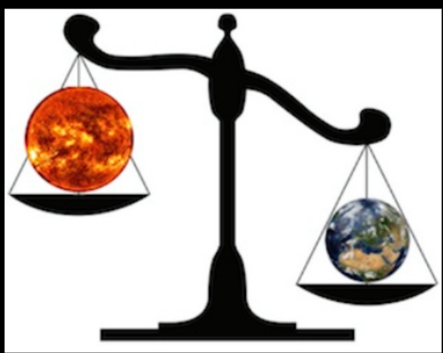
Exoplanetary Atmospheres and Habitability

Thermodynamics, Disequilibrium and Evolution focus group



Abstract book

12 - 16 Octobre 2015

Observatoire Côte d'Azur, Nice

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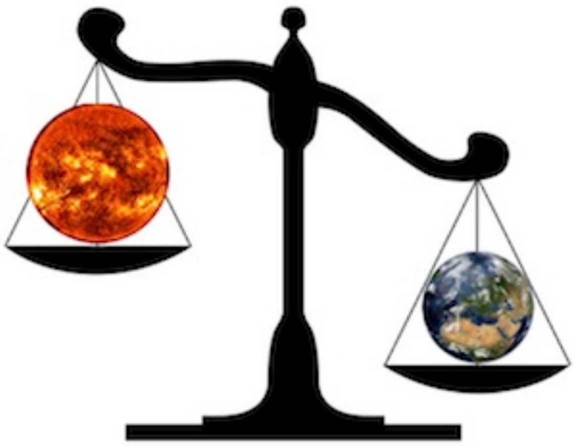

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The Thermodynamics Disequilibrium and Evolution Focus Group

E. Simoncini, L. Barge

1 Introduction

The TDE Focus Group is intended to bridge the gap between researchers working on the theory and experimental aspects of the Origin of Life and astronomers and remote sensing researchers planning future space missions and deciding on future targets for the search for extraterrestrial life. It will concentrate on the entropy and energy requirements for life and planets and how they inform our selection of potentially habitable planets and environments in the cosmos.

Granted by NAI sponsorship in late 2010, the TDE Focus Group has developed relationships worldwide, from US to Europe, from South America to Asia.

Earth displays abundant life that uses solar and chemical energy, the latter partly produced from geothermal energy. The convective mass transfer of heat driven by one or more of these forms of energy, from the very core of our planet through to the upper atmosphere, eventually conduces the interfacing of the chemical tensions appropriate to the nurturing of life. Disequilibrium on a cellular scale is made possible by the cell membrane, which maintains redox and pH gradients that are put to work by the cell. On a supra-cellular scale disequilibrium conditions are created most visibly by colony-formers such as stromatolites and corals, which are multi-cellular (often symbiotic) aggregates on a local scale. On a planetary scale, biological processes such as photosynthesis can establish and maintain disequilibrium conditions. With this understanding of the fundamental character of life (that it depends upon disequilibrium in the environment as a source of energy, that it maintains a state of disequilibrium as a condition of life, and that it can mark its existence in an environment through the presence of disequilibrium) the TDE Focus Group seeks to integrate the astrobiology community around this paradigm to inform our search for life in the universe.

2 Aims

The transdisciplinary questions to be addressed include: *Under what energetic conditions does life start? What are the thermodynamic requirements of its processes? In which environments is it likely to exist? How might we find it?*

To achieve these objectives, the TDE Focus Group integrates its members and facilitates discussion by:

- Creating an e-mail distribution list;
- Distributing a periodic TDE e-Newsletter;
- Holding monthly telecons/videocons utilizing the IT Collaborative tools of NAI Central;

- Developing a series of workshops (1 - 2 per year);
- Organizing focused scientific sessions concerning the objectives of the focus group at larger conferences such as the AbSciCon, the AAS, and the AGU

3 Activities

2015

The next TDE workshop will be held in the Observation Côte d' Azur, Nice, France, from October 12 – 18, with the name: "Exoplanetary atmospheres and habitability" [1] and in collaboration with Dr. Andrea Chiavassa.

The aim of the workshop is to discuss about chemical disequilibrium and its link to planetary habitability. In particular, the Thermodynamics, Disequilibrium and Evolution focus group seeks to understand how disequilibria are generated in geological / chemical / biological systems, and how these disequilibria can lead to emergent phenomena, such as self-organization and eventually, metabolism.

For this meeting, different points of view on planetary habitability are invited to contribute. The search for other inhabited bodies in the Solar System is nowadays focussing on Mars and, moreover, on the icy moons of Jupiter and Saturn. For the latter, it is possible to suggest a plausible emergence of pre - biotic chemistry in hydrothermal vents (mainly on Europa), as on Earth. Further, the discovery of exoplanets is shedding a light on the possibility of assessing habitability with just the analysis of few atmospheric data. Thus, atmospheric modeling is increasing its importance also in this field.

The prospects for planetary atmosphere characterization are excellent with access to large an amount of data for different kind of stars either with ground- or space-based telescopes supported by accurate modeling of the atmospheric compositions and their corresponding spectra. In particular for many discovered exoplanets (hot and gaseous), a large chemical disequilibrium in the atmosphere has been observed, due to the high vertical temperature gradient. Several new studies are now comparing this of vertical-mixing driven disequilibrium with the chemical disequilibrium characterizing the atmosphere of planet Earth, which is mainly due to the presence of life. However, present research on exoplanet's atmospheric disequilibrium is focused on a very small number of compounds (CH_4, CO, CO_2, H_2O), lacking for a generalized and wider methodology. In this workshop we plan to enlarge these studies to a joint effort between the thermodynamics of habitable

[1] http://exoatmo.sciencesconf.org

conditions to the exoplanetary atmospheres.

The workshop at the Observatory of Côte d'Azur (OCA) is the main opportunity in Europe in 2015 to discuss about the connection between planetary habitability and its atmospheric disequilibrium, through the use of some thermodynamic functions. OCA has a long tradition in the field of theoretical planetology. The research are focused on the detection and study of extra-solar planets, protoplanetary disks, and on the formation and evolution of planetary systems. This will ensure an excellent context for local exchanges.

Three principal topics will be tackled during the workshop:

- Icy moons, icy planets and the conditions for the emergence of life
- The modeling and observations of exoplanetary atmospheres: chemistry and physics
- The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets

2014

8^{th} Meeting of the NASA Astrobiology Institute Thermodynamics, Disequilibrium and Evolution (TDE) Focus Group. The meeting was held on November 10 - 14, 2014 in Tokyo at the Earth-Life Science Institute (ELSI). The aim of the workshop was to discuss the conditions for early Earth conducive for the emergence of life. Specifically, geochemical disequilibria generated at seafloor interfaces on wet rocky planets, and in particular, investigating the thermodynamic and chemical phenomena that emerge from this inherent disequilibria at water-rock interfaces [2].

7^{th} International Workshop on Thermodynamics, Disequilibrium and Evolution. Dr. Douglas Galante along with the NAI TDE focus group hosted the 7th International Workshop on Thermodynamics, Disequilibrium and Evolution, on September 24 - 26, in Campinas, Brazil [3].

[2] http://www.elsi.jp/en/research/activities/workshops/2014/09/workshop2014_1110.html

[3] http://astrobiology.nasa.gov/seminars/featured-seminar-channels/conferences-and-workshops/2014/9/24/workshop-on-thermodynamics-disequilibrium-and-evolution-tde/

2013

The 5^{th} TDE Focus Group Workshop: Engines of Life: thermodynamic pathways to metabolism. The Beyond Center hosted the Physics of Living Matter workshop series in association with NAI TDE Focus Group to produce the Engines of Life: thermodynamic pathways to metabolism Workshop. The meeting had a foundational theme, focusing on the interplay of matter, energy and entropy in biological and prebiotic systems, with particular reference to the manner in which the chemical and physical conditions of the ancient environment, such as considerations of redox potentials and stoichiometry, may have constrained the possible pathways to metabolism.

