Labex MILYON

Mathématique et Informatique Fondamentale de Lyon

UNIVERSITÉ DE LYON

BIOMATH SPRING LYON

CONFERENCE

“Mathematical Modeling in Cell Biology”

March 25-29, 2013

http://mathbio2013.sciencesconf.org/

ÉCOLE CENTRALE LYON

ENS DE LYON

Supports

MATHématiqueS
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pour la TERRE

Organizing committee : **Hugues Berry** (INRIA, Lyon), **Vincent Calvez** (UMPA, ENS de Lyon)

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	Monday	Tuesday	Wednesday	Thursday	Friday
09:00-10:00	Welcome	**MOGILNER**	**HOLCMAN**	**GOLDSTEIN**	**DOUMIC**
10:00-10:30	Welcome	Coffee break	Coffee break	Coffee break	Coffee break
10:30-11:00	**BENICHOU**	**FLEGG**	**AMITAI**	**FEDOTOV**	**GABRIEL**
11:00-11:30		**MILISIK**	**LEONCINI**		**GINELLI**
11:30-12:00	**SCHMEISER**	**VERDIER**	**CHAUVIERE**	**FALCONER**	**DUMAIS**
12:00-12:30				**LAGACHE**	
12:30-14:30	Lunch time	Lunch time	Lunch time	Lunch time	Lunch time
14:30-15:30	**HAMANT & BOUDAOUD**	**NEDELEC**		**NEWBY**	
15:30-16:30		**MEUNIER**	*Free afternoon*	**CHATE**	
16:30-17:00	Coffee break	Coffee break	*(Guided tour in Old City)*	Coffee break	
17:00-18:00					

Abstracts of the plenary talks

- Arezki Boudaoud & Olivier Hamant (Ecole Normale Supérieure de Lyon)

Title: Stochasticity in plant growth and morphogenesis: are some cells more equal than others?

Abstract: A number of studies have shown that growing thin sheets undergo buckling and wrinkling by default. In particular, we found that when growth is enhanced near the edge, the equilibrium configuration of the sheet is fractal-like, accounting for the shape of beet or lettuce leaves – mathematically, this amount to the embedding of hyperbolic elastic surfaces in 3D. This default, wrinkled state raises the question of how a flat shape is maintained in leaves, and implies the existence of mechanisms that regulate the homogeneity of growth in plant tissues. We investigated such a mechanism using a combination of biological and modeling approaches. More specifically, we considered growing tissues subjected to a stochastic noise and to a feedback of mechanical stress on cell growth. This led us to counter-intuitive results on stochasticity in plant morphogenesis.

- Olivier Bénichou (Université Paris 6)

Title: First-passage times of diffusion processes and Geometry-controlled kinetics

Abstract: It has long been appreciated that transport properties can control reaction kinetics. This effect can be characterized by the time it takes a diffusing molecule to reach a target - the first-passage time (FPT). We will present a new method of determination of the statistics of the FPT in confined geometries, and show that transport processes as various as regular diffusion, anomalous diffusion, diffusion in disordered media and in fractals fall into the same universality classes. Beyond this theoretical aspect, this result could have potential impact on standard reaction kinetics. More precisely, we argue that geometry can become a key parameter so far ignored in this context, and introduce the concept of "geometry-controlled kinetics". These findings could help understand the crucial role of spatial organization of genes in transcription kinetics, and more generally the impact of geometry on diffusion-limited reactions.

- Hugues Chaté (CEA Saclay, Paris)

Title: Alignment vs noise: simple models for collective motion.

Abstract: I will give an overview of our current understanding of models consisting in self-propelled particles aligning locally, like the celebrated Vicsek model. Particular attention will be paid to the wealth of non-trivial emergent phenomena that even such simple models generically exhibit. I will sketch how faithful continuous theories can be /derived/ from these models in a controlled manner. I will also discuss the possible relevance and limitations of such a simple setting to cell biology.

