Summer School: Advanced Scientific Programming in Python - Latin America

Project Proposal [Draft May 8, 2019]

México City, México July 2020

Scope

The summer school Advanced Scientific Programming in Python (ASPP) - Latin America will follow the structure and curriculum of the previously organized schools in Europe (2008-2019) and the Asia-Pacific region (2018, 2019). This highly successful summer schools have shown that there is a need for teaching scientists the principles of scientific computing and software engineering in the Python programming language. The goal of this intensive programming workshop is to teach a selection of advanced programming techniques and best practices in software development which are standard in the industry, to researchers in the natural and social sciences, engineering and mathematics.

The tools and concepts introduced in this workshop will help researchers spend less time writing, debugging and understanding computer programs. In addition, we expect that after attending this course participants will be able to contribute to the open-source scientific software community. With only a week of lectures, we accept that these ambitious goals will be at best partially realized. Nonetheless, the participants will be exposed to a suite of resources which, if studied and practiced, will help to train a generation of future scientists to be able to write better code, but also to make it reusable and easy to understand in case someone wants to reproduce their results.

The course will consist of lectures and discussions along with practical handson exercises which will supplement the lectures and will let participants practice the techniques. The participants are assumed to have prior knowledge (at the level of a competent user) on some high-level programming language used in scientific computing (for example, C, C++, Java, Fortran, MATLAB, etc.) and a basic knowledge of Python. The lectures will move at a rapid, though pedagogical pace. In general, the material covered will be more than the average amount that a participant can digest in a single week. Therefore, it will be mandatory that the participants familiarize themselves with some (online) prerequisite material that we will provide. Moreover, we encourage participants to continue with further study and implementation of the techniques after the course.

The course will not be an introductory course to the Python programming language, though questions on basic features of the language will be refreshed as we go along the lectures if necessary. It will also not be a specialized course on software engineering or computer science. Rather, the lectures will be focused on the needs of scientists who need to optimize their software work-flow. Correspondingly, there will be a strong hands-on component, where participants are encouraged and expected to participate, discuss and proactively learn not only from the faculty but also from other participants.

Organizing Committee

- Carlos Echeverría Serur, PhD Student at the Institut für Mathematik of the Technische Universität Berlin (Alumnus ASPP-Europe 2018).
- Luis García Ramos, PhD Student at the Institut für Mathematik of the Technische Universität Berlin. (Alumnus ASPP-Europe 2018).
- Josué Martínez Moreno (head), PhD Student at Research School of Earth Sciences of the Australian National University, Canberra (Alumnus ASPP-APAC 2019).
- Ricardo Méndez Fragoso, Professor at Department of Physics, School of Sciences of the National Autonomous University of Mexico, (Invited to ASPP-Europe 2019).
- Florencia Noriega, Professor of Software Engineering at CODE University of Applied Sciences, Berlin (Alumna ASPP-Europe 2016).
- Tiziano Zito, from the Institut für Psychologie of the Humboldt Universität zu Berlin. (Co-Founder of ASPP-Europe)

Faculty

- Tiziano Zito, Institut für Psychologie, Humboldt Universität zu Berlin
- Rike-Benjamin Schuppner, Institute for Theoretical Biology, Humboldt-Universität zu Berlin, Germany.
- Stéfan van der Walt ,Researcher, Leader of the Software Working Group, Berkeley Institute for Data Science, University of California at Berkeley, USA.

- Josué Martínez Moreno, PhD Student at Research School of Earth Sciences of the Australian National University, Canberra, Australia.
- Florencia Noriega, Professor of Software Engineering at CODE University of Applied Sciences, Berlin, Germany.
- Madicken Munk, Postdoctoral Researcher at the Data Exploration Lab, National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign, USA.
- Kathryn D. Huff, Assistant Professor, Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign, USA.
- Fernando Pérez, Assistant Profesor, Berkeley institute of Data Science, University of California at Berkeley, USA.
- Ricardo Méndez Fragoso, Professor of Physics, Faculty of Sciences of the National Autonomous University of Mexico.
- ^{c1}Who else may be interested? Ideally we should invite people from the US, and America Latina

Tutors (Preliminary List)

- Carlos Echeverría Serur
- Luis García Ramos
- Josué Martínez Moreno
- Ricardo Méndez Fragoso
- Florencia Noriega

Note: The budget will fund travel, accommodation and *Per Diem* expenses of lecturers and organizers. Typically, organizers also serve as lecturers. The budget may not allow for funding of organizers who do not actively participate in the school as lecturers. Additional budget will be use to support accommodation or travel expenses of international and local students.

