Scientific Computing Bootcamp

Application to Plasma Physics and Nuclear Fusion

September 14-18th, 2015

4000 Aurora Avenue N., Suites 5 & 6, Seattle, WA 98103

An introduction to the scientific computing tools that plasma physicists use regularly in addressing some of today's most pressing challenges.

Intended audience: undergraduate students with at least some computing familiarity and an interest in pursuing high performance computing in their careers.

Topics:

– Grand challenges in computational plasma physics

– Overall process of computational simulation

– Historical context

– Introduction to plasma physics research & development codes

– Compiling and debugging, including Make, FORTRAN

– High performance computing and best practices

– Visualization and post-processing tools, including Octave and Python

– Finite element method

– Verification and validation in scientific computing

– Contemporary issues

– Exascale computing

For information please see http://www.**woodruffscientific.com/shortcourse**

Applications will be accepted through **Friday, May 29th.**

"Attending the Scientific Computing Bootcamp at Woodruff Scientific was an incredible learning experience, and tons of fun! I was able to connect with industry experts and learn many fundamentals of scientific computing—as well as their respective applications. Even if you have no prior knowledge of plasma physics or nuclear fusion, I highly recommend applying to this opportunity!" Hannah Misenar, BSc Computer Engineering, University of Washington

"Woodruff Scientific Computing Bootcamp was a safe and inviting place to learn about scientific computing basics, plasma physics, and broader applications of the two. Expect to broaden your understanding with in-depth tutorials, great speakers, diverse content, and a lot of fun!" Danielle Lemmon, BSc Physics, University of Washington

"It was a lot of fun and you guys did a great job of exposing the problems in the field and giving us an appreciation for the scale that all of that happens at, from the cost to the temperature, to computing resources, it takes a lot of time. As a CSE student the into to parallelization was really cool and the basic intro to using a unix terminal served me well. I have definitely recommend the camp to friends and would recommend it to anyone in an interest in physics, applied math, or CSE." Ben Gardon, BE Computer Engineering, University of Washington

Scientific Computing Bootcamp 2015 Summary

We have just ended a week of training for students in high performance computing. We had a lot of fun, and I feel a sense of accomplishment: the students were really receptive and appreciative and it seemed like they came away with a good grounding in the subject.

Shown in the Photo is Dr. Alan Glasser - the originator of most of the computer simulation codes that we run at WSI, and next to him is Dr. Erika Harnett who is the coordinator for the WA NASA Space Grant program from which 6 students were offered a place. Dr Kara Olson, a recent CS PhD, is on my right - has been an extraordinary help in putting the program together. We had speakers from all over the world - including the Chair of the IOP plasma physics division in the UK (Prof. Philippa Browning), the director of one of the biggest computing centers in the world (Dr. David Keyes, KAUST), and the DoE program manager that oversees scientific computing in the US (Dr. John Mandrekas), and some of my colleagues in the US (Drs Izzo, Meier, O'Bryan, and Glasser).

Summary by section

SCBC1 – Grand Challenges in Computational Plasma Physics

(a) Computation as third pillar of science

(b) Multi-physics and multi-scales for nuclear fusion simulations

(c) OFES HPC (initiatives, centers, SciDac)

(d) Current research directions globally, nationally, and locally

Duration: 2 hours

In this session, Dr. John Mandrekas called in from the Department of Energy Fusion Energy Sciences headquarters in Germantown to give an overview on the role of advanced computing in resolving some of the most pressing problems for fusion. He showed how simulations cover wide spatial and temporal scales, and how many codes need to work together (as multiphysics codes) to address issues such as plasma disruptions. Dr. Woodruff then spoke about efforts underway at Woodruff Scientific to address some of the main topics brought up by Dr. Mandrekas, in particular the efforts to simulate disruption mitigation schemes currently being explored in experimental campaigns. Dr. Woodruff then highlighted some of the other computational work underway at WSI in support of DARPA and ARPA-E projects exploring compact fusion concepts, and efforts to explore fusion in the private sector (including compact neutron sources under investigation in an IAEA Coordinated Research Project).