- Arnaud Chauvière (Université Joseph Fourier, Grenoble)

Title: Influence of stationary states on biological (reactive) transport

Abstract: Transport in biological systems may be of various natures (e.g., diffusive or convective) and at different scales (e.g., intracellular or multicellular levels). Models of transport in physical sciences are well established and can be used to investigate the spatiotemporal dynamic of specific biological systems. In this talk, we are interested in a particular feature, i.e. the influence of a switch between separate, mobile and stationary states, on transport dynamics. In a first part, we propose a generic mesoscopic model of "particle" (that can be seen as intracellular molecules or cells) transport as a velocity-jump process including resting phases. We derive the corresponding macroscopic formulation and show that anomalous diffusion arises from the switch between the mobile and stationary states. In particular, sub- and super-diffusion regimes can be observed and are governed by a parameter describing intrinsic mobility properties of the particles. In a second part, we present biological applications of this type of model and investigate the spatiotemporal dynamics resulting from the switch between the mobile and stationary states in two different systems: At the multicellular level, we study the spreading and growth of glioma (a very aggressive type of brain tumor) when the switch to quiescence is density-regulated, and we use a combination of numerical and analytical techniques to characterize the development of spatiotemporal instabilities and traveling wave solutions generated by our model; At the intracellular level, we describe coupled motor-cargo transport with attachment/detachment processes along microtubules within the squid giant axon and show the excellent agreement between the model predictions and the experimental data.

- Marie Doumic-Jauffret (INRIA Rocquencourt, France)

Title: Does size or age govern the bacterial growth ?

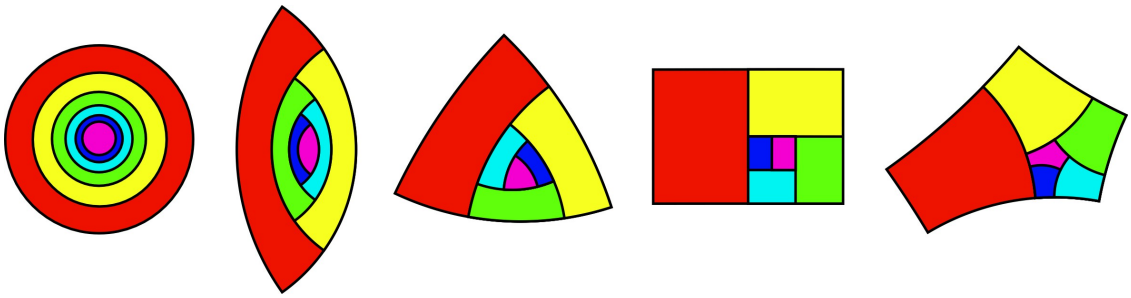
Abstract: Models describing the growth of cell populations have been developed based on assumptions on the stochastic mechanisms underlying growth and division at the single cell level. In particular, two different models have been widely used for decades, assuming that cell division probability depends respectively on cell age (the renewal equation) or cell size (the size-structured or growth-fragmentation equation) - or both. We confront these models with data on E. coli single cells growth, and develop a new estimation methodology, based on nonparametric functional testing within the PDE models, in order to test the hypothesis of an age-dependent versus size-dependent division rate. This is a common work with N. Krell, M. Hoffmann and L. Robert.

- Jacques Dumais (Universidad Adolfo Ibáñez, Chile)

Title: Mechanics and Dynamics of Plant Cell Division

Abstract: The division of eukaryotic cells involves the assembly of complex cytoskeletal structures to exert the forces required for chromosome segregation and cytokinesis. In plants, tensional forces within the cytoskeleton appear to constrain cells to divide according to a small number of area minimizing configurations. We have shown that the probability of observing a particular division configuration increases inversely with its relative area according to an exponential probability distribution known as the Gibbs measure. The distribution is universal up to experimental accuracy with a unique constant that applies for all plants studied irrespective of the shape and size of their cells. Using a maximum entropy formulation, we were able to demonstrate that the empirically derived division rule is predicted by the dynamics of the tense cytoskeletal elements controlling the positioning of the division plane. Finally, by framing this division rule as a dynamical system we

were able to identify several attractors that are predictive of characteristic cell patterns observed in plants. Plant cell division thus offers a remarkable example of how simple mechanical interactions at the subcellular level can lead to subtle behaviors at the cellular or multicellular levels.