The 6^{th} TDE Focus Group organized a workshop Out-of-Equilibrium Systems and Planetary Habitability on October 14th-16th, 2013. It took place at INAF-Astrophysical Observatory of Arcetri, Largo Enrico Fermi, 5, Firenze. A report of the meeting has been published by the Florence University Press in the journal “Il colle di Galileo” (Galileo’s hill): `http://www.fupress.net/index.php/cdg/article/view/14647` .

2012

The group met at the 2012 Astrobiology Science Conference. A report is available in the footnotes [4].

The 4^{th} TDE Focus Group Workshop was held in Granada, Spain, at the Andalusian Institute for Geosciences (IACT - CSIS).

2011

The Thermodynamics, Disequilibrium and Evolution Focus Group held their first organizational meeting from March 1-3, 2011 at the Centro de Astrobiologa in Madrid, Spain. A report and abstracts from the meeting are available in the footnotes [5].

The TDE Focus Group hosted a Workshop at the Osservatorio Astrofisico di Arcetri (Galileo’s House) in Florence (Italy), on September 12-14. Its main goal was to discuss the submission of the proposals discussed in the previous Workshop in Madrid to either US or European Funding Opportunities.

[4] `http://astrobiology.nasa.gov/media/txp_files/THERMODYNAMICS.docx`
[5] `http://astrobiology.nasa.gov/media/txp_files/1stWorkshop_TDE_FG_REPORT.pdf`

4 Publications

List of publications with peer-review achieved by TDE collaborations.

2015

- L. M. Barge, Y. Abedian, M. J. Russell, I. J. Doloboff, J. H. E. Cartwright, R. D. Kidd, I. Kanik. (2015) From Chemical Gardens to Fuel Cells: Generation of Electrical Potential and Current Across Self-Assembling Iron Mineral Membranes. Angewandte Chemie International Edition, 54, 28:8184-8187, DOI: 10.1002/anie.201501663.

- L. M. Barge, S. S. S. Cardoso, J. H. E. Cartwright, G. J. T. Cooper, L. Cronin, A. De Wit, I. J. Doloboff, B. Escribano, R. E. Goldstein, F. Haudin, D. E. H. Jones, A. L. Mackay, J. Maselko, J. J. Pagano, J. Pantaleone, M. J. Russell, C. I. Sainz-Daz, O. Steinbock, D. A. Stone, Y. Tanimoto, N. L. Thomas. (2015) From Chemical Gardens to Chemobrionics. Chemical Reviews, DOI: 10.1021/acs.chemrev.5b00014.

- L. M. Barge, Y. Abedian, I. J. Doloboff, J. E. Nunez, M. J. Russell, R. D. Kidd, I. Kanik. (2015) Chemical Gardens as Flow-Through Reactors Simulating Natural Hydrothermal Systems. Journal of Visualized Experiments, in press.

2014

- Russell, M. J., Barge, L. M., Bhartia, R., Bocanegra, D., Bracher, P., Branscomb, E., Kidd, R., McGlynn, S., Meier, D., Nitschke, W., Shibuya, T., Vance, S., White, L. (2014) The Drive to Life on Rocky and Icy Worlds. Astrobiology,14, 4, 308-343.

- L. M. Barge, T. P. Kee, I. J. Doloboff, J. M. P. Hampton, M. Ismail, M. Pourkashanian, J. Zeytounian, M. M. Baum, J. Moss, C.-K. Lin, R. D. Kidd, I. Kanik (2014) The Fuel Cell Model of Abiogenesis: A New Approach to Origin-of-Life Simulations. Astrobiology, 14(3):254-70.

- Barge, L. M., Doloboff, I. J., Russell, M. J., VanderVelde, D., White, L. M., Stucky, G. D., Baum, M. M., Zeytounian, J., Kidd, R., Kanik, I. (2014) Pyrophosphate Synthesis in Iron Mineral Films and Membranes Simulating Prebiotic Submarine Hydrothermal Systems. Geochimica Cosmochimica Acta, 128, 1-12.

- Cardoso SSS, Cartwright JHE. (2014) Dynamics of osmosis in a porous medium. R. Soc. open sci. 1: 140352. http://dx.doi.org/10.1098/rsos.140352

2013

- Elbert Branscomb, Michael J. Russell. Turnstiles and bifurcators: The disequilibrium converting engines that put metabolism on the road. Biochimica et Biophysica Acta (BBA) – Bioenergetics. 2013 1827 (6): 806. doi: 10.1016/j.bbabio.2012.10.003.
- Julyan H. E. Cartwright, Bruno Escribano, Diego L. Gonzlez, C. Ignacio Sainz-Daz, and Idan Tuval (2013) Brinicles as a Case of Inverse Chemical Gardens. Langmuir 2013 29 (25), 7655-7660, DOI: 10.1021/la4009703
- Simoncini, E., Virgo, N., Kleidon, A., Quantifying drivers of chemical disequilibrium: theory and application to methane in the Earth's atmosphere, Earth Syst. Dynam., 4, 317-331, 2013. doi:10.5194/esd-4-317-2013.
- T. Grassi, S. Bovino, D. R. G. Schleicher, D. Seifried, J. Prieto, E. Simoncini, F. A. Gianturco, KROME - a package to easily embed the chemistry in astrophysical simulations. MNRAS, vol. 439, 3, 2386 - 2419.
- Russell, M. J., Nitschke, W. & Branscomb, E. 2013, The inevitable journey to being. Phil. Trans. R. Soc. Lond. B 368 : 20120254.

2012

- Shawn E. McGlynn, Isik Kanik, Michael J. Russell. Peptide and RNA contributions to iron-sulphur chemical gardens as life's first inorganic compartments, catalysts, capacitors and condensers Phil Trans R Soc A. 2012, 370 (1969): 3007 - 3022. DOI: 10.1098/rsta.2011.0211.

Program

Monday, October 12, 2015

TIME	EVENT
1:00 pm - 2:00 pm	Registration at the observatory - Registration
1:30 pm - 1:45 pm	Opening and presentation of the TDE working group - Eugenio Simoncini
1:45 pm - 3:55 pm	The modeling and observations of exoplanetary atmospheres: chemistry and physics - Andrea Chiavassa
13:45 - 14:25	› Spectroscopic observations of Exoplanet atmospheres - *Angerhausen Daniel, NASA Goddard Space Flight Center*
14:25 - 14:55	› A Report of SEEDS Survey: Direct Imaging Characterizations of Giant ExoPlanet Atmospheres - *Masayuki Kuzuhara, Tokyo Institute of Technology*
14:55 - 15:25	› Turbulent mixing, chemical disequilibrium and cloud formation in substellar atmospheres - *Derek Homeier, Landessternwarte, Zentrum für Astronomie Heidelberg*
15:25 - 15:55	› Charactherization and Interaction of the magnetic field in solar type stars and their planets - *Raissa Estrela, Centro de Radioastronomia e Astrofísica Mackenzie(CRAAM)*
3:55 pm - 4:15 pm	Coffee break
4:15 pm - 6:15 pm	The modeling and observations of exoplanetary atmospheres: chemistry and physics - Daniel Angerhausen
16:15 - 16:45	› New view on exoplanet transits: describing the granulation pattern with three-dimensional hydrodynamical simulations of stellar convection - *Andrea Chiavassa, Observatoire de la Cote d'Azur*
16:45 - 17:15	› "Spectral features of hot Mini-Neptunes and EGP orbiting different stars" - *Yamila Miguel, Observatoire de la Cote d'Azur*
17:15 - 17:45	› A Collisional Origin for the Coexistence of Volatile-Poor Super-Earths and Mini-Neptunes in the Proximity of Stars - *Yasunori Hori, Astrobiology Center, National Institutes of Natural Sciences, National Astronomical Observatory of Japan*
17:45 - 18:15	› Probing the atmospheric properties of transiting exoplanets through light curve analysis and atmospheric models - *Arvind Rajpurohit, Laboratoire d'Astrophysique de Marseille*

