

**Prof. Gilbert DELEAGE**

Director

Ref. MJ/GG/GD

Object : Letter for G. Goret support

Mr Johnson

ILL

Grenoble

Lyon, april 21 avril 2012, 21<sup>th</sup>

Dear Mr Johnson,

I am very pleased to write this letter of support for Dr. Gael Goret. I know him for years when he was a student in biochemistry master at Lyon University. He was actually one of the most interacting students showing high curiosity level. It is my sincere pleasure to offer an expert opinion concerning Dr. Gael Goret's scientific accomplishments and provide testimony that he is a truly outstanding developer worthy of being recruited by ILL. Indeed, I notice you are seeking for "Previous experience working with neutrons or X-rays would be an asset. You are highly motivated and are able to write codes using modern languages such as Python and C and modern tools like the software forge (SVN, Eclipse)."

I would say that Dr. Gael Goret has an apparently natural talent for crossing scientific disciplines and for surmounting technical barriers to produce high impacting and immediately applicable software that can only be described as truly excellent. Dr. Gael Goret has pursued a broad range of projects related to software development applied to biology (one of them in my lab). Now, he is currently the lead developer of VEGA, an excellent software for dynamics structure fitting into cryoEM maps. I think it is a very important feature that he largely contributed to introduce in France under the supervision

of J. Navazza in Grenoble at IBS. I think G. Goret's experience totally fulfils the expertise you are searching for.

Dr. Gael Goret, although rather young, is a very mature computing developer/researcher who published some important publications in journals with very good impact factor. I have no doubt that he will further pursue his career in applied computational biology yielding a continued production of high level software.

Yours sincerely,



P. G. DELEAGE  
Directeur  
IBCP - UMR 5086

Dear Mark,

With Gaël it was the first time I had a student (collaborator) that was only a programmer. Fortunately, it happened that his thesis turned out to be only computational, the kind of things Gaël likes and knows, and I was really satisfied with the result, but I would have liked Gaël felt also concerned with the physics and mathematics used to solve the problems we were considering.

If what you need is a programmer, then Gaël can do the job quite well.

But he will need help for whatever maths and physics is used.

Juan Rodriguez-Carvajal was in the jury of Gaël's PhD. He certainly knows better than I if Gaël's qualifications fit with the position requirements.

Here follows a reference letter. I don't know if this was what you were expecting from me.

Regards,

Jorge

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Jorge Navaza  
MEM , IBS Grenoble  
France

23 April 2012.

To whom it may concern:

Gaël was my PhD student from October 2008 till September 2011. He developed a graphical interface for docking macromolecular atomic models into EM reconstructions, taking into account all point groups and helical symmetries. He wrote this interface in PYTHON, with VTK as the graphical language. This interface was conceived to launch the scientifically relevant applications, already existing, that performed symmetry manipulations, docking, normal mode analysis and other tasks.

As a programmer he is undoubtedly gifted. In particular, he found an efficient way to communicate graphics and results from the calculations, which allowed computing correlations in real time as the models moved within the EM maps. Although his background in applied

mathematics and physics is poor, he was able to incorporate any well-documented (or thoroughly explained) application to his interface. His program, called VEDA, can be downloaded from <http://mem.ibs.fr/VEDA>.

Gaël's profile exactly corresponds to a "Master's degree in computing with experience working in a scientific environment and collaborating effectively with scientists" (mainly biologists), as specified in "qualifications and experience" in the description of the position for the Computing for Science group at ILL.

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On 05/04/2012 15:46, johnson wrote:

Hi Michael

Gael has applied for a software development position with us.

What do you think about him? Has he done a good job for you/Alexis?

Thanks and bon w/e.

M.

Hi, Mark

I think that he good skills, is eager to learn, and is highly motivated if he sees the "grand picture", meaning if he sees the

usefullness of what he is doing. He did a suite of data extraction and fitting routines, and I am quite satisfied with his work.

He is a very pleasant character, open-minded, and pro-active. On Alexei's scale he is too slow, but Alexei is not a fair reference.

I believe it is worthwhile having a look at him, but I suggest to check his technical skills with precise questions.

Cheers, Michael

Hi Mark,

all of them are excellent candidates.