Vision

The Advanced Scientific Programming in Python has been a student initiative with the goal of better understanding how to make scientific source code reproducible, acurate and reusable that many scientists use along their career. The school will bring together sceitnrist from all over Latin-America for the first

^{c1} Josue: Text added.

ASPP in the American continent. During the 7-day intensive course, students will explore and learn the fundamentals ideas of scientific code development from leading experts in the field. The school will be held in a remote location near Mexico City to create a deep, focused learning experience away from distractions and daily routines. Informal chats during shared meals, recreation time and during coding excercises will provide opportunities to all participants to form close professional and personal relationships, fostering future collaborations and openness within the next generation of Latin-American Scientists.

Scope

The Advanced Scientific Programming in Python (ASPP) - Latin America will follow the structure of the previous organized schools in Europe and Asia-Pacific. This intensive programming course aims to teach the rudiments of scientific python and how to use it in a reproducible, efficient and academic way. We are concerned with the current use of programming languages without fully understanding the foundations and their potential. We are also interested in concepts and tools to use programming as an open-source community for the purpose of scientific development. With only a week of lectures, we accept that these broad aims will be at best be partially realized. Nonetheless, the students will be exposed to a suite of resources which, if studied and practiced, will help to train a future scientists able to improve their codes, but also to make it reusable and easy to understand in case someone wants to reproduce their results.

The course will be taught in a traditional manner with spoken lectures and discussions, along with practical sections which will supplement lectures and will encourage students to engage and take advantage of the lectures. The student is assumed to have prior knowledge on any coding language and a basic understanding of Python. The lectures will move at a rapid, though pedagogical pace. In general, the material covered will be more than the average amount an student could digest in a single week. Therefore to take fully advantage of this course, we encourage students to read the pre-course and post-course study. This particular topic requires devoted engagement and interaction not only during the lectures but after the course is finished.

This course is not *per se* a how to code course, though some basics will be cover. This is also not an programming engineering or computer science course. Rather, the lectures are focused on how scientists can optimize their work-flow, as well as to facilitate the reproducibility, collaboration and maintenance of their codes. Correspondingly, there will be a strong hands-on component, where students are encouraged and expected to participate, discuss and proactively learn not only from the faculty but also from other students.

Need

There is a considerable education lack in scientific programming courses. Across many academic and non-academic institutions, programming has become a key skill to conduct research. However, in many cases our interaction with codes ranges from simply copy-paste code found online to developing and running new modules-packages. Whilst many of us are familiar with the basics of programming, less well understand the full capabilities and standards used to facilitate openness and sharability of code. Additionally, the codes we commonly use do not aliviate the generation of bugs which leads to use trial-and-error or rely on advice from others. Therefore, a better understanding on better coding practices as well as the underpins on Python, will provide the required tools to increase the participants efficiency and code robustness while programming.

Participants

Participation is free, i.e. no fee is charged, however participates should take care of travel, living, and accommodation expenses by themselves. We may be able to provide a small travel allowance if resources are sufficient (see "Funding" below).

Admission Requirements

These are the requirements for participating in ASPP - Latin America:

- Applicants should be research students, Masters, PhD students, Postdocs
 or Research Scientists in the natural or social sciences, engineering or
 mathematics, at an institution in South, Central or North America. Priority will be given to applicants from Latin America and applicants from
 underrepresented groups.
- Applicants are absolutely required to know a high-level programming language used in scientific computing (for example, C, C++, Java, Fortran, MATLAB, etc.) and the basics of Python to get the most out of this Summer School.
- Applicants should provide proof of their English proficiency by providing a letter of motivation and a curriculum vitae of the applicant written in the English language. Applicants are not required to provide results from a proficiency test. c1 c2

^{c1} Josue: Is there something else to add? Shall we ask for a reference letter or something? ^{c2} Luis: The application form should require a letter of motivation and a short resume-bio

Lectures

These lectures will build from feedback obtained during the previous ASPP-Europe and ASPP-Asiapacific schools (topics include some of the potential speakers).