Tuesday, October 13, 2015

TIME	EVENT
9:30 am - 10:40 am	The modeling and observations of exoplanetary atmospheres: chemistry and physics - Eugenio Simoncini
09:30 - 10:10	› Chemistry and microphysics with KROME - *Tommaso Grassi, Centre for Star and Planet Formation, Universiy of Copenhagen*
10:10 - 10:40	› The development of an open-source chemical kinetics network: VULCAN - *Shang-Min Tsai, University of Bern*
10:40 am - 11:10 am	Coffee break
11:10 am - 12:00 pm	The modeling and observations of exoplanetary atmospheres: chemistry and physics - Eugenio Simoncini
11:10 - 11:40	› Biosignatures in context - *Franck Selsis, Laboratoire d'Astrophysique de Bordeaux*
11:40 am - 12:00 pm	Discussion
1:00 pm - 2:00 pm	Lunch at the observatory
2:15 pm - 3:55 pm	Icy moons, icy planets and the conditions for the emergence of life - Eduardo Pacheco
14:15 - 14:55	› Habitability potential of icy moons around Jupiter and Saturn - *Athena Coustenis, Laboratoire d'études spatiales et d'instrumentation en astrophysique*
14:55 - 15:25	› N-rich prebiotic chemistry in the atmosphere of Titan - *Nathalie Carrasco, Laboratoire Atmosphères, Milieux, Observations Spatiales*
15:25 - 15:55	› Titan's Complex Atmospheric Chemistry Revealed by ALMA - *Steven Charnley, NASA Goddard Space Flight Center*
3:55 pm - 4:15 pm	Coffee break
4:15 pm - 5:55 pm	Icy moons, icy planets and the conditions for the emergence of life - Eduardo Pacheco
16:15 - 16:55	› Abiotic Organic Synthesis during Low Temperature Serpentinization - *Kirtland Robinson, Arizona State University - ASU (USA)*
16:55 - 17:25	› Molecular chirality in simulated interstellar ices as a probe of photochemically induced asymmetry - *Iuliia Myrgorodska, Synchrotron SOLEIL, University of Nice Sophia Antipolis*
17:25 - 17:55	› Host's stars and habitability - *Florian Gallet, Observatoire de Genève*

Wednesday, October 14, 2015

TIME	EVENT
9:30 am - 10:30 am	Icy moons, icy planets and the conditions for the emergence of life - Kirtland Robinson
09:30 - 10:00	› Targeting water special disequilibrium properties - *Claudia Lage, Rio de Janeiro Federal University*
10:00 - 10:30	› Life based on Methane on Saturn's moon Titan? - *Eduardo Pacheco, Departamento de Astronomia, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, Brazil - Claudia LAge, Instituto de Biofísica Carlos Chagas Filho, Universidade Federal do Rio de Janeiro, Brazil*
10:30 am - 11:00 am	Coffee break
11:00 am - 12:00 pm	Icy moons, icy planets and the conditions for the emergence of life - Kirtland Robinson
11:00 - 11:40	› Does a Possibility of Emergence of Life in Deep Oceans of Icy Moons Meet the Physicochemical Requirements Inferred for Chemical Self-organization Processes? - *Robert Pascal, Institut des Biomolécules Max Mousseron*
11:40 am - 12:00 pm	Discussion
12:30 pm - 2:00 pm	Special banquet at the Observatory
2:00 pm - 4:00 pm	Visit of the Observatory and free afternoon

Thursday, October 15, 2015

TIME	EVENT
9:30 am - 10:40 am	The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets - Tommaso Grassi
09:30 - 10:10	› Disequilibrium analysis of the Earth atmosphere during its geological history - *Eugenio Simoncini, Astrophysical Observatory of Arcetri - INAF*
10:10 - 10:40	› On detecting biospheres from thermodynamic disequilibrium in planetary atmospheres - *Joshua Krissansen-Totton, Department of Earth and Space Sciences*
10:40 am - 11:00 am	Coffee break
11:00 am - 12:00 pm	The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets - Tommaso Grassi
11:00 - 11:30	› Thermochemical Calculations and Modeling on Exoplanetary Atmospheres - *Jasmina Blecic, University of Central Florida [Orlando]*
11:30 - 12:00	› Modeling chemical uncertainties in a pale orange dot - *Eric Hébrard, Oak Ridge Associated Universities, NASA Goddard Space Flight Center*
1:00 pm - 2:00 pm	Lunch at the Observatory
2:30 pm - 4:00 pm	The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets - Eugenio Simoncini
14:30 - 15:00	› A Fully-Consistent 1D Radiative-Convective Equilibrium Model for Planetary Atmospheres - *Benjamin Drummond, University of Exeter*
15:00 - 15:30	› Effect of flares on the chemical composition of exoplanets atmospheres - *Olivia Venot, Institute of Astronomy, K.U. Leuven*
15:30 - 16:00	› Equilibrium and Disequilibrium in Hot Jupiters - *Sarah Blumenthal, Planetary Sciences Group, University of Central Florida [Orlando]*
4:00 pm - 5:00 pm	Coffee break and informal discussions

Friday, October 16, 2015

TIME	EVENT
9:30 am - 11:00 am	Coffee break served during the general discussion
9:30 am - 11:10 am	The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets - Eugenio Simoncini
09:30 - 10:10	› Equilibrium and Disequilibrium Chemistry in Evolved Exoplanet Atmospheres - *Renyu Hu, Jet Propulsion Laboratory*
10:10 - 10:40	› The Open-source Bayesian Atmospheric Radiative Transfer (BART) Code to Model Exoplanet Atmospheres - *Patricio Cubillos, University of Central Florida [Orlando]*
10:40 - 11:10	› Seismo-atmospheric waves observations from the Mars Insight mission - *Lucie Rolland, Géoazur, Mars Science Team*
11:10 am - 12:00 pm	General Discussion - TDE - Eugenio Simoncini, Kirtland Robinson

The modeling and observations of exoplanetary atmospheres: chemistry and physics

Spectroscopic observations of Exoplanet atmospheres

Angerhausen Daniel * [1]

[1] NASA Goddard Space Flight Center (NASA Goddard Space Flight Center) – United States

In my presentation I will give a short introduction to the science of extrasolar planets, in particular to a number of state-of-the art techniques to characterize their atmospheres. I will then focus on exoplanet transit, eclipse and phase-curve spectro-photometry and describe my various projects in this emerging field using the newest spectroscopic and photometric instruments on the largest ground based telescopes, the 'flying telescope' SOFIA (Stratospheric Observatory for Infrared Astronomy) and the Kepler and Hubble space telescopes. Furthermore I will give an overview of upcoming missions (such as JWST, TESS, EXO-C/S) and their potential to advance this field.

*Speaker

A Report of SEEDS Survey: Direct Imaging Characterizations of Giant ExoPlanet Atmospheres

Masayuki Kuzuhara * [1]

[1] Tokyo Institute of Technology – Japan

Observation of exoplanet atmospheres enables us to test and improve the models of planetary atmosphere. Furthermore, this is important for the characterization of exoplanets, which leads to explore their formation and evolution scenarios. Among the techniques to observe exoplanets, direct imaging is currently the most efficient to find and characterize wide-orbit (> ~10 AU) giant planets. In addition, this technique allows for tracing the planet's energy distribution as a function of wavelengths. Indeed, the wide-orbit planets have been discovered with this technique, providing new insights into the exoplanet atmospheres. We have carried out an extensive campaign, SEEDS, to search for wide-orbit exoplanets. This campaign has finished about 120-night observations. We have selected the target samples from nearby field stars and young stars that are associated to moving groups, the Pleiades open cluster, or star forming regions. As a result, it was revealed that the G0-type star GJ 504 has a significantly faint companion (GJ 504b). Based on our age estimate (100–510 Myr) for GJ 504 and theoretical evolution models for giant planets, the companion's mass is calculated to be 3–8.5 Jupiter masses. Furthermore, using the similar way, we inferred its effective temperature to be ~500 K, being consistent to the observed evidence of methane in its atmosphere. We also detected a massive giant planet or brown dwarf companion orbiting the nearby B-type star Kapp And. We here report the SEEDS direct imaging studies for giant exoplanets; then, we place emphasis on the atmosphere studies in our observations.

