Doctoral School Lectures Series 2014

Non-equilibrium thermodynamics: from theory to practice in chemistry, physics and biology

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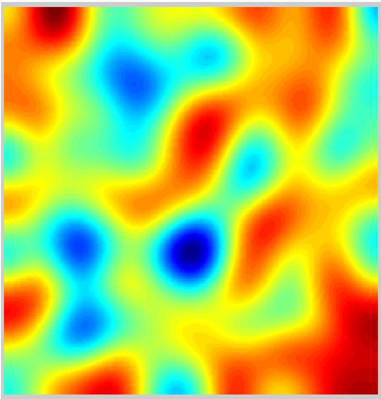

Most of the systems found in the Universe are not in thermodynamic equilibrium, thus they are changing or can be triggered to change over time, and are continuously and discontinuously subject to flux of matter and energy to and from other systems. Systems not in thermodynamic equilibrium offer a large diversity of intriguing behaviors, such as the self-organization processes arising from "disorder" systems, and the autocatalytic reactions in biological systems. Non-equilibrium thermodynamics is a modern scientific theory which aims to describe systems that are not in thermodynamic equilibrium. Even if still under development, this theory already offers a very powerful tool for the understanding of the dynamic physicochemical mechanisms and processes in a large diversity of application domains in Chemistry, Physics and Biology.

This multidisciplinary Doctoral School module introduces the fascinating Non-Equilibrium Thermodynamics Theory and aims to teach the PhD students on how to use it in their day-by-day scientific work to describe, analyze, understand and predict physicochemical mechanisms and processes. Within a highly interactive and comprehensive approach, the lectures aim stimulating the students to think "out of the box" and to develop their creativity within a transversal view of sciences.

The tentative program is detailed below:

- **Lecture 1 (inaugural lecture, 2 h)**: Non-equilibrium thermodynamics as a Theory of "Everything"
  - Non-equilibrium thermodynamics: pillars, concepts and formalism :
    - 1st Pillar: Uncertainty as an intrinsic property of the Universe
    - 2nd Pillar: The concept of Energy
    - 3rd Pillar: Time: concept or reality?
    - 4th Pillar: Entropy, from order to disorder, from disorder to order…
  - Non-equilibrium thermodynamics as an extension of equilibrium thermodynamics
  - Postulates
  - Linear non-equilibrium thermodynamics: mathematical formulations, Osanger's relations
  - Thermodynamic efforts and fluxes
  - Application examples
  - What is the Entropy of the Universe?

- **Lecture 2 (2 h)**: Chaos, the Geometry of the Universe and non-linear non-equilibrium thermodynamics
  - Onsager's regression hypothesis
  - Maxwell's relations
  - Energy conservation and dissipation
  - Entropy production general properties
  - Stability of steady states

- Lyapunov exponents
- Non-linear dynamic systems: random vs. deterministic chaos
- The “Geometry” of the Universe
- Fractals
- Poincaré Maps, Hénon Maps and more
- Phase space diagrams, dissipative structures, attractors
- Chaos in physics, chemistry and biology: examples
- Non-linear non-equilibrium thermodynamics: introduction and application examples
- Non-conservative forces
- *Presentation of the students' dissertations rules: “How Entropy can become my friend?” (dissertations will take place in Lecture 10)*

- **Lecture 3 (2 h)**: the origin of life and the biological systems from the non-equilibrium thermodynamics viewpoint
    - Bifurcations
    - Ergodic theory
    - Horeshoe maps
    - Open theoretical challenges and ongoing efforts in the development of the non-linear non-equilibrium thermodynamics, curiosities
    - Self-organization in chemistry
    - Chemical clocks: theory
    - *Chemical clocks: practice (modeling and numerical simulation)*
    - Turing's structures
    - Propagation waves: reaction-diffusion systems
    - The origin of life
    - Autocatalytic reactions and chirality in biological systems
    - Morphogenesis
    - Non-equilibrium thermodynamics and the Darwin's evolution theory, mutations
    - Sociology and entropy
    - Cooperation vs. competition
    - Game theory and its implication in biology, the human society and ecology
    - Bifurcation vs. catastrophe theories

- **Lecture 4 (2 h)**: Fluids within the framework of non-equilibrium thermodynamics
    - Symmetry vs. asymmetry
    - Statistical Mechanics and its connection with non-equilibrium thermodynamics
    - Self-organization in physics
    - Fluids in Earth, fluids in other planets…
    - Mixing
    - Polymer solutions: multiscale structures
    - Fluid/fluid interfaces
    - Non-Newtonian fluids
    - Micro-fluidics
    - Traffic forecasting and other applications in the human day-by-day life
    - Phase changes: theory
    - Phase field modeling
    - *Phase changes: practice (modeling and numerical simulation)*
    - Weather prediction