- Sergei Fedotov (University of Manchester)

Title: Nonlinear fractional equations and subdiffusive transport in living tissue

Abstract: The standard models for the description of anomalous subdiffusive transport of particles in living tissue are linear fractional equations. The question arises as to how to extend these equations for the nonlinear case involving transport with adhesion, non-linear crowding and chemical reactions. The talk will be concerned with new nonlinear and non-Markovian random walk models developed in the recent years. We discuss the structural instability of fractional subdiffusive equations and nonlinear crowding effects. We derive the nonlinear fractional equations for the density of particles and apply these equations to the anomalous chemotaxis and morphogen gradient formation problems.

- Ray Goldstein (University of Cambridge, UK)

Title: Fluid Dynamics and Self-Organization of Cytoplasmic Streaming

Abstract: First described by Bonaventura Corti in 1774, cytoplasmic streaming, the persistent circulation of the fluid contents of large eukaryotic cells, is now known to arise from the entrainment of fluid by multitudes of molecular motors moving along filamentary tracks. Yet, its role in physiology is still rather mysterious. Is it simply a transport mechanism? Does it play a role in homeostasis? What kinds of self-organization are responsible for the observed highly regular flow geometries? In this talk I will outline recent theoretical and experimental work (both in vivo and in vitro) aimed at answering some of these questions, and suggest that there are interesting parallels to be found between phenomena involved in streaming and in the collective behaviour of motile organisms. There are as well some fascinating fluid-body interactions arising from the coupling of streaming flows to cytoskeletal filaments.

- David Holcman (ENS Paris, France)

Title: Synaptic dynamics: modeling, analysis, stochastic simulations and extraction of features from superresolution data of live cell imaging

Abstract: What defines synaptic strength at a molecular level and how can we compute the synaptic current? To answer these questions, we will present mathematical models that we have developed for estimating the current at excitatory synapse based on the properties of AMPA receptors. We accounted for various geometrical parameters of the synapse and also for receptor trafficking. We will also discuss statistical methods based on the Langevin's equation to extract

local biophysical properties of cell-particle interaction from thousands of individual trajectories. We will focus on AMPA receptor diffusion properties and the strength of their molecular interaction at the sub-diffraction level. Our analysis reveals several attracting potential wells of large sizes, showing that the high density of AMPARs is generated by physical interactions with an ensemble of cooperative membrane surface binding sites, rather than molecular crowding. This talk summarizes our long lasting effort to identify key parameters involved in the regulation of synaptic transmission and plasticity, processes that underlie learning and memory.

- Nicolas Meunier (Université René Descartes, Paris 5)

Title: Modeling Yeast Cell Polarization Induced by Pheromone Gradients

Abstract: In this work, we investigate the dynamics of a non-local model describing cell polarisation. It consists in a drift-diffusion equation set in the half-space, with the coupling involving the trace value on the boundary. We characterize the following behaviours in the one-dimensional case: solutions are global if the mass is below the critical mass and they blow-up in finite time above the critical mass. The higher-dimensional case is also discussed. The results are reminiscent of the classical Keller-Segel system in double the dimension. In addition, in the one-dimensional case we prove quantitative convergence results using relative entropy techniques. This work is complemented with a more realistic model that takes into account dynamical exchange of molecular content at the boundary. In the one-dimensional case we prove that blow-up is prevented. Furthermore, density converges towards a non trivial stationary configuration. Finally a comparison with data provided by M. Piel is performed and this gives rise to a validated model for yeast cell polarization induced by pheromone gradients.