On 4/5/2012 3:03 PM, johnson wrote:

Ricardo Leal  
Gael Goret  
Jerome Roy

They are skilful people and proficient in Python. Ricardo has the largest programming experience among them, followed by Jérôme who used to be until recently a BL scientist. Both wrote interesting (and used) Python applications and have a significant scientific background. I think Trevor has been very happy with Ricardo. Gaël is right now working for the BL of Michael Krisch in collaboration with my group and is making very good progress. He needs however some more on-the-field experience to catch up with the other two.

All of them have worked in one form or the other together with my group and I feel enough confident to recommend you all of them

I guess the choice would however be between the first two for the time being, due to their longer experience, but if both turn down the offer, Gaël should be considered as a very serious spare candidate

Tell me if you need more detailed information

Grenoble, 20 April 2012

To whom it may concern:

**This letter is to support the application of Dr. Ricardo Ferraz Leal for a post in the Computing for Science group at ILL.**

Dr. Ricardo Leal has been working as Postdoc under my supervision since February 2009. He is directly involved in several projects that are mainly concerned with the development of new techniques and instruments for X-ray studies of macromolecular crystal structure using synchrotron radiation. One of aims was to further extend the work that Ricardo undertaken during his PhD thesis - engineer special software for X-ray data collection strategy planning and to apply this to a specific scientific target: the mitigation of radiation damage effects whilst collecting X-ray data from crystals of biomolecules. Ricardo successfully developed an automated procedure for the determination of the radiation damage rate incurred in a crystal, providing calibration and verification of a specific decay model. The information prepared by this method can be then used for definitive X-ray data collection of macromolecular crystals. The application of this method to different conditions, e.g. at room temperature experiments has shown very surprising outcome and we are now finalising a new publication on this subject. Ricardo has also developed in parallel other tasks on 3D crystal modelling from visual images as well as on the effects of the X-ray beam shape on crystal decay. The thorough understanding of these mechanisms is fundamental for developing an adequate data collection strategy planning. He is also participated in the development of data collection strategy using many crystals.

I am very pleased with Ricardo's progress to date. He is becoming a serious scientist, highly motivated, and very able. During the period of his postdoc, he has gone out of his way to learn and develop his knowledge of radiation damage effects on macromolecules and data collection strategy planning. In his first year working, he was awarded the prize of the best poster at 25th European Crystallography Meeting in the domain of Instrumentation. In my view there are too few people left in macromolecular crystallography that have serious insight into the principles and methodologies involved and it is very important to maintain and cultivate such capabilities at the EPN-Campus and also more widely in the crystallographic community. In summary, Ricardo has been an excellent Postdoc and his application to this job position has my full support.

If you would like any further input, please do not hesitate to ask.

Yours faithfully,

Dr. Alexander N. Popov

ESRF ID23-1 Beamline in charge scientist

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**Australian Government**



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In Confidence:

Re: Luis Fuentes- Montero

Dear Mark,

It is with much pleasure that I write to you to support the application made by Luiso for the post of Research Engineer in Programming.

I have known Luiso since he arrived at ANSTO in June 2011 in the context of his current joint appointment between ILL and ANSTO (where his project is related to my work as an instrument scientist on the Laue diffractometer KOALA). Luiso has shown himself to be an excellent colleague and has come to grips with the many scientific issues inherent in the task he has undertaken in this appointment.

It is to Luiso's great credit that he has made significant progress in this project in the context of what I perceive to be unresolved conflicts regarding the very nature and scope of the project and the competing interests of the parties to whom Luiso was answerable at the two institutions. As Luiso came to understand these interpersonal dynamics he endeavoured to manage them with a high degree of diplomacy and respect for the positions which others had adopted and to recognize that it was unlikely that he would be able to resolve them.

In the time Luiso was at ANSTO, he took care to seek out those who would be potential users of his program and enlisted them to test and provide feedback which he discussed with me in a well organized and constructive approach to providing a scientifically correct and user friendly platform. Luiso is unnecessarily modest regarding his language capabilities which in my observation are excellent – his English allowed him to be fully functional at ANSTO from the time of his arrival – you will be better placed to make observations regarding his facility in French! It is clear that he possesses the requisite scientific, technical and interpersonal skills to undertake the advertised position.