*Speaker

Turbulent mixing, chemical disequilibrium and cloud formation in substellar atmospheres

Derek Homeier * [1], Bernd Freytag [2], France Allard [3]

[1] Landessternwarte, Zentrum für Astronomie Heidelberg (ZAH-LSW) – Königstuhl 12 - 69117 Heidelberg Germany, Germany
[2] Department of Physics and Astronomy, Uppsala University – Regementsvägen 1 Box 516 SE-75120 Upssala, Sweden
[3] Centre de Recherche Astrophysique de Lyon, École Normale Supérieure de Lyon (CRAL/ENS-Lyon) – INSU, CNRS : UMR5574, Ecole Normale Supérieure de Lyon, Université Claude Bernard - Lyon I – 46 allée d'Italie, 69364 Lyon cedex 07, France

Cool atmospheres from low-mass stars over brown dwarfs to gas giant planets, hot Neptunes and super-Earths show atmospheric dynamic driven by convective instability and global energy transport. Classical 1D and local 2D and 3D simulations allow, within parameterised approaches like mixing length theory, and radiative hydrodynamics (RHD) the modelling of convective velocity fields, overshoot and phenomena like gravity waves. This description of atmospheric dynamics has been successfully applied in physically detailed 1D models to quantitatively describe molecular advection and condensate formation, reproducing the various cloud formation patterns and non-equilibrium chemistry observed with decreasing temperature in substellar atmospheres. To take into account rotation effects, irradiation in close-in planets and time evolution of atmospheric features however global models are required, where general circulatation models (GSMs) have allowed to estimate the effect of the associated large-scale circulation patterns on local dynamics. But a new generation of global RHD models mapping the vertically and horizontally fully resolved convective structure onto a downscaled model of the entire star, brown dwarf or planet. These models allow us to study convectively driven large-scale structures that may explain the observed variability in many brown dwarfs, and form a new tool for understanding rotating and irradiated planets.

*Speaker

Charactherization and Interaction of the magnetic field in solar type stars and their planets

Raissa Estrela * [1], Adriana Valio† [1]

[1] Centro de Radioastronomia e Astrofísica Mackenzie(CRAAM) – Brazil

The magnetic field of a star plays a crucial role in the star internal mechanisms, as well as in the interactions with its environment. In particular, the star magnetic field can affect the habitability of the exoplanets it potentially hosts. The objective of this project is to characterize the magnetic field of stars and to understand the star-planet magnetic interaction. Moreover, the analysis of solar-type stars is also useful to shed light on the origin of the solar magnetic field. In the Sun, a relation between the magnetic field and the spots temperature has been observed for sometime. We may naturally expect that the same relation holds in other stars of solar type. Provided this hypothesis is true, the study of starspots gives us information about the magnetic field of the star, such as intensity and characterization of the cycle. Using this, we studied the magnetic field of the solar-type stars CoRoT-2, Kepler-17 and Kepler-63. We applied the method proposed by Silva (2003) that characterizes indirectly the spots (radius, intensity, temperature) by the detection of variations in the light curve of a star caused by the occultation of a spot during a planetary transit. The intensity of the spot may then be converted to temperature by considering that both the spot and the stellar photosphere radiates as a black body. The transit fitting yields spots with mean intensity (relative to the central star intensity Ic) of 0.45±0.24Ic, 0.53±0.19Ic, 0.47±0.16Ic respectively for the three stars. Considering an effective temperature of 5625K (5781K, 5576K) for the stellar photosphere, the mean spot temperature is found to be 4600±700K (5000±600K, 4800±400K). This finally gives access to the mean magnetic field of the stars, 1700±700G (1400±700G, 1600±400G).

*Speaker

†Corresponding author: adrivalio@gmail.com

New view on exoplanet transits: describing the granulation pattern with three-dimensional hydrodynamical simulations of stellar convection

Andrea Chiavassa * [1]

[1] Observatoire de la Cote d'Azur (OCA) – Lagrange – B.P. 4229 06304 Nice Cedex 4, France

A potential complication to planet detection technique is caused by stellar surface inhomogeneities (due to the presence of stellar granulation, magnetic spots, dust, etc.) of the host star. Large efforts have been made in recent decades to use theoretical modelling of stellar atmospheres to solve multidimensional radiative hydrodynamic (RHD) equations in which convection emerges naturally. These simulations take surface inhomogeneities into account (e.g., granulation pattern) and velocity fields and are used to predict reliable observables.
3D RHD grid of simulations cover a substantial portion of the Hertzsprung-Russell diagram, including the evolutionary phases from the main sequence over the turnoff up to the red giant branch for low-mass stars.
Modeling the transit light curves implies the importance to have a good representation of the background stellar disk. I will present how the RHD simulations are used to model the temporal fluctuations of the granulation pattern for different kind of stars and how this affect the depth, the ingress/egress causing fluctuations that have to be considered as an intrinsic incertitude, due to the stellar variability, on precise measurements of exoplanet transits of planets with small diameters. In this context, 3D RHD simulations are essential for a detailed quantitative analysis of the transits.
In this context, 3D RHD simulations are essential for a detailed quantitative analysis of the transits.

*Speaker

“Spectral features of hot Mini-Neptunes and EGP orbiting different stars”

Yamila Miguel * [1]

[1] Observatoire de la Cote d'Azur – Observatoire de la Cote d'Azur – 06304 NICE Cedex 4, France

Next exoplanet missions such as CHEOPS, TESS, K2 and PLATO will largely increase our knowledge on exoplanets, increasing the population of known planets as well as getting a better characterization of their parameters. These observations will give us semimajor axis, radius (and mass) of the planets and information about the parent star. With this motivation, we calculated an atmospheric grid for hot mini-Neptune and giant planets, that links these astrophysical observable parameters with the atmospheric composition and spectral features expected in transmission and emission spectra as observed with future instrumentation.
For calculating the composition we calculate disequilibrium chemistry for planets with temperatures between 2700K and 700K and explore the effect of empirical model parameters on the results. We use a line by line radiative transfer code (SAO98) to generate the observable spectra. Our models explore the detectable atmospheric features for a wide range of stellar types from F to M for distances between 0.01AU and 0.1 AU.
Our link between the observed parameters and atmospheric characterization can provide information for the best targets to further follow up with spectroscopy. Our grid can also be applied to characterize exoplanet atmospheres and serves as a reference to interpret atmospheric retrieval analysis results.

*Speaker

A Collisional Origin for the Coexistence of Volatile-Poor Super-Earths and Mini-Neptunes in the Proximity of Stars

Yasunori Hori *† [1,2], Shang-Fei Liu [3], D.n.c. Lin [4], Erik Asphaug [5]

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The Kepler mission has revealed the prevalence of volatile-poor super-Earths and mini-Neptune in the proximity of host stars. Several post-formation processes have hitherto been proposed for explaining the origin of volatile inventory of those planets: a mass loss via a stellar XUV irradiation and Parker wind, degassing of accreted material, and in-situ accumulation of the disk gas. However, the compositional diversity between neighboring planets on adjacent orbits such as Kepler-36 and Kepler-11 systems is puzzling for the three processes. We consider the possibility of a collisional origin for the coexistence of volatile-poor super-Earths and mini-Neptunes in the proximity of host stars.We present the results of three-dimensional hydrodynamic simulations of giant impacts on a super-Earth with a H/He atmosphere. A high-speed collision can strip off most of the original H/He atmosphere, as we expected. A hot and inflated planet after the giant impact cools and contracts so slowly that a protracted state of the extended post-impact atmosphere enhances mass loss via both a Parker wind and subsequent hydrodynamic escape driven by a stellar XUV irradiation. We also found that a low-speed head-on collision results in the appearance of a positive-compositional gradient deep inside the planet which suppresses the efficiency of heat transport in the planetary interior, whereas a high-speed one can homogenize the refractory material above the core inside the planet.