- Alex Mogilner (UC Davis, USA)

Title: Mechanical pathways of cell polarization and motility initiation

Abstract: Animal cells crawl on flat surfaces using lamellipodium – dynamic network of actin polymers and myosin motors enveloped by the cell membrane. Steady motility of keratocytes is well understood, however, explanation of polarization and motility initiation remains elusive. I will present simulations of a 2D model of viscous contractile actin-myosin network with free boundary that, coupled with experimental data, suggests that stick-slip nonlinear adhesion is the key to understanding polarization of the keratocyte cells. On the other hand, epithelial IAR-2 cells polarize better if myosin is inhibited, and combined experiment and theory point out that competition of protruding and contracting actin network coupled with cell movement is the key to the polarization. Furthermore, we found that cells polarize very fast in electric field, with local protrusions and retractions coalescing rapidly into coherent cell front and rear. I will discuss implications of these finding for cell polarization mechanisms.

- François Nédélec (EMBL Heidelberg, Germany)

Title: Design Principles of Yeast Spindles

Abstract: Bundled cytoskeletal arrays are a universal feature of eukaryotic cells. The anaphase B spindle from fission yeast serves as an excellent model system for studying cytoskeletal arrays under compressive forces as it can be perturbed genetically, is easily visualized using electron or light microscopy and has an organization that is highly stereotyped between different cells. We have used calculations based on electron tomographic reconstructions of the spindle to show that the length and organization of microtubules within the fission yeast spindle are optimized to achieve

maximal strength while minimizing the use of material. A combination of simulations and live cell imaging further indicate that the properties of the microtubule cross-linkers are likely to be responsible for such a precise regulation of spindle morphology in fission yeast.

- Jay Newby (University of Oxford, UK)

Title: Uniform asymptotic approximation of diffusion to a small target

Abstract: The problem of the time required for a diffusing molecule within a large bounded domain to first locate a small target is prevalent in biological modeling. I consider this problem for a small spherical target. Uniform in time asymptotic expansions in the target radius of the solution to the corresponding diffusion equation is developed. Our approach is based on combining short-time expansions using pseudo-potential approximations with long-time expansions based on first eigenvalue and eigenfunction approximations. These expansions allow the calculation of corresponding expansions of the first passage time density for the diffusing molecule to find the target.

- Christian Schmeiser (University of Vienna, Austria)

Title: Stochastic filament based simulations vs. deterministic continuum models of lamellipodia

Abstract: A large number of cell types uses actin filament treadmilling as its main motility mechanism. This involves a complex protein machinery performing tasks like polymerization, depolymerization, tethering, branching, capping, cross-linking, contraction, and adhesion. In a description based on individual filaments, these effects can be described and simulated as stochastic processes. There is also strong evidence of significant influences of the cell membrane. A simulation approach will be presented, where the filament dynamics is coupled with an obstacle problem for the membrane. The model produces flat lamellipodia in a stable way without any input concerning the desired geometry, which we consider as a significant breakthrough. These result will be contrasted by recent simulations of a continuum model of a whole cell, which can be seen as an averaged version of filament based models. The goal is a description of the morphological dynamics of cells in connection with polarization and motility.

- Claude Verdier (Université Joseph Fourier, Grenoble)

Title: Time-dependent Cell traction forces as a measure of cell invasiveness

Abstract: Results on cancer cell migration are presented in the context of cell traction force microscopy (TFM). Different cells with various invasiveness are shown to present different migration modes on soft Polyacrylamide gels. Cell tractions also exhibit differences and are compared. These measurements are made thanks to recent improvements of the TFM (Ambrosi et al., 2006, 2009, Peschetola et al., 2013) where it was shown that the adjoint method is more accurate than the classical FTTC method in 2D. The time dependence of these patterns reveals to be quite important for investigating migration. Adhesion complexes are also shown and provide additional information about migration. In the end, it is shown that less invasive cells require larger tractions as compared to more agressive ones.

Ambrosi, D. Cellular Cellular traction as an inverse problem SIAM J. Appl. Math., 2006, 66, 2049-2060,

Ambrosi, D.; Duperray, A.; Peschetola, V. & Verdier, C. Traction patterns of tumor cells J. Math.

Biol., 2009, 58, 163-181,

Peschetola, V.; Laurent, V.; Duperray, A.; Michel, R.; Ambrosi, D.; Preziosi, L. & Verdier, C. Time dependent traction force microscopy for cancer cells as a measure of invasiveness Cytoskeleton, 2013, in press.

