SCIENCE ASCEND

22-28 October 2024

Highlights

Astrophysics: Robust Stellar Limb Darkening estimation with the Kipping-Sing three-parameter law

Analytical Chem.: Novel non-targeted substance detection with the trapped ion mobility spectrometry

Remote Sensing: Physical Law Embedded Cloud Synthesis to generate realistic clouds for model training

Environmental Chem.: Greener quaternary ammonium salts with extensive toxicology tests

Data Decomposition: Parsimonious Dynamic Mode Decomposition

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Science Ascend

Rising to New Heights of Discovery!

Science Ascend teleports you to the frontiers of science. It compiles and discuss the scientific research preprints from arXiv and chemRxiv just from the previous week to be cognizant of the state-of-the-art of knowledge in astrophysics, analytical chemistry, environmental chemistry, remote sensing, and applied statistics/data science. Light from the Science Ascend will keep brightening the dark horizon beyond the limits of our comprehension. FIRE Araştırma Eğitim Ltd. Şti. guarantees the weekly publication and dissemination of this journal, and make it available for everyone at most fifteen days after its publication freely.

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Bilim Yükselişi

Keşfin Yeni Yükseklerine Ulaşmak!

 $Science$ $A \,s\,c\,n d$ sizi bilimin sınırlarına ısınlar. Astrofizik, analitik kimya, cevre kimyası, uzaktan algılama ve uygulamalı istatistik/veri bilimi alanlarındaki bilgi birikiminin en son $durumu$ hakkında bilgi sahibi olmak için arXiv ve chemRxiv'den sadece bir önceki haftaya ait bilimsel araştırma ön baskılarını derler ve tartışır. Bilim Yükselişi'nden gelen ışık, kavrayışımızın sınırlarının ötesindeki karanlık ufku aydınlatmaya devam edecektir. FIRE Araştırma Eğitim Ltd. Sti. bu derginin haftalık olarak yayınlanmasını, dağıtılmasını ve yayınlandıktan en geç on bes gün sonra ücretsiz olarak herkesin erişimine açılmasını garanti eder.

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Tüm hakları saklıdır.

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Foreword

Greetings everyone!

This issue covers the preprints between October 22-28, 2024.

I am applying a change to the general format of the Science Ascend, and it will be mature starting with the December preprints. The bulk of the preprints will be summarized by no more than one sentence, and there will be an overall assessment for each sections, and potentially for large subsections in some cases.

Moreover, I will look for ways to include other authors, and especially referees to increase the quality.

See you next week! Güray Hatipoğlu

Last week in Astrophysics

Author: Yasin Güray Hatipoğlu

The preprints summarized here were published between October 22 - October 28, 2024. These are from arXiv's astro.EP cross-fields

Reviews

Liu et al.[\[1\]](#page-13-0) examined presolar grains for hints at supernova nucleosynthesis, using $44Ti$ decayrelated and nonradiogenic $44Ca$ excesses with the data from the Cameca NanoSIMS instrument. They discussed different types of supernovae and nucleosynthesis pathways. This review study focused on Type II, Type Ia, and electron-capture Supernovae (ECSNe).

Mathur and Santos[\[2\]](#page-13-1) discussed interesting knowledge gaps in stellar physics, especially for late-type stars, and provided a discussion for a prioritization for future space programs. They listed the key gaps as rotation evolution and coreenvelope coupling in solar-like stars, faster-thanexpected rotating Kepler stars, angular momentum transport (especially lacking some important physics for older stars models), Red Giants mass loss, and binary star evolutions.

Renggli et al.[\[3\]](#page-13-2) provided a comprehensive view of sulfur in the Moon and Mercury provided for The Role of Sulfur in Planetary Processes: from Cores to Atmospheres edited book as a chapter.