*Speaker
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Probing the atmospheric properties of transiting exoplanets through light curve analysis and atmospheric models

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We have taken significant step toward the understanding exoplanetary atmospheres. We took the advantage of the high photometric precision and long temporal coverage the CoRoT and Kepler light curve offer to carry out studies dedicated to the analysis of the atmospheric properties of close-in planets. With the PHOENIX model atmosphere we have calculated irradiation effects under varying incident angles which adds an entire new dimension to the models for individual planets for which we have phase light curves and precise photometry from Kepler. We have calculated theoretical phase fluxes using the PHOENIX atmosphere code (Allard et al 2013) and compared to published phase curves and secondary transit of CoRoT and Kepler planets. We explored different assumptions concerning the redistribution of absorbed stellar flux over the planet's day hemispheres. Our study gives valuable information regarding the cloud and thermal properties of those planets.

*Speaker

Chemistry and microphysics with KROME

Tommaso Grassi * [1]

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Interpreting the large number of available observations requires accurate modelling using ground-breaking computational simulations coupled with advanced numerical techniques and detailed chemistry and microphysics.
To this aim I have recently developed an open-source code called KROME (http://kromepackage.org), which embeds most of the relevant physics for a large set of astrophysical environments (see Grassi et al. 2014). KROME is a state-of-the-art code to treat
microphysics, and is uniquely flexible in the way it interfaces to other computational codes.
In this talk I'll give an overview of the code and of its main features.

*Speaker

The development of an open-source chemical kinetics network: VULCAN

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I will present VULCAN, a 1D chemical kinetics code suited for the temperature and pressure range relevant to the observable exoplanetary atmospheres. The chemical network is based on a set of reduced rate coefficients including C/H/O mechanism. Most of the rate coefficients can be found on the NIST online database. The kinetics network is compared with the thermodynamic equilibrium code, and the difference between the experimentally measured rates and the thermodynamic reverse rates is examined. Some test runs of VULCAN are shown in a hierarchical way: pure H, H+O, H+O+C. Controlled experiments are performed with a simple analytical temperature-pressure profiles. Different parameters, such as the stellar irradiation, atmospheric opacities and albedo are explored, in order to understand how these properties affect the temperature structure and hence the chemical abundances. I will also discuss the "transport-induced-quench" due to vertical mixing and the limitation of this approximation.

*Speaker

Biosignatures in context

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Biological activity has changed the Earth environment on a global scale. One metabolism - oxygenic photosynthesis - is responsible for changing the face of the Earth by converting 0.1% of the solar flux received at the surface into chemical energy. Most of the biosphere depends on this primary production of organic matter. Alternative primary biological production by chemo-autotrophic life relying on the internal heat flux has a negligible impact on the global geochemical cycles.

Considering life as we know it, global-scale biosignatures are thus expected to be tightly linked with the possibility for life to use starlight. As an important consequence, the surface liquid water "Habitable Zone" - while narrower than the region where life can exist - corresponds to the region where remote spatially-unresolved characterization could reveal the signs of biological activity.

Knowing where to search does not, however, mean that we know what to look for. The most general way to search for signs of life may be to search for a strong thermodynamical disequilibrium in the atmosphere, which cannot be maintained by non-biological processes only. This being said, measuring this disequilibrium requires the knowledge of the elemental atmospheric composition as well as contraints on pressure and temperature. Detecting, or even measuring the amount of one or a few atmospheric species is in general insufficient to quantify this disequilibrium.

Therefore, we emphasize that a detailed characterization of a planetary environment must precede any attempt to identify biosignatures. The fact that spectral features are known to be of biological origin on Earth (like the O3/O2 bands) should not interfere with the choice of forthcoming instruments for characterizing exoplanets. The in-depth exploration and understanding of the existing diversity of planetary environments/atmospheres should be seen as a prerequisite for the search for signs of life.

*Speaker

Icy moons, icy planets and the conditions for the emergence of life

Habitability potential of icy moons around Jupiter and Saturn

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Looking for habitable conditions in the outer solar system our research focuses on the natural satellites rather than the planets themselves. Indeed, the habitable zone as traditionally defined may be larger than originally conceived. The strong gravitational pull caused by the giant planets may produce enough energy to sufficiently heat the interiors of orbiting icy moons. The outer solar system satellites then provide a conceptual basis within which new theories for understanding habitability can be constructed. Measurements from the ground but also by the Voyager, Galileo and the Cassini spacecrafts revealed the potential of these satellites in this context, and our understanding of habitability in the solar system and beyond can be greatly enhanced by investigating several of these bodies together [1]. Their environments seem to satisfy many of the "classical" criteria for habitability (liquid water, energy sources to sustain metabolism and chemical compounds that can be used as nutrients over a period of time long enough to allow the development of life).
Indeed, several of the moons show promising conditions for habitability and the development and/or maintenance of life. Europa, Callisto and Ganymede may be hiding, under their icy crust, putative undersurface liquid water oceans [2] which, in the case of Europa [3], may be in direct contact with a silicate mantle floor and kept warm by tidally generated heat [4]. Titan and Enceladus, Saturn's satellites, were found by the Cassini-Huygens mission to possess active organic chemistries with seasonal variations [5], unique geological features and possibly internal liquid water oceans. Titan's rigid crust and the probable existence of a subsurface ocean create an analogy with terrestrial-type plate tectonics, at least surficial [6], while Enceladus' plumes find an analogue in geysers. As revealed by Cassini the liquid hydrocarbon lakes [7] distributed mainly at polar latitudes on Titan are ideal isolated environments to look for biomarkers. Currently, for Titan and Enceladus, geophysical models try to explain the possible existence of an oceanic layer that decouples the mantle from the icy crust. If the silicate mantles of Europa and Ganymede and the liquid sources of Titan and Enceladus are geologically active as on Earth, giving rise to the equivalent of hydrothermal systems, the simultaneous presence of water, geodynamic interactions, chemical energy sources and a diversity of key chemical elements may fulfill the basic conditions for habitability.

Titan has been suggested to be a possible cryovolcanic world due to the presence of local complex volcanic-like geomorphology and the indications of surface albedo changes with time [8,9]. Such dynamic activity that would most probably include tidal heating, possible internal convection, and ice tectonics, is believed to be a pre-requisite of a habitable planetary body as it allows the recycling of minerals and potential nutrients and provides localized energy sources. In a recent study by [4], we have shown that tidal forces are a constant and significant source of internal deformation on Titan and the interior liquid water ocean can be relatively warm for reasonable amounts of ammonia concentrations, thus completing the set of parameters needed for a truly

*Speaker

habitable planetary body.

Such habitability indications from bodies at distances of 10 AU, are essential discoveries brought to us by space exploration and which have recently revolutionized our perception of habitability in the solar system.

In the solar system's neighborhood, such potential habitats can only be investigated with appropriate designed space missions, like ESA's L1 JUICE (JUpiter ICy moon Explorer) for Ganymede and Europa [10].

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N-rich prebiotic chemistry in the atmosphere of Titan

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The quest for exoplanets of astrobiological interest is driven by the possibility of the presence of liquid water, but also of an efficient organic chemistry. Titan, the largest moon of Saturn, with a global structure similar to the Earth (a solid surface with liquid areas, and a dense atmosphere mainly composed of nitrogen) is one of the most interesting models for defining the astrobiological interest of exoplanets through possibly associated exomoons. An intense atmospheric chemistry is indeed being revealed by the ongoing Cassini-Huygens space mission. Photo-dissociation and ionization of its major constituents, N2 and CH4, initiate a complex network of reactions, leading to solid organic aerosols responsible for an organic smog surrounding permanently the satellite. In this work we will discuss how far this complex organic chemistry involving nitrogen is understood and the impact for the production of atmospheric aerosols.

