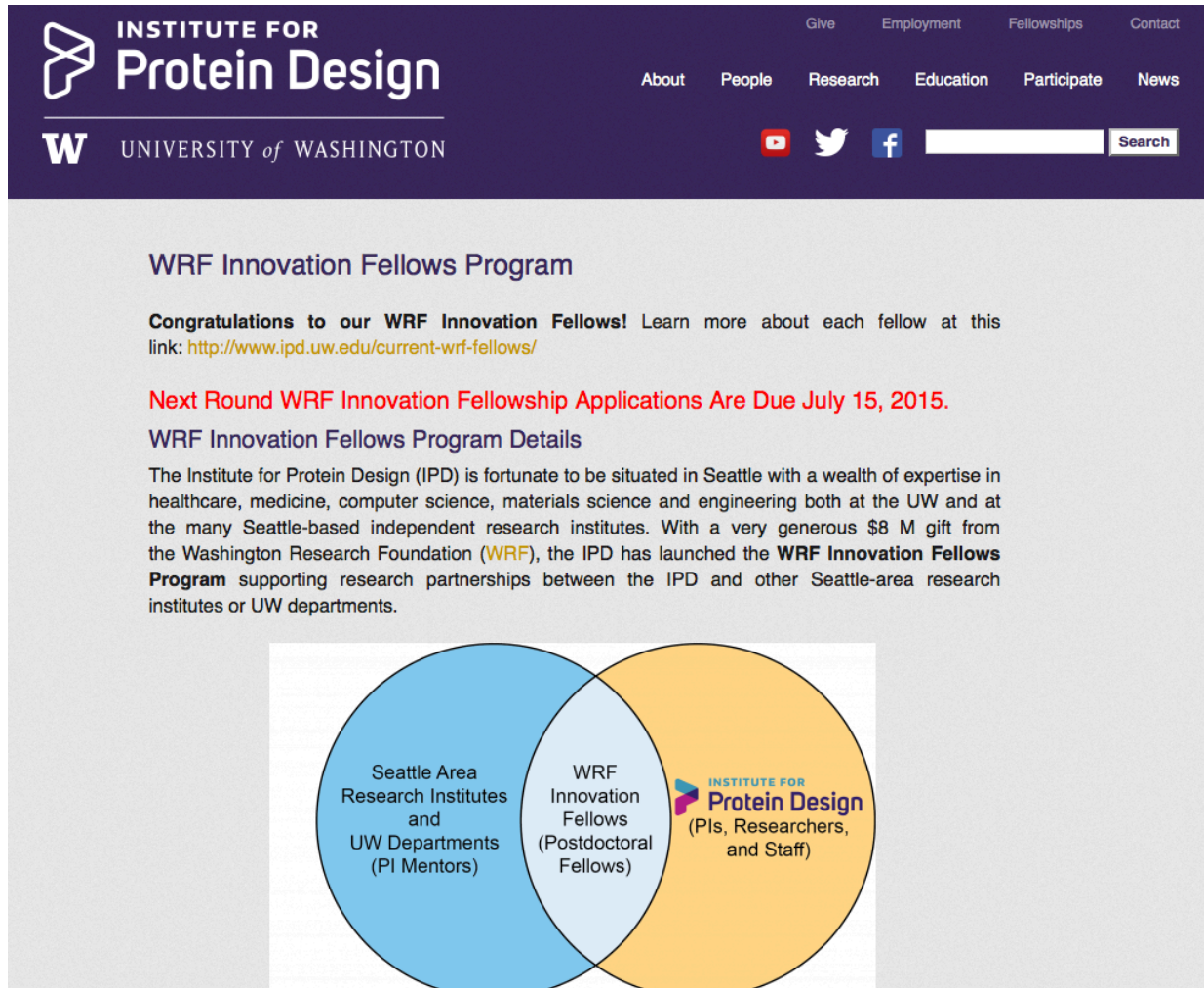


Examples of existing training programs: recent WRF investments

The screenshot shows the top navigation bar of the University of Washington eScience Institute website. The navigation bar includes links for 'UNIVERSITY of WASHINGTON', 'UW HOME', 'DIRECTORIES', 'CALENDAR', 'LIBRARIES', 'MAPS', and 'MY UW'. Below the navigation bar, the eScience Institute logo is displayed, along with the text 'UNIVERSITY of WASHINGTON eScience Institute' and 'ADVANCING DATA-INTENSIVE DISCOVERY IN ALL FIELDS'. The main content area features a large heading 'WRF and Moore/Sloan Postdoctoral Fellows' and a sub-heading '2015 WRF and Moore/Sloan Postdoctoral Fellows'. A search bar is visible on the right side of the page, and a sidebar contains a section titled 'Also in... What We Do' with a link to 'Appliance Gallery' and a brief description: 'Find and use the eScience Institute's virtual machines equipped with software useful for specific applications.'