Abstracts of the short lectures

✗ Assaf Amitai (ENS Paris, France)

Title: The Mean Encounter Time between two polymer sites – Application to DNA looping and modeling the encounter of DNA breaks in the nucleus.

Abstract: The encounter between sites on chromosomes in the cell nucleus can trigger gene regulation, the exchange of genetic material and the repair of DNA breaks. By forming a DNA loop, a protein located on the DNA can trigger the expression of a gene located far along the chain. We computed asymptotically and using Brownian simulations the mean time between two polymeric sites to meet using the classical Rouse polymer model, in which the polymer is described as a collection of bead monomers connected by harmonic springs. When two monomers come closer than a distance epsilon, the search process ends. The novel asymptotic relies on the expansion of the spectrum of the Fokker-Planck operator as a function of epsilon. The key of the asymptotic is the explicit computation of the Riemannian volumes for Chavel-Feldmann formula which gives the shift in the spectrum of the Laplacian operator with Dirichlet boundary condition on a compact manifold, when a submanifold of small volume has been removed. We have shown that the encounter time is Poissonian (due to the small target) and obtained an asymptotic expression of the mean first encounter time as function of the polymer length and epsilon. When the polymer is a DNA diffusing in the confinement nucleus, we further investigated the encounter process which defines one of the characteristic times for the double stranded DNA break repair process.

References:

1. A. Amitai, I. Kupka and D. Holcman, Computation of the Mean First-Encounter Time between the Ends of a Polymer Chain, Phys. Rev. Lett. 109, 108302 (2012).
2. A. Amitai, I. Kupka and D. Holcman, Analysis of the Mean First Looping Time of a Rod-Polymer, Multiscale Model. Simul. 10, 612 (2012).
3. A. Amitai, C. Amoruso, A. Ziskind and D. Holcman, Encounter dynamics of a small target by a polymer diffusing in a confined domain. J. Chem. Phys. 137, 244906 (2012).

✗ Steven Falconer (University of Manchester, UK)

Title: Morphogen gradient formation, under subdiffusion

Abstract: Subdiffusion happens when the mean squared displacement grows sublinearly with time. The study of morphogen gradient formation under subdiffusion requires the use of fractional derivatives. The standard equation used to model this, the fractional Fokker-Planck equation (FFPE), is not structurally stable and therefore its modification is needed. It is essential to consider the degradation of morphogens. In this talk, I will begin with an introduction to morphogen gradient formation under subdiffusion. I will then talk about the problem with the FFPE, and the modification we have proposed. To finish, I will briefly talk about how this can be extended to a non-linear case, which allows for crowding effects etc to be taken into account.

✗ Mark Flegg (University of Oxford, UK)

Title: Matching stochastic reaction-diffusion simulations of different scales.

Abstract: Simulation of spatial-dependent chemical kinetics in biology can often involve small copy numbers of chemical species rendering traditional deterministic approaches such as ODEs and PDEs inappropriate. Stochastic simulation techniques are usually defined by whether or not the simulation is performed on a lattice. On-lattice simulation techniques involve molecular jumping between nodes where reactions may take place while off-lattice simulation involves molecular diffusion to occur in continuous space and reactions are based on molecular proximity. In this talk, we will discuss methods for combining stochastic simulation techniques with each other and with the PDE reaction-diffusion equation via an interface separating domains to be described using different scales.

✗ Pierre Gabriel (University of Versailles, France)

Title: Modeling the aggregation of misfolded proteins

Abstract: The aggregation of misfolded proteins is responsible of several neurodegenerative diseases as Creutzfeldt-Jakob, Alzheimer, Parkinson, but is also involved in the aging of E. Coli bacteria as shown by recent studies. The aim of this talk is to present partial differential equations models for these aggregation processes. The polymerization-fragmentation equation is widely used in the context of neurodegenerative diseases. Using entropy methods, we show in both a linear and nonlinear framework that the solutions of this equation converge to a steady-state distribution. Then we build a spatial model based on the Smoluchowski coagulation equation in order to investigate the influence of the heterogeneity of the intracellular medium on the protein aggregation. It is observed experimentally that the large aggregates appear preferentially in the less crowded zones of the cells. The numerical simulations of our model allow to recover and explain this phenomenon which is a key point in the aging of E. Coli.