*Speaker

Titan's Complex Atmospheric Chemistry Revealed by ALMA

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Titan is Saturn's largest moon, with a thick (1.45 bar) atmosphere composed primarily of molecular nitrogen and methane. Atmospheric photochemistry results in the production of a wide range of complex organic molecules, including hydrocarbons, nitriles, aromatics and other species of possible pre-biotic relevance. Titan's carbon-rich atmosphere may be analogous to that of primitive terrestrial planets throughout the universe, yet its origin, evolution and complete chemical inventory are not well understood. Here we present spatially-resolved maps of emission from C2H5CN, HNC, HC3N, CH3CN and CH3CCH in Titan's atmosphere, observed using the Atacama Large Millimeter/submillimeter Array (ALMA) in 2012-2013. These data show previously-undetected spatial structures for the observed species and provide the first spectroscopic detection of C2H5CN on Titan. Our maps show spatially- resolved peaks in Titan's northern and southern hemispheres, consistent with photochemical production and transport in the upper atmosphere followed by subsidence over the poles. The HNC emission peaks are offset from the polar axis, indicating that Titan's mesosphere may be more longitudinally variable than previously thought.

*Speaker

Abiotic Organic Synthesis during Low Temperature Serpentinization

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Serpentinization is a common water-rock reaction in our solar system, and is likely responsible for producing reducing conditions capable of driving abiotic organic synthesis on the early Earth, and potentially on icy worlds such as Enceladus and Europa. Accordingly, knowledge of this process is fundamental to directing and understanding our observations of extraterrestrial bodies, which may possess surface signatures as a result. This potential for abiotic organic synthesis makes modern low temperature serpentinizing systems attractive sites to investigate for understanding volatile production, prebiotic chemistry, and for characterizing the propensity of serpentinization to generate habitable conditions. Because low temperature terrestrial systems can support life, however, it is very difficult to disentangle which organic compounds measured in natural systems are produced biologically, thermogenically (breakdown of biomass), or abiotically. Experiments are a very useful tool, especially for getting after reaction rates, but at low temperatures certain abiotic reactions which may occur over geologic time scales cannot be observed. Nevertheless, headway in the field is being made via a multi-pronged approach whereby thermodynamic analyses, stable isotope tracer/tracking methods, and chemical mechanism probing techniques are applied to field measurements, abiotic experiments, and biological cultures. I will discuss the progress and caveats of these techniques in the context of natural systems.

*Speaker

Molecular chirality in simulated interstellar ices as a probe of photochemically induced asymmetry

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The physicochemical selection and enrichment of one chiral form over its mirror image isomer (enantiomer) occurred under non-equilibrium conditions. This selection is presumed to be an important step towards the origin of self-organization leading to the emergence of life. Life, as it is known to us, uses exclusively l-amino acid and d-sugar enantiomers for the molecular architecture of proteins and nucleic acids. Therefore, molecular symmetry was broken at some moment of time in the prebiotic world, most probably in a suitable planetary environment. The asymmetric photolysis of extraterrestrial organic matter with circularly polarized light is considered as a possible source of the initial symmetry breaking [1].
Comets and asteroids are interplanetary objects that have preserved a chemical record of the early Solar System at a time when molecular cloud material was abundant in circumstellar disks. In order to gain accesses to the information about the chemical nature of the organic extraterrestrial matter, the Murchison meteorite sample and cometary ice analogues were analysed in our laboratory by two-dimensional gas chromatography (GCGC). In the Murchison meteorite more than 60 amino acids were identified, while some of them such as -leucine and several *N*-alkylated amino acids have never been detected before. Some of the identified chiral amino acids expressed enantiomeric disequilibrium of several %. The following analysis of the organic residues resulting from laboratory simulation of photo/thermo-chemical processes in astrophysical ices allowed for the identification of 10 aldehydes, including the sugar-related glycolaldehyde and glyceraldehyde—two species considered as key prebiotic intermediates in the synthesis of ribonucleotides [2]. These identifications brought a wealth of information on the chemical composition of comets and meteorites, and allowed us proceed to the next step: the asymmetric photochemistry of laboratory organic residues at synchrotron SOLEIL.

In November 2014 five organic residues resulting from H2O:CH3OH:NH3 (12:3.5:1) ice mixtures were separately irradiated at synchrotron SOLEIL with left- and right-handed circularly polarized UV light. The ongoing analysis of photoprocessed residue will provide data on the enantiomeric enrichment of glyceraldehyde. The obtained data will allow us to develop the theory on the role of cpl in creating local enantiomeric disequilibrium.

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Host's stars and habitability

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With more than 2000 exoplanets discovered within a bunch of quite different configuration of distance from the star, size, mass, and atmospheric conditions, the probability to found habitable planets should increase dramatically. While the habitable zone is usually only seen as a snapshot to assess habitability, the intrinsic evolution of the stellar parameters must be taken into account to study the past and future evolution of the habitable zone limits. Indeed, this evolution can strongly affect the notion of habitability currently used in the literature, especially through the definition of the continuous habitable zone required for the emergence of complex life.

The aim of this talk is to highlight the impact of stellar parameter such as metallicity, mass, and rotation on the habitable zone limits and to show that the intrinsic evolution of the stellar parameters should not been neglected anymore.

*Speaker

Effects of the internal regulation of simplified biospheres on atmospheric processes and their significance for habitability

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In the search for an habitable planet we will have to take into account different kind of biospheres. The most probable biosphere that humans would see at first, would be more simplified than ours. In this work we take into account some models of simplified biosphere and their effect of the planetary atmosphere. The principles of population ecology provide the basis for formulating predictive theories and tests that follow simplified population models. In the present study we focus on a Lotka-Volterra model that describes a prey-predator interaction in which natural sources are limited. Predation plays a critical role in population dynamics as it determines the biomass transferred. This kind of ecological interaction was linked with the production and/or consumption of $O2$ and $CO2$ to all populations. We modeled different kind of simplified biosphere and different scenarios were considered, in order to obtain useful information about the interaction between atmosphere and biosphere during time. We finally discuss the results provided for the present Earth's atmosphere in order to compare them with other planetary atmospheres.

*Speaker

Targeting water special disequilibrium properties

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We present some physical and chemical properties of the water molecule. The Helmholtz free energy formalism is used to study some of those properties as thermal ones of the single-phase region and of the vapor–liquid phase boundary, including the phase-equilibrium condition (Maxwell criterion), the caloric properties specific isochoric heat capacity, compressibility and the thermal expansion, specific isobaric heat capacity, speed of sound and differences in the specific enthalpy and in the specific internal energy. By the other hand, water and ice coexist at a thermodynamic equilibrium at all temperatures in the 230-272 K range. The temperature dependence of the equilibrium constant of the water < > ice interconversion in a macromolecular-rich milieu (an important condition for astrobiology) does not obey the Gibbs-Helmholtz equation, and this indicates a strong interaction of macromolecules with water. Among the contributions to the enthalpy and entropy change on cooling and annealing at subfreezing temperatures, the largest contribution remains that from water's crystallization in hydrated macromolecules. We point out that the effect of impurities overcomes the importance of H-bond interaction with macromolecules. The thermodynamic parameters of liquid water are derived in the frame of the Frank and Wen "flickering cluster" model. Various models proposed for the structure of liquid water are reviewed, and the advantages of the Frank—Wen model are stressed. Consequences for astrobiology of some of the results are pointed out, as specific water absorption bandshifts due to organics in the vicinity.

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Life based on Methane on Saturn's moon Titan?

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ABSTRACT. We aim to check the conditions for the possible existence of microbial life on Saturn's moon Titan, in the light of the results obtained by the Cassini space mission. In spite of the fact that Cassini-Huygens mission is not equipped to provide evidence of biosignatures or complex organic compounds, it has already produced hints suggesting that the Titan environment is similar in some aspects to that proposed for the early Earth with the important exception of the lack of water vapor and the presence of hydrocarbons. Although all living beings on Earth (including methanogenic archaeas) use liquid water as a solvent, it is speculated that life on Titan could use a liquid hydrocarbon such as methane or ethane. McKay and Smith (2005) argued that if there is methanogenic life on Titan's surface, it would likely have a measurable effect on the troposphere of the moon satellite: hydrogen levels and acetic acid or its derivatives would be lower than expected. Although to date methane-based forms of life are just hypothetical, we can imagine the possibility of this kind of life be formed somewhere. Chemical signatures found on the surface and atmosphere of Titan reinforce the argument for the existence of a primitive, exotic form of life, which could have also been a precursor of life on Earth. In this poster we will discuss this issue in several aspects.

