



Paris, 6 June 2017

Sixth ISCD Summer School, July 17-Aug. 11, 2017 Scientific Visualization - Data Analytics Roscoff Marine Station, France

Dear Participant,

On behalf of the scientific committee, I am very pleased to extend a warm welcome to the 2017 Summer School on Bioinformatics and visual data analysis.

# Institut des sciences du calcul et des données

FED 3/2017 Dossier suivi par : Pascal FREY, Agnès MISKIEWICZ

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Adresse postale: 4, Place Jussieu Boîte courrier n° 380 75252 PARIS Cedex France By joining our summer program, you will actively work on a number of areas of bioinformatics and visual data analytics in lectures, workshops and supervisions. You will experience approaches to these challenging topics, meet and interact with students from other universities and academic centres attending this school. Faculty who are acknowledged experts in their research disciplines will teach lectures and mini-courses.

To help you prepare your visit, we are providing this package of additional information about the programme, the conference centre and Roscoff. Please read through this information before your arrival. To assist you in finding the information you need, please do not hesitate to contact us.

We look forward to welcoming you to Roscoff personally and to your participation in this summer event.

Yours truly,

Pr. Pascal Frey, director

Parcel For.

# ISCD Summer School 2017 in Bioinformatics and Visual Data Analysis

ISCD Summer Schools "Computational Challenges at the Interfaces" seek to promote academically motivated young students by strengthening their methodological understanding in linking theory and numerical experiments. They convey the excitement of new progress in computational sciences through the stimulus of learning. The objectives are to train and attract new undergraduate and newly graduate students interested by working at the interfaces between disciplines.

This year Summer School will provide theoretical lectures and hands-on training in bioinformatics and visual data analysis. The concrete application of theories in innovative research projects is a task which is far from trivial. It involves a good understanding of the theory, but it also requires skill, creativity and sensitivity for their adjustment to experimental contexts. Our lecturers will help the students to face and take into account these challenges.

#### The course of the programme

The summer school consists of a fourweek programme covering two active research fields, alternating lectures and hands-on sessions. Students will get a thorough introduction to the main concepts in bioinformatics and visual data analysis, and to the underlying mathematical and computational methods applied to these topics. In each period, we tackle the key methodological challenges that arise in almost all research efforts, with consideration within concrete fields of applied research. The modules of the first and second week follow certain didactical course respectively.



Participants, summer school Roscoff 2016.

The detailed programme will be posted at the beginning of every period.

#### **General information**

#### Contact ISCD

Sophie Fassy, Pr. Pascal Frey: + 33 (0)1 44 27 51 02

In case of emergency, after hours or during weekends, please dial: 02.98.29.23.90

#### Location

The Roscoff Station is a CNRS Conference Centre and offers all infrastructure for organising university-level courses and hands-on sessions. All courses will take place in the conference room (auditorium) located on the second floor of Yves Delage building. Hands-on sessions will be carried out in the computer room located in the Hotel de France building.

#### Accomodation in residence

The Gulf Stream residence has 41 single rooms and 6 double rooms available to student participants. The restaurant is open for lunch and dinners for guests as well as for the Marine Station staff. It is famous among the community for the quality of its food and its service. An access code will be given to you upon your arrival to allow you to enter the Gulf Stream hotel.

To facilitate your travel plans, you are welcome to arrive at the station the day before the school starts (i.e. on Sunday July 17<sup>th</sup> for students attending the first or both sessions, or on July 31<sup>st</sup> for students attending the second session only) and leave the day after its ending (Saturday August 13<sup>th</sup>).

The room numbers will be posted at the entrance of the residence. The rooms are open and keys are inside.

**Note**: the code **41706** will give you access to the residence and to the lecture/computer rooms.

#### Meals for residents

Your meals (breakfasts, lunches and dinners) for the duration of the summer school are included Monday to Friday. Breakfast will be served between **7:45** and **8:45**. Lunch will be served at **12:30** and dinner at **19:00**. On weekends (Saturday-Sunday), you will need to make your own arrangement for breakfast, lunch and dinner (allow approx. 60 euros / weekend meals).

#### Computers and electronics

The Gulf Stream and all facilities at Roscoff Marine Station are equipped with a wireless network. You will be registered as UPMC students during the summer school and will be provided with a login and password to connect. If you have problem connecting to the network, please contact the teaching assistants that will notify the Roscoff Station's IT officer.

#### Wifi access codes:

Gulfstream residence: user= ICS2017 passwd= sbroscoff
The codes for the lecture/meeting rooms are listed in the attached document.

#### Coming to Roscoff

If you have chosen to travel by train you will arrive at the Roscoff train station. Departure is scheduled at Paris Montparnasse train station. Train platform will be announced 20 minutes before departure. Take the TGV train to Morlaix and then change for a regional express train (or a bus, if indicated).



