Group D: Big Data & AI

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UQ and Numerical Methods in Kinetic Theory

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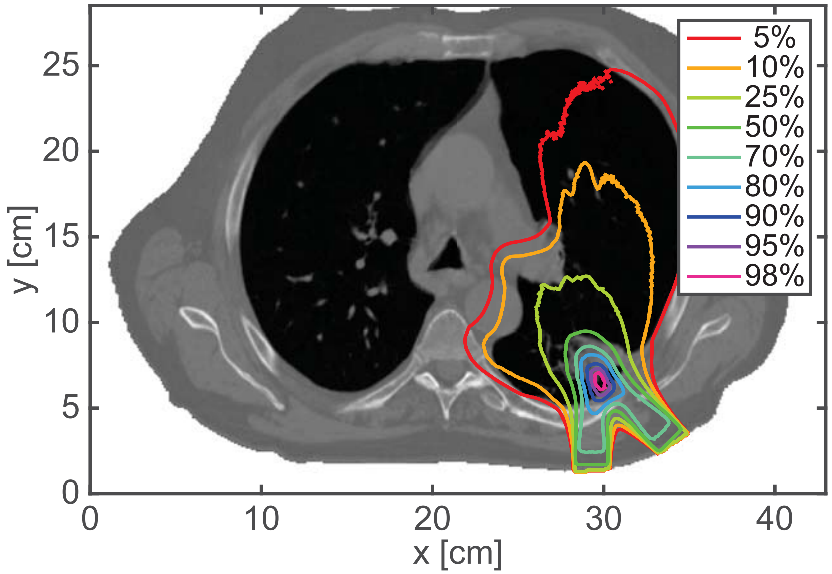
Karlsruhe Institute of Technology

What we are doing...

1. Design numerical schemes for solving PDEs
2. Application in radiotherapy
3. Quantification of uncertainties



Dose distribution by K. Küpper

Challenges we are facing...

Designing numerical schemes:

1. ”optimal” parameters are often hard to find by theory
2. which methods works best in which cases?

UQ:

1. single simulation is already costly
2. therefore hard to measure sensitivities of outputs w.r.t inputs
3. too much data to deduce (or even quantify) dependencies

How Big Data & ML might help...

Designing numerical schemes:

1. run experiments with different parameters and label outputs
2. use this data to train ML algorithms to make predictions
3. only feasible with high performance machines

UQ:

1. cluster medical data and reduce dimensionality
2. train with given experimental / simulation data
3. triggering dependencies without running full simulations