- Version control (GitHub) -
- $\bullet\,$ Tidy data analysis and visualization Rich $^{\rm c1}$
- Testing and debugging scientific code Luis
- Advanced NumPy Carlos
- Organizing, documenting, distributing scientific code and continuous integration -
- Advanced scientific Python: context managers and generators -
- Writing parallel applications in Python -
- Profiling and speeding up scientific code with Cython and numba -

Schedule

Monday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-9:30	Introduction		
9:30-11:00	Git & Github		
11:00-11:30		Coffee Break	
11:30-13:00	Git & Github		
13:00-14:00	Lunch Break		
14:00-15:00	Git & Github		
15:00-16:00	Data visualiza-	Ricardo Méndez	
	tion		
16:00-16:30	Coffee Break		
16:30-18:00	Data visualiza-	Ricardo Méndez	
	tion		

c1 Josue: Perhaps change the structure and remove Tidy data?s

Tuesday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-9:30	Testing & debug-		
	ging		
9:30-11:00	Testing & debug-		
	ging		
11:00-11:30		Coffee Break	
11:30-13:00	Testing & debug-		
	ging		
13:00-14:00		Lunch Break	
14:00-15:00	Advanced		
	Numpy		
15:00-16:00	Advanced		
	Numpy		
16:00-16:30		Coffee Break	
16:30-18:00			

c1

Wendsday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-11:00	Organizing, documenting, distributing & CI		
11:00-11:30		Coffee Break	
11:30-13:00			
13:00-XX:XX		Social activity	

c2

Thursday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-10:30	Parallel Python		
10:30-11:00		Coffee Break	
11:30-13:00	Parallel Python -		
	Pycuda		
13:00-14:00		Lunch Break	
14:00-14:30	Project Intro-		
	duction		
14:30-16:00	Programming		
	Project		
16:00-16:30		Coffee Break	
16:30-18:00	Programming		
	Project		

 $^{^{\}rm c1} Josue$: I would like to add some Scipy, what do you think? $^{\rm c2} Josue$: Do we want a social activity?

Friday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-10:30	Profiling,		
	Cython &		
	numba		
10:30-11:00		Coffee Break	
11:30-13:00	Profiling,		
	Cython &		
	numba		
13:00-14:00		Lunch Break	
14:00-16:00	Programming		
	Project		
16:00-16:30		Coffee Break	
16:30-18:00	Programming		
	Project		

Saturday XX July 2020			
Time	Topic	Speaker	Tutors
9:00-10:30	Programming		
	Project		
10:30-11:00	Coffee Break		
11:30-13:00	Programming		
	Project		
13:00-14:00	Lunch Break		
14:00-16:00	Programming		
	Project		
16:00		Repository Freeze	
16:00-16:30	Coffee Break		
16:30-16:45	How to con-		
	tribute to ASPP		
16:45-17:00	Programming project - Learning report		
17:00-18:00	Friendly Tournament		
18:00-XX:XX	Final Social Event		

c1 c2

Estimated Costs

The budget will fund travel, accommodation and daily expenses of lecturers and organizers. Organizers can also serve as lecturers or tutors since the budget may not allow for funding of organizers who do not actively participate in the school

c1 Josue: I've removed 1 hour from the lunch break so people can go earlier home, do you think we should use that hour or shouldn't?

 $^{^{\}mathrm{c}2}Luis$ and Carlos: We think they should have two hours of lunch break (to be discussed)

as lecturers. Additional resources will be used to support accommodation or travel expenses of international and local students.

Estimated costs per Faculty Member (should be covered by the organizers)

• Flight (from Europe or US): Approx. 800USD

• Accommodation in CDMX: Approx. 400USD

• Local Transport: Approx. 100USD

• Food for the entire duration of the conference: Approx. 200USD

Estimated costs of Organization (sholuld be covered by the organizers)

- Computer Rental (40 computers): Approx. ???USD
- Venue Rental: Approx. ???USD
- Social Activity (Trip to Teotihuacán): Approx. ???USD
- Airport-Venue Transport: Approx. ???USD

Estimated average costs per Participant (should be covered by the participants)

- Flight (From a Latin American Country): Approx. 500USD
- Accommodation in CDMX: Approx. 300USD
- Local Transport: Approx. 50USD
- Food for the entire duration of the conference: Approx. 150USD

Tentative Partner Organizations (Sponsors/Funding)

- Secretaría de Ciencia, Tecnología e Innovación de la CDMX.
- Faculty of Sciences (FCIENCIAS-UNAM).
- Instituto de Investigaciones en Matemáticas Aplicadas (IIMAS-UNAM)
- Consejo Nacional de Ciencia y Tecnología (CONACYT)
- Instituto Latinoamericano de la Comunicación Educativa (ILCE)
- Instituto Politécnico Nacional (IPN)

Policies

Inclusiveness

We are striving hard to obtain a group of participants which is international and gender-balanced.

Behavior

See https://numfocus.org/code-of-conductCode of conduct