✗ Francesco Ginelli (University of Aberdeen, UK)

Title: Collective motion with topological interactions

Abstract: Voronoi tessellation has been recently proposed as a modeling tool for cell tissue dynamics, with interactions between cells taking place at the cell contact borders. This implies that interactions, while being local, have a topological nature rather then a metric one. Based on recent experimental evidence, topological, metric-free interactions have also been found to play a role in the collective dynamics of social vertebrates as bird flocks, fish schools and human crowds. In this talk we discuss the features exibited by simple models for collective motion when inter-particles interactions are based on Voronoi tessellation rather then on metric cut-off as in earlier literature.

✗ Thibault Lagache (ENS Paris, France)

Title: Modeling the endosomal escape of viruses

Abstract: Widely disparate viruses enter the host cell through an endocytic pathway and travel the cytoplasm inside an endosome. In order for the viral genetic material to be delivered into the cytoplasm, these viruses have to escape the endosomal compartment, an event triggered by the conformational changes of viral endosomolytic proteins. We focus here on small non-enveloped viruses such as adeno-associated viruses (AAV), that contain few penetration proteins. The first

time a penetration protein changes conformation defines the slowest time scale responsible for the escape. To evaluate this time, we construct a biophysical model based on a stochastic approach, that accounts for the small number of proteins, the endosomal maturation and the protease activation dynamics. We show that the escape time increases with the endosomal size, while decreasing with the number of viral particles inside the endosome. Finally, we compute the probability that viruses escape when the number of proteases in the endosome is in the optimal range of 250-350, and predict that this probability is maximal (~60%) for three viral particles, demonstrating a possible positive cooperation between enclosed viruses.

✗ Emanuele Leoncini (INRIA Rocquencourt, France)

Title: Stochastic Gene Expression in Prokaryotes: A Point Process Approach

Abstract: The protein production, also referred to as gene expression, is a fundamental process within prokaryotic and eukaryotic cells and has been studied over decades by biologists. Experiments have given direct proof of the stochastic nature of the gene expression. As a consequence, the concentration of a given protein shows stochastic fluctuations, which may be costly given that the whole protein production process consumes 80% of the resources of a prokaryotic cell.

In order to anayse the fluctuations of the number of copies of a specific protein, we present a new modeling approach of the gene expression based on marked Poisson point processes. We investigate a generalized version of some classic Markovian models, which gives analytic close formulas of mean and variance of the main. The main assumption of the classic models is that each step of the production process have an exponentially distributed duration. Nevertheless, it is well-known that some steps of the gene expression, such as the protein elongation, are not exponentially distributed, showing an almost deterministic duration.

Our results show in particular that the exponential assumption may, surprisingly, underestimate significantly the variance of the number of proteins when some steps are not exponentially distributed with smaller fluctuations than an exponential random variable. This counter-intuitive result stresses the importance of the statistical assumptions in the protein production process.
Joint work with: Vincent Fromion (MIG team - INRA - vincent.fromion@jouy.inra.fr) and Philippe Robert (RAP team - INRIA - philippe.robert@inria.fr).

✗ Vuk Milisic (University Paris 13, France)

Title: On the asymptotic regime of a model framework for friction mediated by transient elastic linkages

Abstract: In this presentation we will briefly introduce motility due to actin filaments in the lamellipodia of living cells. We present its mathematical modelling and specify issues that the model can deal with [Oelz, et al, 2008]. We will then insist more on the transient elastic linkages from the cell to the substrate. We present a system of an integral equation of Volterra type coupled to an original renewal equation. The integral equation describes the trajectory of a binding site which is connected via transiently remodelling linkages to the substrate and which evolves driven by a given force. The renewal model accounts for the remodelling process of linkages which attach and break with given probabilities. We give a framework for solutions of such a coupled system and provide a rigorous justification of the asymptotic limit of infinitesimally rapid turnover of linkages. We present a simple example and comment some preliminary numerical simulations.