Rauscher[\[4\]](#page-13-3) presented a chapter on the fundamental physics and chemistry behind a planetary atmosphere with atmospheric equilibrium and disequilibrium chemistry, vertical temperature profiles, energy balance, aerosols, differences in different types of planets, and surface presence/absence.

Hue et al.[\[5\]](#page-13-4) reviewed the studies on the Jovian/Jupiter atmosphere's polar stratosphere in terms of magnetosphere-ionosphere coupling, atmospheric models, and stratospheric chemical distributions in general.

Astrochemistry

Lynas-Gray et al.[\[6\]](#page-13-5) provided ExoMol Line Lists of LXII of propadienedylidene (C_3) in its ground electronic state (basically with a Lewis structure like this: $:C=C=C$:). They reported rotationalvibrational (ro-vibrational) energy levels and related line strengths. Semenov et al.[\[7\]](#page-13-6) provided the ExoMol line lists - LXIV for the rotationalvibrational spectra of phosphorus mononitride in the IR and UV region.

Colmenares et al.[\[8\]](#page-13-7) studied the DoAr 33 solar mass, low-accretion rate T Tauri star with the James Webb Space Telescope Disk Infrared Spectral Chemistry Survey (JDISCS) Mid-Infrared Instrument-Medium Resolution Spectroscopy to check the carbon-rich chemistry in its disk (see more information at the subsection Protoplanetary - Circumstellar Disks).

Villa et al.[\[9\]](#page-13-8) studied the ice properties in cases similar to Uranus and Neptune with molecular and experimental methods. They provided ab initio computer simulations for the H_3NO_4 material over 150 to 700 GPa pressure and 500 to 7000 K temperatures. Their method included molecular dynamics simulations, shock Hugoinot calculations, and XRD to probe further into ice structures, and their phase changes under different environmental conditions.

Robare and Shock[\[10\]](#page-13-9) separated organic molecules according to their potential as biosignature using their thermodynamic stability. In essence, a thermodynamically unstable compound's high concentration may indicate a biosignature, while a thermodynamically stable one would rather be produced by abiotic pathways. They examined the Enceladus (Saturn's Moon)' plume gas and hypothesized that they are to be favorably synthesized by abiotic means.

Stellar Systems - Populations - Clusters

Micolta et al.[\[11\]](#page-13-10) studied the innermost disk calcium abundance of 70 T Tauri stars from the star-forming regions of Chamaeleon I, Lupus, and Orion OB1b for refractory element inference with the Very Large Telescope's X-shooter spectrograph and discussed the Ca depletion in disks for different cases.

Cantalloube et al.[\[12\]](#page-13-11) presented the second phase results of the Exoplanet Imaging Data Challenge (where the participants were tasked with spectrophotometry and astrometry of each injected planets), which utilized the Gemini-S/GPI and VLT/SPHERE-IFS high-contrast integral field spectrograph datasets.

Sun et al.[\[13\]](#page-13-12) worked on the host star's planetary engulfment using the excess lithium abundance in the star from the 125 co-moving pairs of stars with the spectra from the Magellan Telescope, the Keck Telescope, and the Very Large Telescope.

Du et al.[\[14\]](#page-13-13) worked and provided 5105 Mtype star spectra with homogeneous atmospheric parameter labels, used Gaia EDR3 stars as reference standards, utilized a 5-layer neural network to check the label stellar atmosphere label reliability and 1365 of high Signal-to-Noise ratio spectra with their labels were introduced to LASPM stellar parameter pipeline.