• by train: the nearest TGV train station is Morlaix.

Regional express train Morlaix - Roscoff takes 29 minutes.

Bus (SNCF) Morlaix - Roscoff takes 35 minutes.

Roscoff train station:+33 (0)298 697 020

TGV train Paris - Morlaix: departure Paris Montparnasse station.

Train journey takes about 3 hours.

#### • by air:

From Paris Charles de Gaulle airport to Paris Montparnasse train station:

locate Paris by bus - Air France (web link):

Terminal 1: Exit 32 on the Arrivals level.

Terminal 2A-2C: Exit C2. Terminal 2E-2F: Exit E8 or F9.

Terminal 2G: this terminal is linked to Terminal 2F (Entrance 2.10) by the free N2 shuttle bus.

The N2 shuttle bus runs from 05:30 to 23:00.

Maximum service frequency: every 6 minutes. Average journey time: 15 minutes.

Terminal 3: get off at Terminal 1 and take the free CDGVAL shuttle train to Terminal 3 stop.

Fares: 17 euros (single), 14.5 euros (group, > 4 persons).

#### **Arrival in Roscoff**

Walk from the train station to the hotel "The Gulf Stream" (see map below). The list of room assignments will be posted in the lobby of the hotel.





- Station Biologique SALLE DE CONFERENCES.
  - Hôtel restaurant « le Gulf-Stream » .
  - Hôtels de France. Salles de réunions.



#### **ACCES WIFI**

<u>**Gulf Stream**</u>: le code Wifi sera commun à tous les participants. réseau : "sbr\_public " - Identifiant : ICS2017 - Mot de passe : sbroscoff

 $\underline{\textbf{Hôtel de France:}} \ \text{Réseau "wifi-guest", les identifiants et code wifi sont dans les chambres.}$ 

Salle de conférence : Utiliser le réseau "wifi-guest"

il vous appartient de remettre un identifiant et mot de passe de liste

	Identifiant	Mot de passe	Personne	
l	ics1	Sxw347Zi	Vecchio	Federica
2	ics2	PCe3i2e7	Gervasoni	Federica
	ics3	42rNA9xw	Meng	Huqi
	ics4	U9Zwwm42	Letcher	Brice
;	ics5	3Fp87xrC	Renaux	Demir
;	ics6	YWtg83o8	Ribeiro Sabidussi	Emanoel
,	ics7	Ff3D4q4s	Thimonier	Chloé
3	ics8	4u4J8fRe	Verkin	Louise
)	ics9	Qn18hMm1	Wang	Yishu
0	ics10	d0gEb77K	Mansour	Yasmine
1	ics11	q64HvTx9	Perrot	Maxime
2	ics12	24M1Dsfs	Gueda	Moussa
3	ics13	Y816epmC	Quesnel	Emeric
4	ics14	el9l2Yo5	Manneheut	Léa
5	ics15	yFKhz871	Dubois	Léonard
6	ics16	p94j6TYj	Seol-Kong	Kim
7	ics17	dPdA369m	Kocova	Pavlina
8	ics18	94Ck6Tle	El Yaagoubi	Anaas
9	ics19	40kK8iNy	Norgeot	Loïc
0	ics20	oR5G8g1q	Fekete	Jean Danie
1	ics21	tj0TVf48	Baaden	Marc
2	ics22	nSUx115m	Frey	Pascal
3	ics23	D6U01zsz	Laine	Elodie
4	ics24	8iC2oV0e	Carbone	Alessandra
5	ics25		Bernardes	Julia
6		6oQGy3z1	Chauvot de Beauchêne	Isaure
7	ics26	2q7WqM3q	Chikhi	Rayan
8	ics27 ics28	fv2P6Bn7	De Vries	Sjoerd
		h42jll5p	Lopes	Anne
9	ics29	G1M02diz	Rizzi	Raffaella
0	ics30	3u2ooF7H	Shaw	
1	ics31	1pvh61JH		Sophie
2	ics32	k1cG8Yw7	Straatman	Dirk Elin
3	ics33	H9J4n0qg	Teppa	
4	ics34	47jKj1Jw	Vicedomini	Riccardo
5	ics35	1DVye56s	Aït Ahmlat	Adel
6	ics36	vp2T2jZ9		
7	ics37	yZVd2y36		
8	ics38	c1eU0Xo3		
9	ics39	5NoS1c0t		
0	ics40	3Y8n7wyQ		
1	ics41	3chKmS96		
2	ics42	10pC2ab9		
3	ics43	94I5Unbl		
4	ics44	WZs57z8o		
5	ics45	mS70ml3u		
6	ics46	v0Nm44kB		
7	ics47	xuNXi027		
8	ics48	3tw6BuM0		
9	ics49	1h9ptCU4		
0	ics50	6dx4YIn8		
1	ics51	jh1QI79y		
2	ics52	V8l09Ube		
3	ics53	6vcC48Ud		
4	ics54	xbhM5Z78		
5	ics55	oX55Pub2		
6	ics56	LZ4w1ll5		
7	ics57	ifb08306		
8	ics58	rJc1m3A2		
9	ics59	hPX6y50w		
0	ics60	HO8kw8t0		