Examples of existing training programs: recent WRF investments



The screenshot shows the website for the Institute for Protein Design at the University of Washington. The header includes the logo, navigation links (About, People, Research, Education, Participate, News), and social media icons. The main content area features the title "WRF Innovation Fellows Program" and a congratulatory message with a link to the current fellows page. A red headline states "Next Round WRF Innovation Fellowship Applications Are Due July 15, 2015." Below this is a section titled "WRF Innovation Fellows Program Details" with a paragraph explaining the program's purpose and funding. At the bottom, a Venn diagram illustrates the partnership between Seattle Area Research Institutes and UW Departments (PI Mentors) and the Institute for Protein Design (PIs, Researchers, and Staff), with WRF Innovation Fellows (Postdoctoral Fellows) at the intersection.

INSTITUTE FOR Protein Design
UNIVERSITY of WASHINGTON

Give Employment Fellowships Contact
About People Research Education Participate News

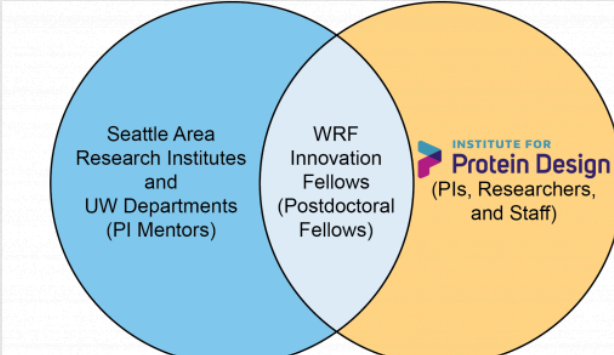
WRF Innovation Fellows Program

Congratulations to our WRF Innovation Fellows! Learn more about each fellow at this link: <http://www.ipd.uw.edu/current-wrf-fellows/>

Next Round WRF Innovation Fellowship Applications Are Due July 15, 2015.

WRF Innovation Fellows Program Details

The Institute for Protein Design (IPD) is fortunate to be situated in Seattle with a wealth of expertise in healthcare, medicine, computer science, materials science and engineering both at the UW and at the many Seattle-based independent research institutes. With a very generous \$8 M gift from the Washington Research Foundation (WRF), the IPD has launched the **WRF Innovation Fellows Program** supporting research partnerships between the IPD and other Seattle-area research institutes or UW departments.



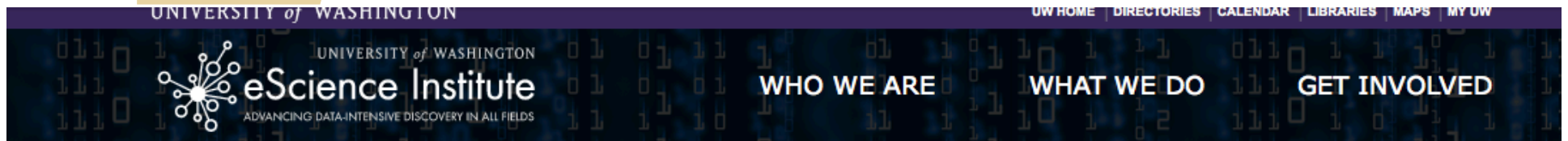
Seattle Area Research Institutes and UW Departments (PI Mentors)

WRF Innovation Fellows (Postdoctoral Fellows)

INSTITUTE FOR Protein Design (PIs, Researchers, and Staff)



Examples of existing training programs: NSF-funded training



Integrative Graduate Education and Research Traineeship (IGERT) in Big Data and Data Science

The IGERT program brings together departments and students to educate an *interdisciplinary cohort of scientists*. IGERT is a PhD program with two key goals:

- **Education and Training:** To produce a new generation of interdisciplinary scientists, versed in computer science, statistics and the domain sciences; capable of developing and using Big Data tools and models that will enable fundamental discoveries in a data intensive world.
- **Cyberinfrastructure Development:** To develop and release open-source tools and Cloud services that can be deployed and utilized by researchers across many domains for managing, analyzing and visualizing Big Data.