*Speaker

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Does a Possibility of Emergence of Life in Deep Oceans of Icy Moons Meet the Physicochemical Requirements Inferred for Chemical Self-organization Processes?

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The common wisdom about the origin of life in the astrobiology community defines habitability as the presence of liquid water at the surface of a planetary body. It has become usual to define a habitable zone as the range in which a temperature compatible with liquid water can be maintained at the surface without leading to a runaway greenhouse effect. The requirement for the presence of liquid water is based (*i*) on the need of a solvent to facilitate migration of reactants originating from different environments, (*ii*) on the very specific properties of water in promoting hydrophobic interactions that have an essential role in molecular recognition and structure formation and (iii) on its specific ability to dissolve ions and to facilitate proton exchanges occurring during many organic reactions. The observation of terrestrial life present far from the surface of the ocean raised the hypothesis that life could emerge in the proximity of hydrothermal systems considered of potential sources of reducing power and organic matter. The astrobiology relevance of this hypothesis was strengthened by the discovery of deep oceans under the surface of icy moons of Jupiter and Saturn. However, this possibility is challenged by the recent introduction of an analysis of conditions for chemical self-organization. In agreement with the view that far from equilibrium conditions are essential for dissipative processes, the reproduction pathways on which life is based must proceed in a kinetically irreversible way. It is concluded that systems capable of delivering the corresponding energy potential could hardly be present in the environment of deep oceans.

*Speaker

The chemical disequilibrium in planetary atmospheres: from hot Jupiters to habitable planets

Disequilibrium analysis of the Earth atmosphere during its geological history

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The study of the habitability of planetary atmospheres is gaining an increasing interest in the last decades, due to the discovery of many extrasolar planets.

It has long been observed that Earth's atmosphere is uniquely far from its thermochemical equilibrium state in terms of its chemical composition. Studying this state of disequilibrium is important for its potential role in the detection of life on other suitable planets.

A methodology to calculate the extent of atmospheric chemical disequilibrium has been developed [1, 2]. This research allows us to understand how life affected geochemical processes on Earth, leading a thermodynamic tool able to be applied to other planets, moons and exoplanet to deeper study their habitability.

This methodology has been developed using the KROME package to solve chemical kinetics [3].

In this work we present an analysis of Earth's atmospheric disequilibrium during its geological history, showing the decreasing contribution of photochemistry due to the rise of a biosphere. Further, we tested different model of simplified ecosystems in order to study the effect of the complexity of trophic chains on the atmospheric disequilibrium.

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*Speaker

On detecting biospheres from thermodynamic disequilibrium in planetary atmospheres

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Earth's atmospheric composition is profoundly altered by the biosphere. All the major constituents (except Ar) are cycled by biology, and the resultant mixture of gases is not in thermodynamic equilibrium. Consequently, atmospheric chemical disequilibrium has been proposed as a method for detecting extraterrestrial biospheres from exoplanet observations. However, disequilibrium can also be maintained by abiotic processes such as photochemistry or volcanic outgassing, and so inferring life from disequilibrium is a question of degree and context. Here, we present the first rigorous calculations of the thermodynamic chemical disequilibrium in the atmospheres of Solar System planets, in which we quantify the difference in Gibbs free energy of an observed atmosphere compared to that of all the atmospheric gases reacted to equilibrium. The purely gas phase disequilibrium in Earth's atmosphere, as measured by this available Gibbs free energy, is not unusual by Solar System standards and smaller than that of Mars. However, Earth's atmosphere is in contact with a surface ocean, which means that gases can react with water, and so a multiphase calculation that includes aqueous species is required. We find that the disequilibrium in Earth's atmosphere-ocean system (in joules per mole of atmosphere) is more than an order of magnitude larger than the disequilibria of all other atmospheres in the Solar System. Disequilibrium in other Solar System atmospheres is driven by abiotic processes, and we identify the key disequilibria in each atmosphere. Earth's thermodynamic disequilibrium is biogenic in origin, and the main contribution is the coexistence of N2, O2 and liquid water instead of more stable nitrate. In comparison, the coexistence of O2 and methane is a small contributor to Earth's atmosphere-ocean disequilibrium. Our metric requires minimal assumptions and could potentially be calculated using observations of exoplanet atmospheres. Our Matlab source code and associated databases for these calculations are available as open source software.

*Speaker

Thermochemical Calculations and Modeling on Exoplanetary Atmospheres

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We present an open-source, Thermochemical Equilibrium Abundances (TEA) code that calculates the molecular equilibrium abundances of the species present in planetary atmospheres. There are two methods to calculate chemical equilibrium: with kinetics by using equilibrium constants and reaction rates or by minimizing the free energy of the system. Chemical equilibrium can be calculated almost trivially for several reactions present in the system; however, as their number increases, it becomes difficult to solve the large number of equilibrium-constant relations. An advantage of the free-energy-minimization method is that each species present in the system can be treated independently. The complicated sets of reactions do not need to be specified and just a limited set of equations needs to be solved. TEA uses Gibbs-free-energy minimization calculation with an iterative Lagrangian optimization scheme based on White et al. (1958) and Eriksson (1971). The code, written in Python, is modular and documented and available to the scientific community via https://github.com/dzesmin/TEA.
TEA initializes the atmospheric retrieval calculations in the open-source Bayesian Atmospheric Radiative Transfer (BART) code. BART characterizes planetary atmospheres based on the observed spectroscopic information. It initializes a planetary atmosphere model, performs radiative-transfer calculations to produce models of planetary spectra, and by using a statistical module compares models with observations.

*Speaker

Modeling chemical uncertainties in a pale orange dot

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The past 20 years have revealed an unexpected diversity of exoplanets in our galactic neighborhood. From afar, these planets are only pale dots of various colors, but future technologies will enable high-resolution spectroscopy. The scientific returns from these observations will depend on our ability to translate these spectroscopic observations into physical (dynamics, pressure and temperature) and chemical (molecular abundances) conditions, and vice versa.
Earth, the only world known, so far, to harbor Life, would currently look like a "pale blue dot" from a distant vantage point [1]. However, Earth may not have been always so blue. Instead, it is becoming increasingly more acknowledged that early Earth had a lower atmospheric pressure [2,3], and a periodically haze-rich atmosphere [4-8] which would have substantially modified the observable features of our home planet in its past. Thus, making it closer to a "pale orange dot" [9]. Additionally, such an organic haze would have produced dramatic effects on the early climate, on the primitive atmospheric chemistry, and on the biochemistry of the very first living organisms.

1D and, more recently, 3D photochemical-climate models have been widely used to assess exoplanetary physical and chemical conditions and/or to define mission/instrument priorities through simulated spectral observations. Such tools self-consistently treat the atmospheres, the surface environments and the spectral features of these planets with a wide variety of parameters. The predicted results are therefore highly dependent on the model input parameters. Except for the very hottest exoplanets, chemical equilibrium does not hold. As a consequence, the atmospheric compositions are controlled by hundreds to thousands of individual chemical reactions. Chemical reactions are based on empirical parameters that must be known at temperatures ranging from 100 K to above 2500 K and at pressures from millibars to hundreds of bars. Derived or - more often - extrapolated from experiments, calculations and educated-guessed estimations, these parameters are always evaluated with substantial uncertainties.