Single Star System (Star, Exoplanet)

Krenn et al.[\[15\]](#page-13-14) simulated an Earth-like transit over real data from Solar Dynamics Observatory's Helioseismic and Magnetic Imager (HMI) with injection-retrieval techniques. The purpose was to see the extent of short-term solar-like variability's impact on the Planetary Transits and Oscillations of stars (PLATO) mission's detection potential of an Earth-like planet transiting a solar-like star. Variabilities in this data with ¡5 hours timescale were removed with a smooth Savitzky-Golay filter, and a noise model was added by PlatoSim. Then, they tried to retrieve transits with a transit least squares algorithm similar method. They reported that with a V magnitude at least 10.5 or brighter may be detected by PLATO reliably, while fainter ones might require further processing. Their artificial transit lightcurves can be retrieved from [here.](https://zenodo.org/records/13939257)

Piotto et al.[\[16\]](#page-14-0) zeroed in on TOI-561 exoplanetary system architecture with the new CHEOPS and TESS observations and presented the expected transiting exoplanets, their estimated characteristics and stability analysis of TOI-561 f.

Tyler et al.[\[17\]](#page-14-1) used 126 new radial velocity measurements from the MAROON-X spectrograph observations to investigate the TOI-1266 system further and they were able to put constraints on the mass and density of their exoplanets.

Galarza et al.[\[18\]](#page-14-2) presented the lowest detected lithium-containing young Solar twin HIP 8522 with the observations from the McDonald Observatory, the National Astronomical Observatory of Japan, the Las Campanas Observatory, and the Observatoire de Haute-Provence.

Kavanagh et al.[\[19\]](#page-14-3) studied the magnetic field of the T8 dwarf WISE J062309.94-045624.6 with their new methodology to understand sub-stellar magnetospheres with several different observations and radio modelling.

Unni et al.[\[20\]](#page-14-4) presented the low-resolution transit spectroscopy with the 2m Himalayan Chandra Telescope's Himalayan Faint Object Spectrograph Camera (HFOSC) for HAT-P-1b, KELT-18b, and WASP-127b.

Keers et al.[\[21\]](#page-14-5) worked on three different ways, the quadratic, power, and Kipping-Sing threeparameter law, for accounting stellar limb darkening effect in the exoplanet characteristics retrieval, and with important insights they recommended the Kipping-Sing three-parameter law for more robust retrievals.

Exoplanet Atmospheres

Mukherjee et al.[\[22\]](#page-14-6) tweaked the exoplanetary metallicity, C/O ratio, intrinsic and equilibrium temperatures, and K_{zz} (1D eddy diffusion coefficient) values in hydrogen-dominated atmosphere cases to see the results in the atmospheric profiles. For this purpose, they used photochem and PI-CASO models individually and also explored the fully-coupled radiative-convective-photochemicalequilibrium models using both. They stated further constraints on several chemical species and ratios under different temperatures and K_{zz} values and other relations-dependences.

Boehm et al.[\[23\]](#page-14-7) observed the inflated hot Jupiter WASP-127b with the Hubble Space Telescope Wide Field Camera 3/UVIS G280 and hinted at high altitude clouds and combined it with archival HST WFC/IR and STIS for sodium (Na) evidence.

Kiefer et al.[\[24\]](#page-14-8) studied the cloudy warm exo Saturn HATS-6b with expeRT/MITgcm 3D general circulation model iterations and calculated local cloud opacities and the dis-equilibrium H/C/O/N gas-phase chemistry.

Pelletier et al.[\[25\]](#page-14-9) studied the ultra-hot Jupiter WASP-121b with CRIRES+ and ESPRESSO for volatile and refractory species estimations and constrained C, O, Fe, and Ni further and provided additional insights into the WASP-121b atmosphere.

Smith et al.[\[26\]](#page-14-10) used the Gemini South IGRINS spectrometer (R=45000) to observe WASP-121 b atmosphere and presented the estimated C/O ratio, refractory/volatile ratio, and chemical species velocity offsets.

Braam et al.[\[27\]](#page-15-0) simulated the Proxima Centauri b atmosphere with a 3D coupled Climate-Chemistry Model with 1:1 and 3:2 spin-orbit resonances and attempted to uncover spin-orbit resonance effect on atmospheric dynamics.