Latest eScience News

[Preface to Python Data Science Handbook \(Early Release\)](#)

2 days 2 hours ago

[Data Science for Social Good: Week Two - Welcome ALVA Students!](#)

3 weeks 5 days ago

[Study Shows Alaska Glacier Melt Contributing to Sea Level Rise](#)

4 weeks 46 min ago

[The Promise of Big Data: Q&A With](#)



Our vision: focus on a regional partnership that is people focused

We can do more together, we can do it better (*selected examples*):

- > Undergraduates: a regional REU program that connects computational scientists at all three institutions
- > Graduates: Grow/find/create new resources to develop trainees and the next generation of computational scientists
- > Diversify the pipeline: Leverage institutional strengths to increase participation of women and persons from URM backgrounds in computational science

Available Programs

Gaussian

[Gaussian](#) is one of the most robust and powerful software packages for modeling quantum chemical problems. The Gaussian09 (G09) binaries are available on Hyak for all UW Seattle students. You must be a member of the 'ligroup-gaussian' Unix group in order to access the program. Access can be requested by contacting Prof. Xiaosong Li at xqli@uw.edu.

Users must load the g09.d01 module in order to set up the proper environment. These two lines should be included in your submission script. Note that this module sets up the /scr folder as your scratch directory, which has ~100 Gb limit.

```
module load contrib/g09.d01
.$g09root/g09/bsd/g09.profile
```

Now you can submit your calculation with the g09 command.

```
g09 job.com
```

You can find scripts to help you submit your calculation [here](#). The g09sub.sh and g09lsub.sh scripts will help you set up a single node and a cross node job. Gaussian uses Linda parallelization to run across multiple nodes and needs to know which nodes are being utilized. The g09lsub.sh script will modify a line in your submission script

```
%LindaWorker=Linda_nodes
```

to reflect the nodes allocated by the Hyak scheduler. The gdvsub.sh and gdvlsub.sh scripts can be used to run a development version of Gaussian, which is not available to most users. You must be part of the 'ligroup-gdv' Unix group to access the development version of Gaussian.

Search for:



PAGES

- [Available Programs](#)
- [Getting Started on Hyak](#)
- [Home Page](#)