Although practical, few models of planetary atmospheres have considered these underlying chemical uncertainties and their observational consequences. Recent progress has been made that now enables us (1) to evaluate the accuracy and precision of 1D models of planetary atmospheres and quantify uncertainties on their predictions for the atmospheric composition and associated spectral features; (2) to identify the 'key parameters' that contribute the most to the modeled predictions and should therefore require further experimental or theoretical analysis, (3) to reduce and optimize complex chemical networks for their inclusion in multidimensional atmospheric models.

*Speaker

Here, we consider these chemical uncertainties in modeling a haze-rich Archean Earth. We rely on recent 1D photochemical-climate simulations of Archean Earth with fractal hydrocarbon hazes. These hazes are consistent with geochemical data and account for the lower end of paleopressure estimates (0.5 bar) [9]. This detailed "case study" of Archean Earth provides us with an example of a habitable planet for which the propagation of chemical uncertainties may have major climatic and observational effects, due to a chemically-produced global haze that may have been present at the time.

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The Open-source Bayesian Atmospheric Radiative Transfer (BART) Code to Model Exoplanet Atmospheres

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Multi-wavelength secondary-eclipse and transit depths probe the thermochemical properties of exoplanet atmospheres. In recent years, several research groups have developed retrieval codes to analyze the existing Spitzer, HST, and ground-based data and study the prospects of future facilities. However, the scientific community has limited access to these packages. Here we present the open-source Bayesian Atmospheric Radiative Transfer (BART) code (github.com/exosports/BART). We will discuss the key aspects of the BART components: the Thermochemical Equilibrium Abundances code, TEA (github.com/dzesmin/TEA), to calculate species mixing ratios by minimizing the system's Gibbs free energy; the one-dimensional line-by-line radiative-transfer code, Transit (github.com/exosports/transit), to calculate transmission or emission spectra; and the statistical package Multi-core Markov-chain Monte Carlo, MC3 (github.com/pcubillos/MCcubed), to estimate best-fitting parameters and posterior sampling using Bayesian principles. We apply the BART retrieval code to the HAT-P-11b transmission data to constrain the planet's molecular composition. We will compare our results against those of Fraine et al. (2014).

*Speaker

Seismo-atmospheric waves observations from the Mars Insight mission

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InSight (Interior Exploration using Seismic Investigations, Geodesy and Heat Transport) is a NASA Discovery Program mission that will place a single geophysical lander on Mars to study its deep interior. This mission is planned to be launched in March 2016, with first data expected by the end of the year. Meteorological sensors onboard the lander will provide a continuous dataset of pressure, air temperature and wind speed and direction. The unprecedented sensitivity of the pressure sensor should allow catching signatures of infrasound sources (dust devils, bolides, etc.). In this presentation, we will show how acoustic waves propagates in the atmosphere of Mars, not only much more tenuous (~ 6 mbar) than the Earth atmosphere but also CO2-rich and extremely windy. We will also investigate how the internal structure of Mars impacts the coupling mechanisms between infrasound sources and the planet surface. These are potential external sources that could excite seismic waves to be sensed by the Insight seismometer SEIS and thus illuminating the interior of the planet.

*Speaker

Equilibrium and Disequilibrium in Hot Jupiters

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Signatures of disequilibrium chemistry can provide new insights into the complex dynamical and radiative environments in hot exoplanets (Cooper & Showman 2006, Showman et al. 2008, Moses et al. 2011), and may eventually provide a strategy for determining whether Earth-like exoplanets are inhabited by using the Gibbs' free energy as a metric (Krissansen-Totton Catling 2015). To begin to study departures from chemical equilibrium (CE), we first compare results for CE calculations from several existing models: CEA (Gordon & McBride 1994), TEA (Blecic et al. 2015, submitted), and Venot (Venot et al. 2012). We then compare the CE results to Venot models including disequilibrium processes such as photochemistry, and extend the Gibbs' free energy calculations from Krissansen-Totton & Catling to Hot Jupiters. We also present preliminary results on distinguishing spectral features between equilibrium and non-equilibrium chemistry in HD209485b and HD189733b using the open-source spectral modeling code, transit (www.github.com/exosports/transit/), and discuss future work on probing spectral variation across new regimes of planetary parameter space. As we near the advent of higher spectral resolution provided by missions such as JWST and E-ELT, we hope this preliminary study will provide another stepping stone in understanding a broader range of planetary environments.

*Speaker

Equilibrium and Disequilibrium Chemistry in Evolved Exoplanet Atmospheres

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It has been found that sub-Neptune-sized planets, although not existing in our Solar System, are ubiquitous in our interstellar neighborhood. This revelation is profound because, due to their special sizes and proximity to their host stars, Neptune- and sub-Neptune-sized exoplanets may have highly evolved atmospheres. I will discuss helium-dominated atmospheres as one of the outcomes of extensive atmospheric evolution on warm Neptune- and sub-Neptune-sized exoplanets. Due to depleted hydrogen abundance, the dominant carbon and oxygen species may not be methane or water on these evolved planets. Equilibrium and disequilibrium chemistry models are used to compute the molecular compositions of the atmospheres and their spectral features. Applications to GJ 436 b and other Neptune- and sub-Neptune-sized exoplanets will be discussed. As the observations to obtain the spectra of these planets continue to flourish, we will have the opportunity to study unconventional atmospheric chemical processes and test atmosphere evolution theories.

*Speaker

Effect of flares on the chemical composition of exoplanets atmospheres

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M stars are very abundant in our Galaxy, and very likely harbour the majority of planetary systems. A particularity of M stars is that they are very active. They experience stellar variability such as flares for instance. These violent and unpredictable outbursts originate from the photosphere and are caused by magnetic processus. During such an event, the energy emitted by the star can vary by several orders of magnitude for the whole wavelength range. It results in an enhancement of the H alpha emission and of the continuum. Some studies on the effect of flares on exoplanets have already been conducted (Segura et al. 2010, Tofflemire et al. 2012). Here we are interested in the effect of a flare on the atmospheric composition of a super-Earth orbiting around an M star. Using the stellar flux of AD Leo recorded during a flare event (Hawley & Pettersen 1991, Segura et al. 2010) and the chemical model of Venot et al. 2012, we have studied the impact on the planetary atmosphere. We have also computed the synthetic spectra assuming that such an event occurs during a transit to see in which extent a flare can influence observational data. We will present these results.

*Speaker

A Fully-Consistent 1D Radiative-Convective Equilibrium Model for Planetary Atmospheres

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I will present new results from a study of non-equilibrium chemistry in exoplanet atmospheres under conditions relevant to highly irradiated exoplanets. I will show the effects of vertical mixing and photodissociations on the chemistry and the subsequent impact on the temperature structure and on the spectra of these hot atmospheres. Non-equilibrium chemistry can introduce important differences to the calculated transmission and emission spectra that must be considered when analyzing observational data. We have developed a 1D radiative-convective atmosphere model, called ATMO, which couples consistently hydrostatic equilibrium, radiative transfer and equilibrium and non-equilibrium chemistry. I will also briefly discuss our current developments, the implementation of our non-equilibrium chemistry code in the Met Office UM, a sophisticated general circulation model (GCM), an important next step in understanding the inherently non-symmetric atmospheres of close-in, tidally locked planets. Our model includes non-equilibrium chemistry allowing us to consistently calculate the pressure-temperature profile. Previous studies either assume chemical equilibrium or do not allow non-equilibrium chemistry to feedback on to the background atmosphere, and none so far have included chemical kinetics in a 3D GCM.

*Speaker
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Building an atmosphere from first principles: a revision of chemical cores applied to atmospheric models.

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We present the latest development in our effort to develop a model that relies on a minimal number of observational parameters. In order to account for the multiple physico-chemical processes necessary to such endeavor we take advantage of the efficiency of the KROME chemical solver. KROME has the ability to solve large number of chemical species interconnected by a complex reaction network. In this report we present a photochemical dynamic core capable of solving ultraviolet opacities and photo-dissociation reaction rates at each step of the calculation. The stability and robustness of the code has been tested for a large network with more than 500 reactions interlinking more than 40 chemical species. The results obtained so far have been contrasted with the most common chemical codes available in the literature for benchmark.

*Speaker

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