# **Summer School "Computational Trends at the interfaces"**

# **Bioinformatics - Visual data analysis**

July 17 - August 11, 2016, Roscoff

# **Week 1: Protein and Protein Complex Structures**

## Mon. Jul 17 D. Straatman

09:00 - 12:00 Introduction to protein and protein complex structures

14:00 - 17:00 Visualisation/manipulation of structures

## Tue. Jul 18 S. De Vries & I. Chauvot de Beauchêne

09:00 - 12:00 Molecular docking, concepts and algorithms

14:00 - 17:00 Manipulation of different docking tools I

### Wed. Jul 19 S. De Vries & I. Chauvot de Beauchêne

09:00 - 12:00 Protein-nucleic acid docking, flexibility in docking

14:00 - 17:00 Manipulation of different docking tools II

## Thu. July 20 A. Lopes & E. Laine

09:00 - 12:00 Evolution of protein complexes

14:00 - 17:00 Analysis of docking results I

## Fri. July 21 A. Lopes & E. Laine

09:00 - 12:00 Promiscuity versus specificity, identification of cellular partners

14:00 - 17:00 Analysis of docking results II

# Week 2: Sequence analysis and genomics

### Mon. Jul 24 R. Chikhi & S. Shaw

09:00 - 12:00 Introduction to sequence analysis, main algorithms (suffix trees / BWT / backward search, graphs for DNA assembly

14:00 - 17:00 Implementation and usage of BWT

# Tue. Jul. 25 J. Bernardes & R. Vicedomini

09:00 - 12:00 Protein domain annotations/identification

14:00 - 17:00 Application on genomic and meta-genomic datasets

#### Wed. Jul. 26 R. Rizzi

09:00 - 12:00 Gene annotation and GTF file format

14:00 - 17:00 Development of python code to manipulate GTF, for full-length transcript & CDS reconstruction

### **Thu. Jul 27** A. Ait-Hamlat

09:00 - 12:00 Gene regulatory networks (GRN), main algorithms

14:00 - 17:00 Manipulation/Analysis of expression data and GRNs

## Fri. Jul 28 A. Carbone & E. Teppa

09:00 - 12:00 Phylogeny and co-evolution

14:00 - 17:00 Application of coevolution to protein analysis

# **Summer School "Computational Trends at the interfaces"**

# **Bioinformatics - Visual data analysis**

July 17 - August 11, 2016, Roscoff

# Week 3: scientific visualization

14:00 - 17:00 Hands-on session V

Mon. Jul 31	P. Frey
09:00 - 12:00	introduction to scientific visualization definition, purposes, motivations, technological aspects
14:00 - 17:00	Hands-on session I
Tue. Aug 1	P. Frey
09:00 - 12:00	Computer graphics primer quest for realism, illumination models
14:00 - 17:00	Hands-on session II
Wed. Aug 2	P. Frey
09:00 - 12:00	Mathematical primer geometric transformations, affine/projective transformations
14:00 - 17:00	Hands-on session III
Thu. Aug 3	P. Frey
09:00 - 12:00	Surface representation and approximation curves and surfaces introduction, differential geometry, triangulations
14:00 - 17:00	Hands-on session IV
Fri. Aug 4	P. Frey
09:00 - 12:00	Data analysis and visualization data structures, scalar/vector/tensor fields

# Week 4: scientific visualization

# Mon. Aug 7 J.D. Fekete

- 09:00 12:00 Introduction to Information Visualization
- 14:00 17:00 Hands-on session (D3.js + Python/Pandas as backend)

## Tue. Aug 8 J.D. Fekete

- 09:00 12:00 Introduction to Visual Analytics
- 14:00 17:00 Hands-on session (Python with Scikit Learn, the Jupyter Notebook)

# Wed. Aug 9 M. Baaden

- 09:00 12:00 Introduction. Principles of scientific illustration
- 14:00 17:00 Hands-on session on molecular visualization (UnityMol, VMD)

## Thu. Aug 10 M.Baaden

- 09:00 12:00 Molecular simulations
- 14:00 17:00 Hands-on session on analysis of molecular simulation data (VMD, Paraview)

# Fri. Aug 11 M. Baaden

- 09:00 12:00 Introduction to interactive visualisation and manipulation of molecular models
- 14:00 17:00 Hands-on session on interactive simulations, virtual and augmented reality (UnityMol/HireRNA, VMD/BioSpring, UnityMolVR)