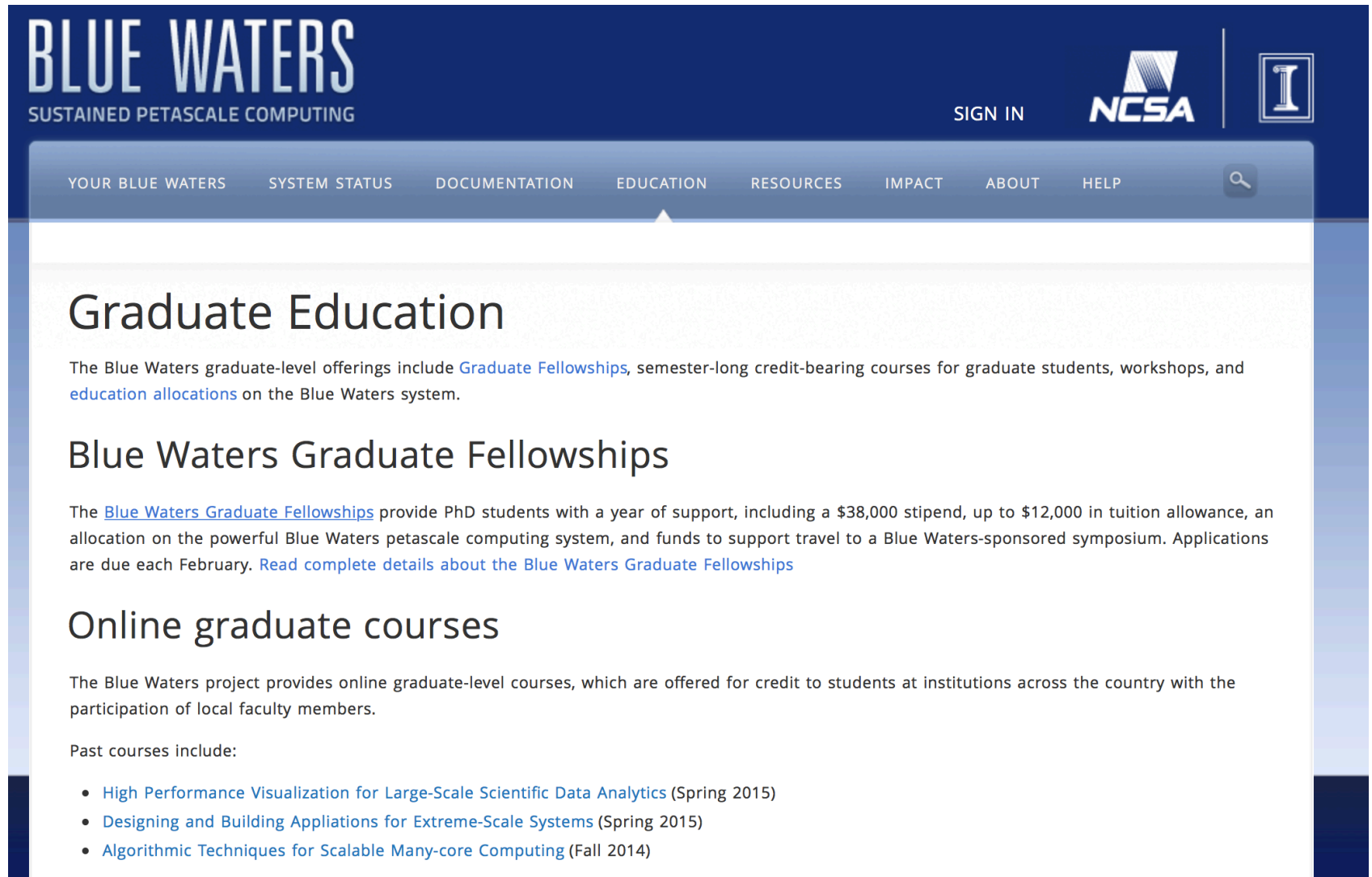
RECENT COMMENTS

- [The High Performance Computing Club is up and running | UW HPC Club on Getting Started on Hyak](#)
- [Mr WordPress on The High Performance Computing Club is up and running](#)

CATEGORIES

- [News](#)

Example of executing a people focused vision: Blue Waters Grad Fellows



The screenshot shows the Blue Waters website with a dark blue header. The header contains the text "BLUE WATERS" and "SUSTAINED PETASCALE COMPUTING" on the left, and "SIGN IN", "NCSA", and a logo on the right. A navigation bar below the header lists: "YOUR BLUE WATERS", "SYSTEM STATUS", "DOCUMENTATION", "EDUCATION", "RESOURCES", "IMPACT", "ABOUT", "HELP", and a search icon. The main content area is white and features the following sections:

Graduate Education

The Blue Waters graduate-level offerings include [Graduate Fellowships](#), semester-long credit-bearing courses for graduate students, workshops, and [education allocations](#) on the Blue Waters system.

Blue Waters Graduate Fellowships

The [Blue Waters Graduate Fellowships](#) provide PhD students with a year of support, including a \$38,000 stipend, up to \$12,000 in tuition allowance, an allocation on the powerful Blue Waters petascale computing system, and funds to support travel to a Blue Waters-sponsored symposium. Applications are due each February. [Read complete details about the Blue Waters Graduate Fellowships](#)

Online graduate courses

The Blue Waters project provides online graduate-level courses, which are offered for credit to students at institutions across the country with the participation of local faculty members.

Past courses include:

- [High Performance Visualization for Large-Scale Scientific Data Analytics](#) (Spring 2015)
- [Designing and Building Applications for Extreme-Scale Systems](#) (Spring 2015)
- [Algorithmic Techniques for Scalable Many-core Computing](#) (Fall 2014)

Our vision: focus on a regional partnership that is people focused

We can do more together, we can do it better (*selected examples*):

- > Advanced trainees: A competitive postdoctoral scholars program to bring the best and brightest to the region
- > Advanced application support and development: A “regional computational science helpdesk” to support nascent and advanced users
- > More collaboration: Build on the goals of NIAC to bring researchers together, more often, with actual human resources to conduct science (*a seed grants program*)

Our vision: focus on a regional partnership that is people focused

But what about hardware?

- > There are more seats at the table (many more seats)
- > Hyak users are *extremely* satisfied, so why not bring more people into the fold?
- > Expanding capacity (mid-scale) computing, and its support at UW is critical to our future science vision
- > No need to reinvent the wheel (but why not get bigger rims?)
 - We have demonstrated an awesome model that we love!

An exciting time for supercomputing in the PNW...

