

Computational Statistics and Molecular Simulation

A Practical Cross-Fertilization

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Aim and organization of the week

- **Trying to mix two communities...**
 - who have been discussing a lot in the past (Metropolis)
 - discussed less in the recent times... (HMC, MALA)
 - nowadays discussing more again (PDMPs)
- **How to get to know each other?**
 - “hands-on” sessions → pedagogical presentation of an actual problem & **open discussion** [what would you have done in that situation?]
 - short presentations
 - **time to talk!**

Who are the people in the room?! (tentative classification)

- (Rather) statistical physics
 - Andrea Agazzi (Duke University)
 - Josh Fass (Memorial Sloan Kettering Cancer Center)
 - Carsten Hartmann (BTU Cottbus-Senftenberg)
 - Alessandra Iacobucci (Universite Paris Dauphine)
 - Tony Lelièvre (Ecole des Ponts)
 - Jianfeng Lu (Duke University)
 - Anton Martinsson (University of Edinburgh)
 - Luc Rey-Bellet (University of Massachusetts)
 - David Sanders (Universidad Nacional Autonoma de Mexico)
 - Chus Sanz-Serna (Universidad Carlos III de Madrid)
 - Gabriel Stoltz (Ecole des Ponts)
 - Eric Vanden-Eijnden (Courant Institute)
 - Arthur Voter (Los Alamos National Laboratory)
 - Jonathan Weare (Courant Institute)
- In-between
 - Miranda Holmes-Cerfon (Courant Institute)
 - Jonathan Mattingly (Duke University)

Who are the people in the room?! (tentative classification)

- (Rather) statistics side
 - Christophe Andrieu (University of Bristol)
 - Igor Barahona (Universidad Nacional Autonoma de Mexico)
 - Angela Bitto-Nemling (WU Vienna University of Economics and Business)
 - Yang Chen (University of Michigan)
 - Alain Durmus (ENS Cachan)
 - Gersende Fort (Université de Toulouse & CNRS)
 - Jeremy Heng (Harvard University)
 - Florian Maire (Universite de Montreal)
 - Gael Martin (Monash University)
 - Kerrie Mengersen (Queensland University of Technology)
 - Matt Moores (University of Wollongong)
 - Marcelo Pereyra (Herriott Watt)
 - Murray Pollock (University of Warwick)
 - Sam Power (University of Cambridge)
 - Christian Robert (Universite Paris Dauphine)
 - Gareth Roberts (University of Warwick)
 - Scott Schmidler (Duke University) ???

Some burning questions for the week

- Variance reduction for rare events beyond the large deviations regime
- Design and analysis of Markov Chain Monte Carlo in high dimension
- Same question when the target distribution has heavy tails
- Quantify systematic uncertainty in predictions from MD?
- Sampling metastable dynamics/rare events/multimodal distributions
- Statistical coarse-graining techniques: Generative Adversarial Networks, clustering, diffusion maps, auto-encoders, etc...
- Variance reduction/convergence of non-reversible MCMC algorithms
- Temperature control (tempering, thermostats, etc.) in sampling
- Variance reduction when invariant measure unknown (nonequilibrium)
- Sampling measures concentrated near lower-dimensional manifold
- Proper sampling of trajectories linking metastable states without prior knowledge of these states?
- Can MC methods be useful for deterministic dynamical systems?
- Can methods from interval analysis offer any useful tools in computational statistics / statistical physics?

A few organizational points

- There is wifi! “CMO” + password cmo_oaxaca
- Send your slides to Miguel Altamirano: maltamirano@im.unam.mx
- Excursions:
 - Monte Alban (archeological site with great views)
 - Mitla (archeological site) + Mezcal factory, wool weavers of Teotitlan, ...

Payment by cash only (320 Mexican Pesos). At least 11 persons for excursion to take place.