- **Lecture 5 (2 h)**: The application of non-equilibrium thermodynamics to the Electrochemical Science
  - The fascinating history of the Electrochemistry Science
  - Electrochemistry in biological systems
  - Quantum-electrochemistry
  - Inconsistencies within the classical electrochemistry usage vs. the non-equilibrium thermodynamics theory
  - Electrochemical affinity and kinetic rates
  - Multi-step chemical and electrochemical reactions, autocatalytic and self-oscillating (electro-) chemical reactions, electrochemical interfaces
  - Reaction-transport systems in electrochemistry: theory
  - *Reaction-transport systems in electrochemistry: demonstration with the LRCS simulation package "MS LIBER-T"*
  - Electrodeposition, fractal crystals growth
  - Magneto-electrochemistry
  - Chaos in electrochemistry

- **Lecture 6 (2 h)**: Complexity and thermodynamic networks
  - Complexity vs. simplicity
  - Tellegen's theorem
  - Negative resistances and inductances: physical meaning?
  - Causality and the time arrows
  - Thermodynamic networks within the 1st order Non-Equilibrium Thermodynamics perspective
  - Thermodynamic networks within higher order Non-Equilibrium Thermodynamics
  - Graphs theory
  - The theory of languages and the Bond Graphs
  - Bond Graphs: application examples
  - The Biosphere within the framework of network thermodynamics
  - *Students' challenge: "Find your Bond Graph!" (game exercise)*
  - Fluctuations and mean field approximations: validity
  - Multiscale modeling through mean field approaches
  - On-the-fly coupling between atomistic with continuum modeling paradigms: possible or impossible?
  - An existential question…

- **Lecture 7 (2 h)**: Non-equilibrium thermodynamics in electro-magnetism and mechanics
  - Classical mechanics and electro-magnetic theory revisited
  - Impossible machines (perpetual motion)
  - Is the Universe in perpetual motion?
  - Granular media theories
  - Chaotic scattering
  - Self-oscillation and chaos in mechanical and electro-magnetic systems
  - The celestial mechanics: galaxies mechanics
  - Black holes and entropy
  - Chaos synchronisation
  - Control of chaos
  - *Non-equilibrium thermodynamics formulation and numerical simulations of cases of interest for the students PhD research topics (practice).*

- **Lecture 8 (2 h)**: Non-equilibrium thermodynamics as an interpretation tool of the History dynamics, quantum chaos
    - o Markovian vs. non-markovian processes
    - o Diverging degrees of freedom and spatiotemporal chaos
    - o Lindy effect
    - o Cliodynamics (or History dynamics)
    - o Economics and network thermodynamics
    - o Information theory revisited
    - o Neural networks
    - o Non-equilibrium thermodynamics and informatics
    - o Non-equilibrium thermodynamics vs. general and special theories of relativity
    - o Non-equilibrium thermodynamics vs. quantum mechanics
    - o Quantum chaos as another view of deterministic chaos

- **Lecture 9 (2 h)**: Key concepts revisited and something more…
    - o Non-equilibrium thermodynamics: key concepts revisited
    - o *Chaotic lottery wheel: game…*
    - o What Prof. Franco did not tell you yet…(sshh ! that's a secret…)

- **Lecture 10 (2 h)**: Student's dissertations: "How Entropy can become my friend?"
    - o Student's dissertations
    - o Prizes and surprise…
    - o Concluding remarks by Prof. Franco

Audience: this Doctoral School module is devoted to PhD students on Chemistry, Physics and Biology. The module is highly interactive, enriched with epistemological concepts and designed in a fully comprehensive/understandable way by both theorists and experimenters. PhD students on Mathematics and Informatics are also very welcome. Some basic skills on classical thermodynamic concepts are required. Skills on modeling and numerical simulation are not necessary.
As the audience is expected to be diverse, two levels of learning are possible all along these lectures: 1) "starter" (any or few mathematics), 2) "deep" (some mathematics). Appropriate references for each learning level are provided all along the lectures.

- **Note 1:** presentation materials will be provided prior or after each lecture, by email, or in some cases, through **www.modeling-electrochemistry.com**.
- **Note 2:** scientific computational software will be provided to the students during the corresponding lecture.

➔ **ONLINE QUIZZES (approx. 1 every 2 lectures) :**
- ❑ Quiz announced via email after Lecture N and to be done before Lecture N+1.
- ❑ Quizzes in www.modeling-electrochemistry.com
- ❑ Do not consult internet or other bibliography when replying ! The goal is checking that you understand what is presented in the lectures.
- ❑ Not noted, just for advice. Your answers will be appreciated!
- ❑ Correct answers will be provided and commented in

Lecture N+1.

Duration of the lectures-series: 20 hours.

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