Simulation of Implanted Muons in high-Tc Superconductor System, $YBa_2Cu_3O_6$

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$YBa_2Cu_3O_6$

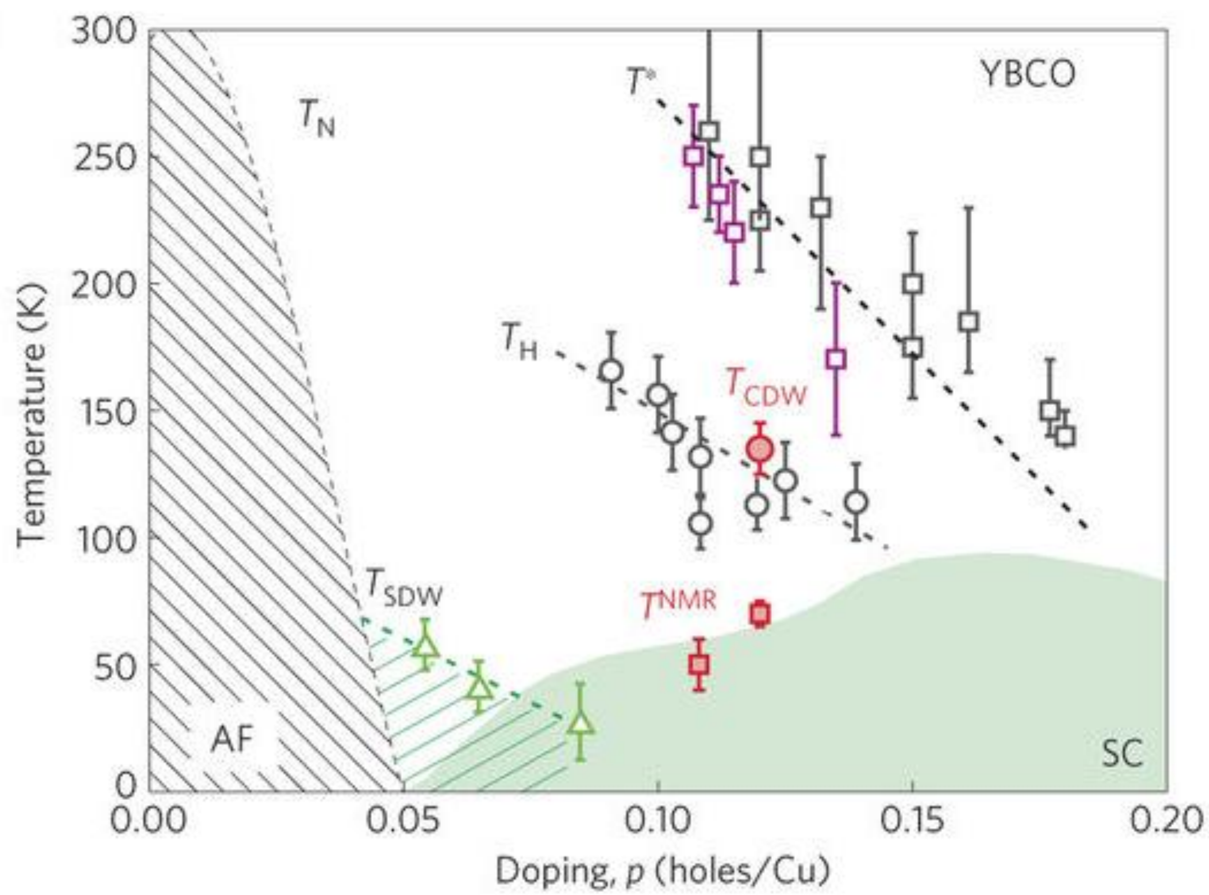
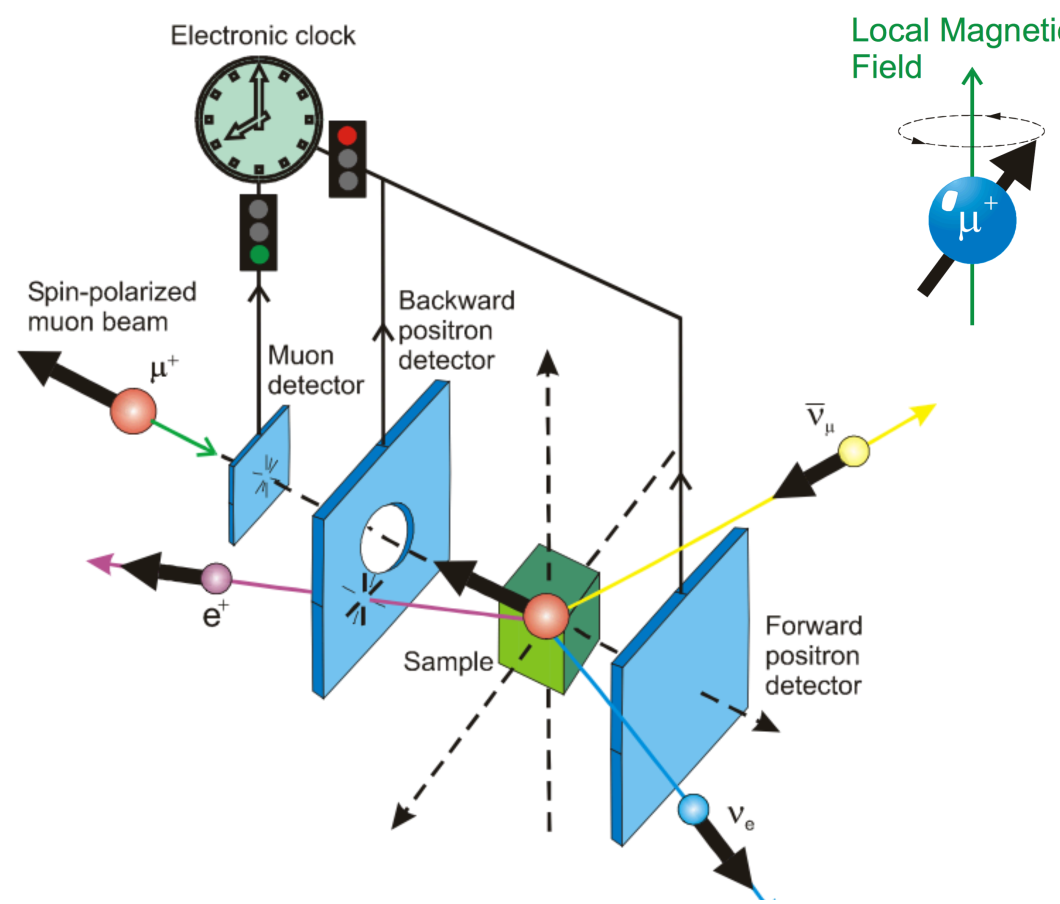