Guez and Claire[\[28\]](#page-15-1) presented their novel Molecule Agnostic Spectral Clustering technique by using 42 JWST MIRI similar synthetic transit transmission spectra, denoising them, normalizing and splitting into bands, and applying HDBSCAN clustering algorithm, and reported that exoplanetary characteristics might be retrieved from the correlations between these characteristics and the cluster results.

MacDonald[\[29\]](#page-15-2) presented the POSEIDON code in the Python environment for multidimensional atmospheric retrieval from the exoplanet spectra.

Petit dit de la Roche[\[30\]](#page-15-3) focused on the hot Jupiter WASP-69b's transit spectra with the VLT-FORS2 instrument data and detected an unocculted faculae on the respective star.

Mullens et al.[\[31\]](#page-15-4) provided an extensive opensource Atmospheric Mie Scattering database for cross-section and optical properties, and a way to account for them in the POSEIDON retrieval code, especially for the complex scattering, reflection, and absorption spectra, and then, they applied it to HD 189733 b's transmission spectrum.

Maguire et al.[\[32\]](#page-15-5) injected the ESPRESSO high-resolution optical observations with planetary transmission spectra and utilized the two most common methods, MOLECFIT and PCAlike SysRem to remove the telluric component from the signals and presented the caveats of using them under different cases.

Protoplanetary - Circumstellar Disks

Wu and Chen[\[33\]](#page-15-6) performed a 2D simulation of protoplanetary disks to check the impact of magnetohydrodynamic disc winds on the planetary accretion (see the subsection Magnetohydrodynamics and Hydrodynamics for more information).

Calcino et al.[\[34\]](#page-15-7) utilized 3D smoothed particle hydrodynamics (SPH) to simulate the streamer-disc interactions of a prograde streamer among protoplanetary discs (see the subsection Magnetohydrodynamics and Hydrodynamics for more information).

Colmenares et al.[\[8\]](#page-13-7) studied the DoAr 33, 1.1 times solar mass, low-accretion rate T Tauri star with the James Webb Space Telescope Disk Infrared Spectral Chemistry Survey (JDISCS) Mid-Infrared Instrument-Medium Resolution Spectroscopy to check the carbon-rich chemistry in its disk. They reported water, hydroxyl, and carbondioxide detections, along with two- and four-carbon molecules. They estimated that this carbon-rich chemistry originated from the sublimation of carbon-rich grains near the soot line. They used local thermal equilibrium slab models from spectools ir to retrieve column density, temperature, and emission area best fits for each detected molecule, with HITRAN database lines. The disk was modeled using Dust and Lines thermochemical code (DALI). They chose to use the AS 209 stellar spectrum with a modified far UV emission and a viscous accretion disk. They proposed that these results might come from an unusually low M-star-like accretion rate of the central star.

Kuwahara et al.[\[35\]](#page-15-8) examined the potential of dust rings and gaps in protoplanetary disks even though there are no clear gas-carving gaps from the planets. After their simulations, they also compared it to the observations by Atacama Large Millimeter/submillimeter Array (ALMA) surveys. To understand the implications of exoplanetary orbital distance, mass, and parameters

regarding dust, they made time-dependent (not steady state) models, a 3D hydrodynamic model (nonisothermal, with the Athena++ code) around embedded planets and resulting gas velocity field, the radial drifted velocity of dust perturbed by the gas flow, then calculating dust surface density in steady state with a 1D advection-diffusion equation. They reported the expected dust rings and gaps with thermal mass equal to or greater than 0.05 (approx. $1/3$ Earth mass at 1 au or 1.7 Earth mass at 10 au), and other spatial and temporal dynamics related to these parameters and turbulence conditions.

Adibekyan et al.[\[36\]](#page-15-9) attempted to find hints to the relations between the primordial composition of planet-building disks, present-day rocky planet composition, and stellar abundances with interesting results on Fe/Mg ratio overall temporal stability and other insights.