Luiso's training in engineering sees him well equipped to pursue a career in scientific programming and I give my wholehearted endorsement to his present application. Please feel free to phone me on +61409310045 should there be any further endorsement I can offer to this application or to discuss any issues arising from it.

Yours sincerely

Alison Edwards  
B.Sc.(hons) Ph.D.

Senior Research Scientist and  
Instrument Scientist

Bragg Institute





Grenoble, April 23<sup>rd</sup> 2012

Dear Mark,

This is to recommend Dr. Jerome Roy for the post of a programming researcher available at the ILL. I work as a second scientist at the ID32 beamline at the ESRF and it was always a pleasure to work with and co-supervise Jerome for more than 4 years. He was first a post-doc and then a young scientist in our group. He was the person who introduced me into the operation of our beamline as he's been there since 1 year before I arrived.

Since the beginning Jerome showed a particular interest in and understanding of the technical and computing issues of the beamline operation. This more technical focus has distracted him sometimes from more scientific work. During his stay at ID32 he has developed from a rather impatient and unfocused post-doc into a persistent and concentrated young scientist who keeps track of the scientific goal even when deeply immersed in the technicalities of the subject. During his last appointment as an executive leader of a long-term project (X-ray standing wave on zeolite microcrystals) he has shown capabilities to manage a technically very challenging scientific project – by organizing instrument development and/or loans, by careful planning and developing various experimental approaches, and especially by optimizing those by computer simulations. Despite meagre scientific results from his mission he was able to produce important results in the form of technique-based papers.

One of the main activities of Jerome during his young scientist appointment was development of Python-based data analysis and simulation code for X-ray standing wave technique called PyXSW. The X-ray standing wave (XSW) is a technique that combines structural and spectroscopic information about matter thus allowing to refine crystal structures and adsorbate geometries with chemical state and atomic species selectivity. The data analysis requires determination of the phase of the standing wave which is not possible by simple fitting to an analytical function but it is accessible only via dynamical theory of diffraction and includes the simulation of the phase change over the whole optical path. Development of a computer code for data analysis thus requires extensive knowledge in optics and in scientific computing. Based on the zeolite project and other users' demands, Jerome has developed, almost on his own, a very versatile package in Python that illustrates his abilities in scientific programming. Being a Python-literate scientist (and a contributor to one of the tool scripts in PyXSW) I also appreciate his approach that uses the maximum of available resources without duplicating them (DABAX database, CIF structure files, standard ESRF data formats, least-square fitting routines) which is a "good practice" in scientific computing sometimes neglected by scientists. Jerome's code is very well documented including a tutorial and examples which allow even a beginner Python user to write personalized scripts that go beyond capabilities of other existing XSW data analysis codes. I will not exaggerate if I say that with this package one can analyze any XSW data today. For me, it has become an indispensable tool in my scientific work.

Jerome has a very strong sense of collaboration and appreciates mutual help and distribution of tasks between scientists in a project. He can work both independently or in collaboration, depending on the requirements of the problem. He usually tries to find a solution alone (or, in

the case of Python, by documentation and forum search) but he is not afraid to ask others for help on more complex issues. As an example I can mention his collaboration with J. Kieffer and C. Ferrero (Scientific Computing Group at the ESRF) for issues including the code's internal structure, maintenance and distribution.

I think Jerome is a very suitable candidate for the proposed job. He will be very attentive to the main issue of the project which is, in my view, the various types of data (and possible resulting data formats) to deal with. Having experience from a technique that combines two (or more) very different signals (diffraction and various spectroscopic signals) he will be able to generalize and anticipate needs of the software to develop. He also has got experience from developing scientific software for a user community, not only for himself.

I highly recommend Jerome for the announced post not only based on his scientific computing capabilities but also taking into account his collaboration skills.

Should you need more information, don't hesitate to contact me by phone at 04.76.88.27.76 (office) or 04.76.88.26.65 (beamline), I will be happy to discuss my recommendations in more detail.

Sincerely,

Blanka Detlefs

scientist at ID32 beamline, ESRF