SCBC2 – Some Computer Science Considerations

(a) Modeling & simulation, and why

(b) Overall process of computational simulation

(c) Sources of approximation, including computer arithmetic*

(d) Numerical (in)stability

(e) Accuracy versus precision

Duration: 1 hour (* can be hands-on)

Dr. Kara Olson introduced some of the foundational aspects of scientific computing and how one begins even to develop a model and a simulation, explaining some semantics. Some surprising aspects of how computers handle numbers was highlighted with matlab scripts. Some of the over-arching themes of accuracy and error were introduced (to be expounded on later in the week).

SCBC3a – Using UNIX

(a) Introduction to the UNIX command line

(b) Introduction to make

Duration: 4 hours interactive hands-on

Proto-Dr. Jens von der Linden took us through an engaging hands on session for those who had never used a command promt in a unix environment, changing and making directories, file handling, all of the way through to the contents of a make file, and compiling code.

SCBC3b – Introduction to R&D Codes

(a) Introduction of some codes we use and why

(b) FORTRAN syntax

(c) Compiling and debugging

(d) Revision control and repositories

Duration: 3 hours lecture + hands-on

To start this session students logged on to their NERSC training accounts, went to the NIMROD directory and launched the make file to start the compilation of one of the state-of-the-art R&D MHD codes. Dr. Woodruff explained some of the differences and similarities between the various MHD codes in use at WSI, both in terms of their time-dependence and time-independence. Some equations were discussed! As the code compiled, we switched to the scratch directory at NERSC and launched a batch script. We took one case example from a current contract to work on and each student was given license to make changes to the input deck. With parallel jobs running on the now 62nd fastest supercomputer in the world, students were directed to a new directory in which the NIMROD code had been broken. A prize was awarded to the first student to get the code to compile, with hints being given and references made to an online F90 textbook.

SBC4 – High Performance Computing

(a) Parallel computing, scalability

(b) Schedulers, jobs, batching, queue handling

(c) Hands-on: running an R&D code at NERSC, retrieving data

(d) Local facility tour (2015: Hyak@UW)

Duration: 4 hours lecture + hands-on + tour

Job handling on parallel architectures was discussed with reference to both the SLURM and TORQUE schedulers. James Stuber presented a short introduction and oriented students for further information on version control, and for NERSC resources (e.g. MOTD, modules). There followed an outstanding tour of the Hyak – the 10,000 processor HPC facility, led by Stephen Fralich and David Cox. Students were given the opportunity to experience the heat and the noise generated by the cluster, and think through energy management.

SCBC5 – Post-Processing

(a) VisIt introduction, tutorial, application to SCBC4 generated data

(b) ParaView introduction, tutorial, application to SCBC4 generated

data

(c) Scripting with Octave

Duration: 4 hours lecture + hands-on

Dr. Woodruff presented a short overview of post-processing that outlined which methods are of use for visualization, introducing typical useful plotting including contours, glyphs, streamlines. Then there was a hands-on session for post-processing the data obtained from runs at NERSC. Students were given freedom to explore with VISIT and Paraview, with many making movies of the time-series. Scripting was introduced only briefly, however we made reference to the synthetic diagnostic script that Danielle Lemmon had developed.

SCBC6 – Solving PDEs Numerically with Finite Elements

(a) Partial differential equations background, as needed

(b) Equation sets most regularly used in plasma physics

(c) Spatial and temporal discretization

(d) Common time advance methods

(e) Demonstration of Fluxgrid, CUBIT*

Duration: 4 hours lecture (* can be hands-on)

The PDE/FEM section of this course was cancelled due to illness, however, the spatial discretization was demonstrated by example: fluxgrid (one of Glasser's codes) was used to pack a 2D grid, and then we showed how we have optimized a grid for a stellarator for the HiFi code. The final examples were given by use of Cubit, which is a 3D meshing package allowing for unstructured meshes (that can be read for example into NIMROD or HiFi).