Participants

A

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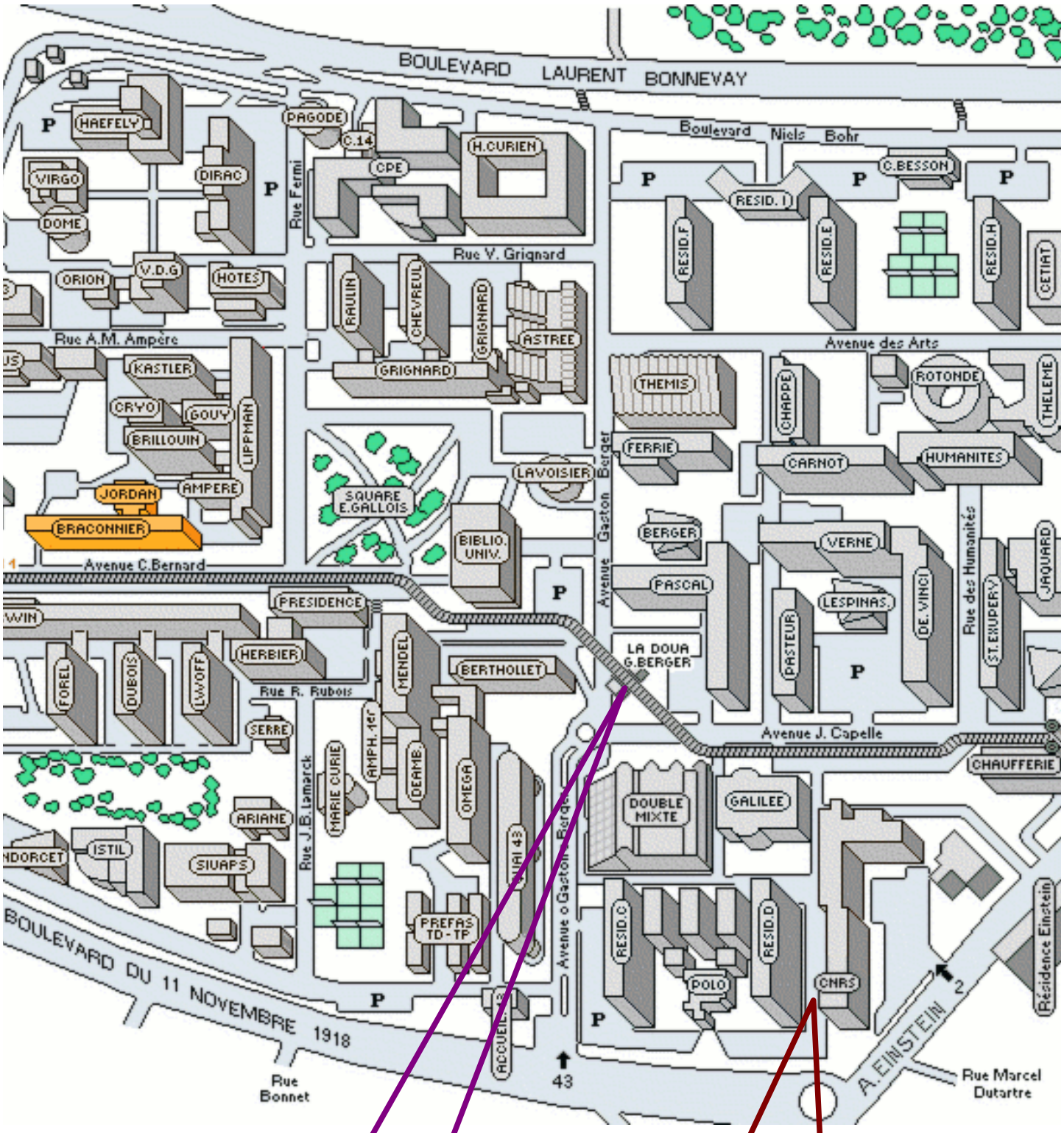
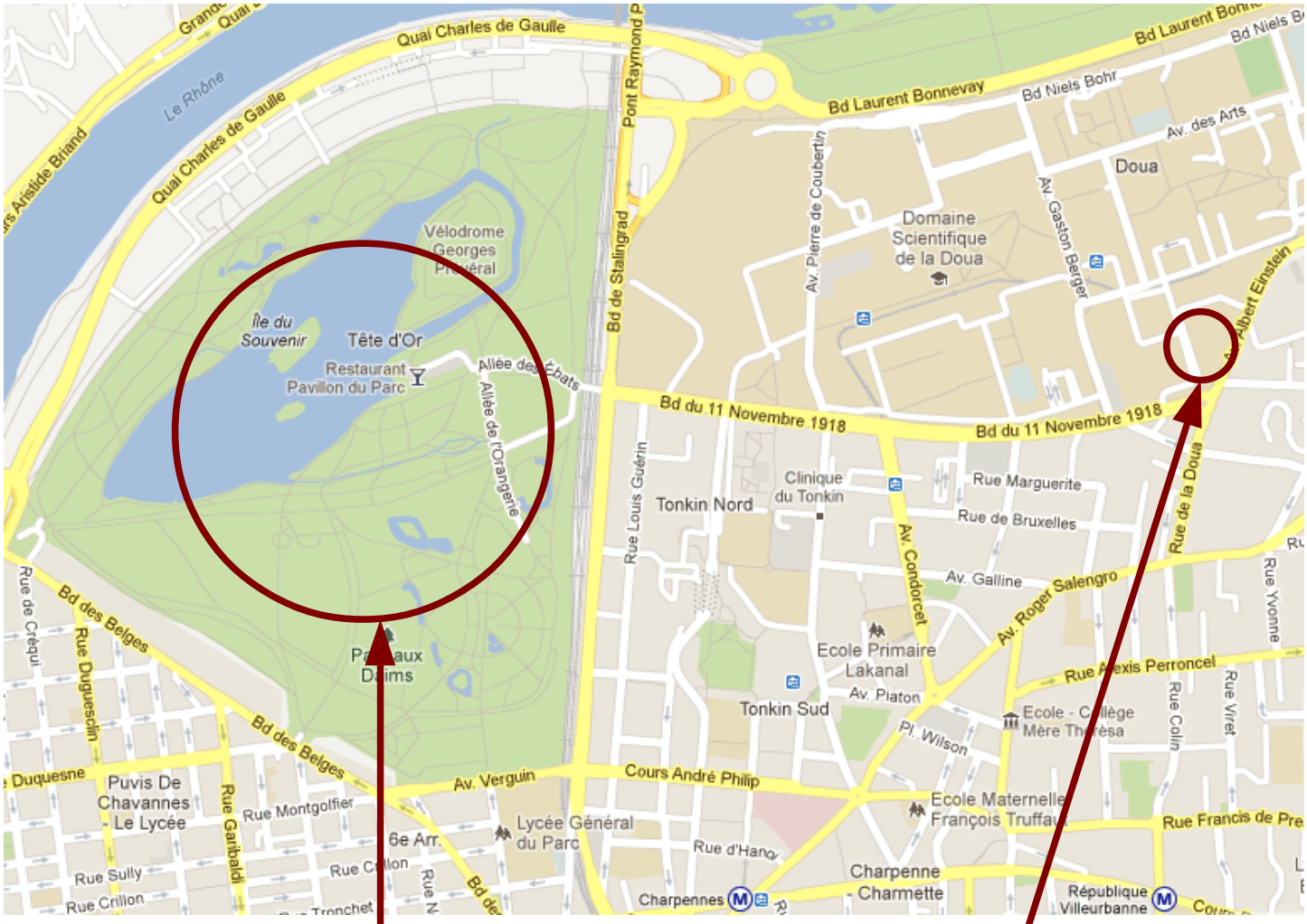
Map of the scientific campus Lyon I



Tram station T1
« La Doua
Gaston Berger »

Conference room
Amphithéatre CNRS

Map of the neighbourhood



Parc de la Tête d'Or (main park in Lyon) 10 min by walk

Conference