Figure 1. Phase diagram of YBCO6+x
(Chang et al., Nat. Physics, 8, 2012)

Superconductivity
⇕
Magnetism
(Spin fluctuation)



- Antiferomagnetic Mott insulator at x=0
- Magnetic ordering is disappear with emergence of superconductivity.
- SDW coexistence with SC

Probe the microscopic magnetism by μSR technique

Our Work

- Magnetic order parameter ==> Muon stop position
- Try solve that problem by using computing approach
- Supercell calculation to simulate muon behavior in the system (~ 384 atom, 3200 electron and more), high performance computing plays important role.
- We need tons of calculation and analysis amount big data in different doping concentration (x) and parameters to propose an explanation of high-Tc superconductivity mechanism that driven by spin fluctuation

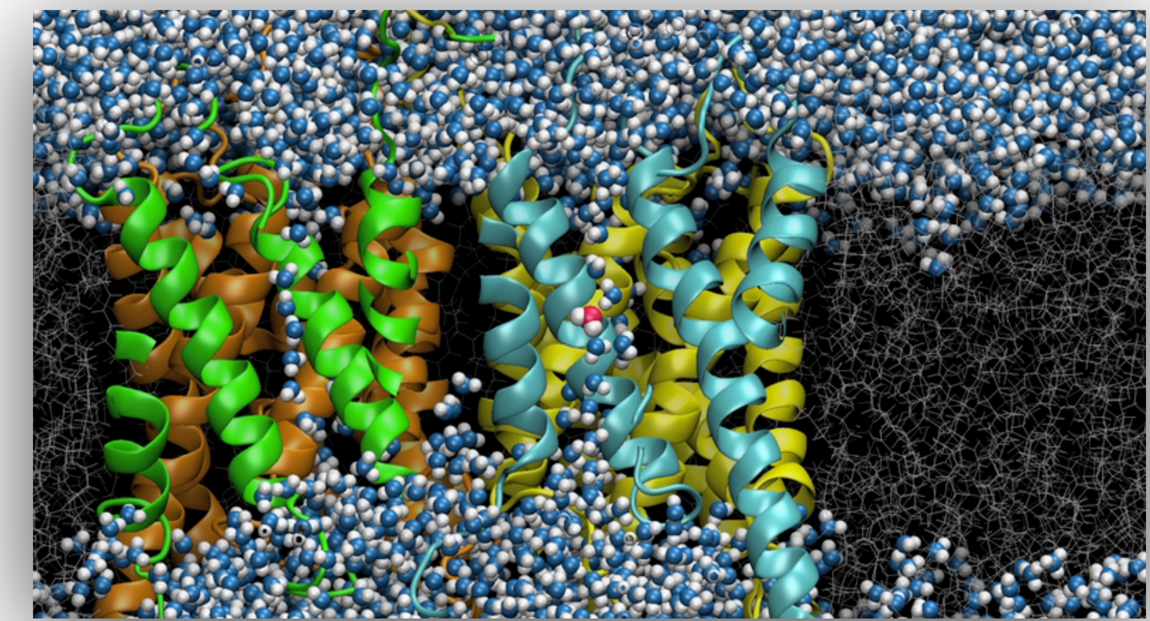
All-atom molecular dynamics

Reproduce the dynamics of a system by using atomic model

Newton's equation of motion

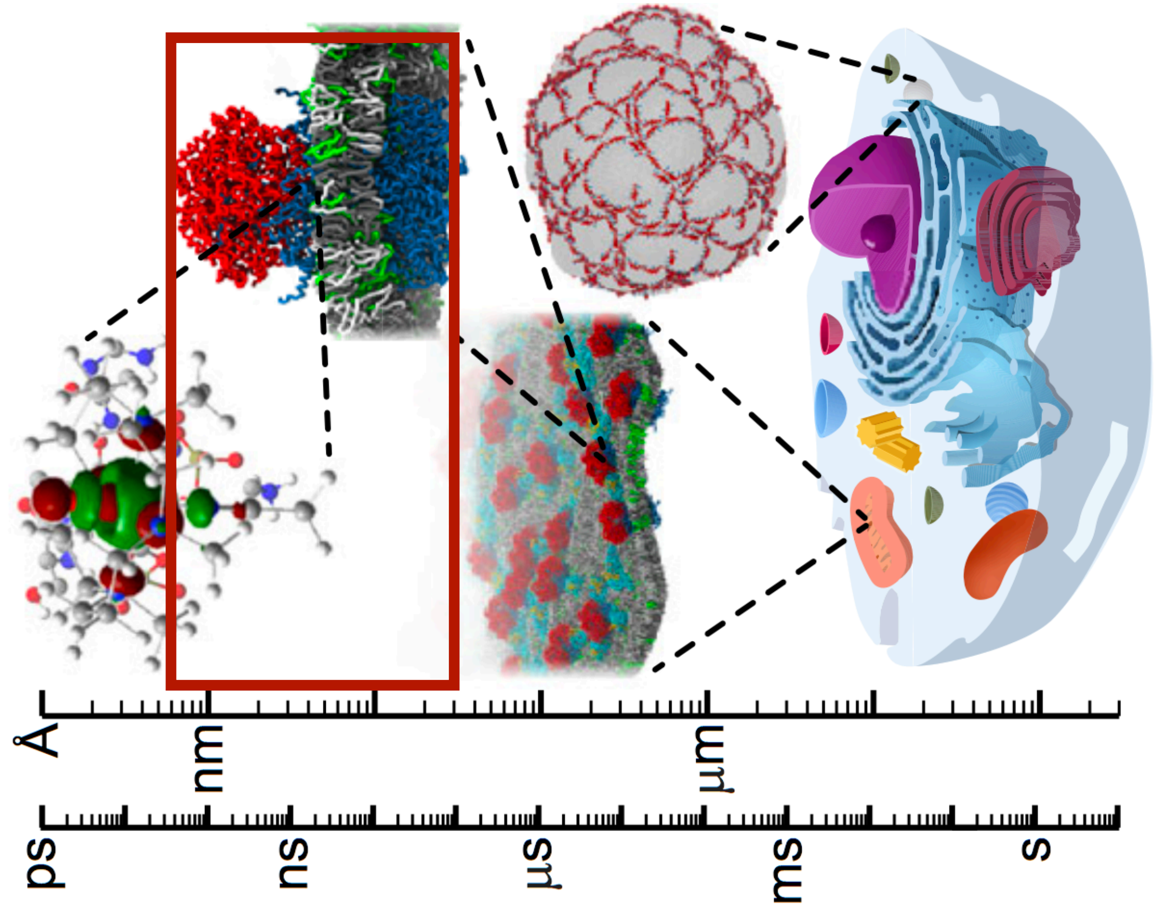
$$m\frac{d^2\boldsymbol{r}}{dt^2} = \boldsymbol{F}$$

Water in aquaporin



[2]

This make it possible to analyse a phenomenon in a atomic scale



[1]

Calculation cost is high

[1] H. I. Ingólfsson, C. Arnarez, X. Periole and S. J. Marrink, *J. Cell. Sci.* **129**, 257 (2016).
[2] E. Yamamoto, T. Akimoto, Y. Hirano, M. Yasui, and K. Yasuoka, *Phys. Rev. E.* **89**, 022718 (2014).