SCBC7 – Verification and Validation in Scientific Computing

(a) Verification & validation

(b) Predictive capabilities, restrictions

(c) Synthetic diagnostics

(d) Reproducibility of results

Duration: 3 hours

Dr. Woodruff presented two talks that had great impact on him at an ICC workshop in 2013. The first was by Dr. Bill Oberkampf, the author of 'Verification and Validation in Scientific Computing' that mapped out a very formal semantic approach to verification and validation. Equipped with the terminology, the next talk was one given by Martin Greenwald that showed how V&V was being brought into practice. The contrast between the two talks was discussed. Danielle Lemmon called in to present a short talk on her development of synthetic diagnostics here at WSI during her internship in the last year. Synthetic diagnostics were then presented as part of the

SCBC8 – Contemporary Issues in Plasma Physics and Nuclear Fusion Anticipated but not limited to:

(a) Multi-fluid modeling (mixed neutral-plasma models)

(b) Multi-physics (Fokker-Plank coupling to MHD)

(c) Adaptive solvers

(d) Flux-source expression of dominant equations

Duration: 3-4 hours (anticipated 6-8 presentations)

The Thursday afternoon had a fast-paced session, with presenters from around the US and the UK calling in over skype to give 15 minute introductions to their research. We heard from Prof. Philippa Browning at Jodrell Bank in the UK on plasma merging simulations, from Dr. Peter Buxton on spectral finite difference methods, from Dr. Valerie Izzo on disruption mitigation simulations, from Dr. John O'Bryan at UMBC on his use of NIMROD to find a more efficient formation scheme for spheromaks, from Dr. Eric Meier on his new modeling efforts with SOLPS, from Dr. Alan Glasser on his ongoing efforts to develop a new resistive MHD stability code with amazing speed, then from Dr. Woodruff on one of the MHD code applications to adiabatic compression of compact tori. Students were given opportunity to ask questions, and the discussion was lively. Early the next morning Prof. Randy Leveque from the U. Washington gave a very interesting talk on CFD modeling of Tsunamis and how sensitivity analysis is built in to each run campaign, the title of his talk however was 'Reproducible Research' and introduced the challenges in computational science for making codes available for scrutiny when publishing results.

SCBC9 – Future of Scientific Computing

(a) Exascale roadmap

(b) Hardware/software, architecture/algorithms gap

(c) Algorithmic considerations & foresight

Duration: 2 hours

We had great fortune to have Dr. David Keyes call in (2nd year in a row), again very late in the evening for him. Dr. Keyes is the director of the Extreme Computing Research Center at the King Abdulla University of Science and Technology, home to Shaheen II (now ranked 7th fastest supercomputer in the world). He presented the motivation and philosophy of moving to exascale computing, and how this move will impact both the chip architecture and force the development of new algorithms. The discussion that followed was very lively, and participants were hungry for more information on the algorithm development (for which we may develop a separate 2 day workshop in the future).

SCBC10 – [Optional] Retrospective: A Beginning History of Computers

(a) First computers, languages, processors

(b) Tour of Living Computer Museum

Duration: 3 hours

To end the day and the course we arranged to visit the Living Computer Museum, now home to many of the computers that have influenced Paul Allen. As a primer to the tour, Dr. Olson gave a short introduction to some of the computers we would see, as well as a humorous set of slides on the early advertisements for minicomputers. A special mention should be made here to Dr. Hermann Hauser. Dr. Hauser has been following our fusion development story for the last few years due to a family connection, and is the founder of Acorn – essentially the UK equivalent of Apple. Acorn developed the BBC Microcomputer which was used in most schools in the UK during the 1980's as the platform for teaching computer literacy (and was the computer that sparked an interest in computing for Woodruff). When he learned that we were visiting the Living Computer Museum and that they didn't currently have a BBC Microcomputer, he sought get one sent from the Cambridge Computer Museum. We are enormously grateful to Dr. Hauser for making this donation, and very glad that next time we go to the LCM we will get to use a Beeb.