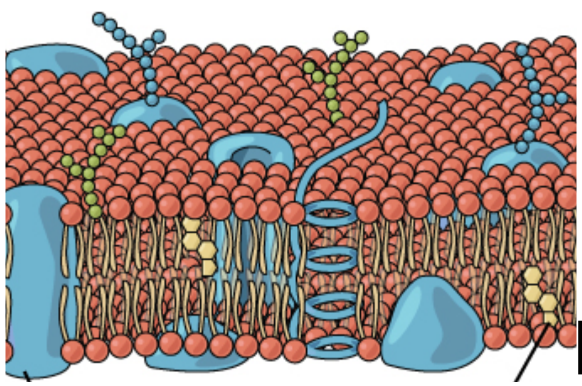
Challenge: Analysis by machine learning

Analyse the atomic data which is obtained by molecular simulation

Analysis example

Short time simulation

Predict the long-time-scale property


[3]

Motion
Fluidity
etc.

Learn

$\mathrm{ns} \sim \mu\mathrm{s}$

ms

Cut the simulation cost

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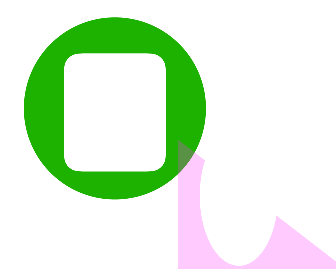
data of something

make a physical interpretation

Learn

Shape of something



Make it easier

[3] http://oerpub.github.io/epubjs-demo-book/resources/0303_Lipid_Bilayer_With_Various_Components.jpg

Uncertainty Quantification for Tsunami-drafted objects Based on Big Data

2018/02/06
RIKEN AICS HPC Youth Workshop FY2017

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1st year of Master's Program
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Introduction: Uncertainty Quantification

- In my master's program, we have tried to quantify uncertainties for objects drafted by tsunami waves.
- Tsunami waves are generated by a lot of uncertain factors such as earthquakes, volcanic eruptions, and underwater landslides[*1].

Behaviors of tsunami-drafted objects damage certain structures in an uncertain way.

A Ship Drafted by Tsunami Waves [*2]

[*1] A. Sarri, S. Guillas, and F. Dias, "Statistical emulation of a tsunami model for sensitivity analysis and uncertainty quantification", 2012.

[*2] http://www.asahi.com/special/10005/TKY201104070204.html

Uncertainty Quantification and Big Data

- Big data related to these uncertainties enables us to analyze behaviors of tsunami-drafted objects.
- Bayesian framework is one of the possible approaches to infer the behaviors based on such big data [*1].

Uncertainty quantification has a strong potential to mitigate damage caused by tsunami-drafted objects.

[*1] A. Sarri, S. Guillas, and F. Dias,
"Statistical emulation of a tsunami model for sensitivity analysis and uncertainty quantification", 2012.

How Big data and Deep learning may replace traditional compilers in HPC

Ksander EJJAAOUANI - 2nd year PhD student – Inria & Maison de la Simulation (CEA)

Thesis director	Michel MEHRENBERGER	Senior lecturer at University of Strasbourg / IRMA researcher
Thesis supervisor	Julien BIGOT	CEA researcher
Co-supervisor	Olivier AUMAGE	Inria researcher
Collaborator	Katharina Kormann	IPP researcher

06/02/18

My motivation

- Lot of approaches exists to write efficient code:
  - DSLs,
  - Runtimes,
  - Libraries, …
- Although they are great, they have flaws:
  - Rely on compiler (may not take the best choices)
  - Imply overheads
  - Ask for lot of information
  - ...

Current work

1. Improve collaboration between domain scientists & optimization specialists
   - Through a DSL specifying the application's semantics

2. Assists optimization specialists in the simulation code optimization processing
   - Using the semantics and source-to-source compiler
     - Asking for information not specified in the semantics
   - Nothing automatic
     - You know what you want to do, I help you achieve this goal

➢ But what if I could guess this information ?

Current work to infinity...

- I would know:
  - what to do (semantics)
  - how to do it (optimization choices)
  - parameters to do it efficiently
- It would ease optimization specialists job
  - Thus increase productivity
- How can I find these parameters ? Big data !
  - F(semantics, choices) = Parameters

...and beyond !

- But data may not be enough
  - We have to analyze it
  - Could make mistakes
- Let’s use Deep learning for that
  - Find correlation impossible to make for us
- Next level
  - Compilers can’t make next to optimal choices in every situation
  - Deep learning may achieve that:
    - Give it what you want to do (semantics)
    - And it will generate how it should be done for efficiency