Pascucci et al.[\[37\]](#page-15-10) studied four young stars with the edge-on disks from the Taurus star-forming regions with the JWST/NIRSpec spectro-imaging and presented the results regarding wind morphology, and structure.

Nekrasov et al.[\[38\]](#page-15-11) examined the planetary migration in a non-stationary alpha-disk with changing mass inflow using a numerical model from the MESA ode to model the binary system, and stated that the primary component's mass loss rate at the late evolutionary stages has a significant impact on the planetary system structure.

Solar System

Pan and Gallardo[\[39\]](#page-15-12) explored 1:1 mean-motion resonance within the Solar system, filtered through NASA Horizons asteroid catalogs, and discussed 169 objects found to be in co-orbital resonant motions with several solar system planets (excluding Jupiter).

Mercury

Arkhypov[\[40\]](#page-15-13) stressed the case of Mercury as similar to the Moon on transient phenomena with previous and currently shelved information (as Forgotten pre-cursors) on interior or impact outgassing, dust plumes, dust clouds, and global dust envelope.

Mars

Jackson et al.[\[41\]](#page-15-14) used Mars 2020 Ingenuity data to profile near-surface Martian winds while also comparing it with the Mars 2020 Perseverance rover's MEDA meteorology package.

Solar System Gas Giants

Dietze and Read[\[42\]](#page-16-0) explored singular Riemannian manifolds and the concentration of highfrequency eigenfunctions' accumulation at the boundaries. After working through asymptotics and boundary conditions and providing the proof, they applied this to the acoustics of gas giant planets. Later, they provided the acoustic mode accumulation rate for such gas planets, where their speed of sound approaches zero near the planetary boundaries.

Sarkango et al.[\[43\]](#page-16-1) studied the ion dynamics in Jupiter's magnetosphere and provided insights on several bands in this magnetosphere corresponding to ion species mappings from the observations of Juno's Jovian Auroral Distributions Experiment ion sensor (JADE-I).

Solar System Ice Giants

Villa et al.[\[9\]](#page-13-8) studied the ice properties in cases similar to Uranus and Neptune with molecular and experimental methods (see details in the subsection Astrochemistry).

Near-Earth Objects - Asteroids - Comets

Kasianchuk and Reshetnyk[\[44\]](#page-16-2) examined the orbits of more than 35000 near-Earth objects (for 2024) for potential interplanetary space missions between Earth, Venus, and Mars and provided 120 candidates for one-way fast transfers in 180 days and 2 candidates for double transits.

Mazur et al.[\[45\]](#page-16-3) presented the meteor-tracking spectrograph at the Canadian Automated Meteor Observatory, CAMO-S.

Pluto

Desoubrie and Vienne[\[46\]](#page-16-4) studied the dynamics of Pluto-Charon satellites with the REBOUND nbody simulator and its IAS15 integrator, applied a frequency map analysis and interpreted their 3 body and 6-body analysis results.

Hyperion

Goldberg and Batygin[\[47\]](#page-16-5) studied the Hyperion in terms of nutation-orbit resonances and stated that it does not tumble chaotically according to their Hamiltonian derivation without planar or principal axis rotation and averaging spin period and observations were stated to be in line with this result.

Jupiter and Saturn Moons

Mura et al.[\[48\]](#page-16-6) used the Juno/JIRAM observations to estimate the vertical and temporal structure of the H_3^+ emission and presented interesting results.

Boccelli et al.[\[49\]](#page-16-7) studied the sealing time of Europa's ice fractures and vents by passing vapor from the plume and found their modeled sealing was compatible with the HST observed 7-hour plume in 2012.

Earth - Space relationship

Yoshida et al.[\[50\]](#page-16-8) performed numerical analyses of UV absorption in the ancient Earth atmosphere and reported that this self-shielding of UV absorption by organic molecules both suppressed the water photolysis and enhanced the life-essential complex organic molecules deposition.

Magnetohydrodynamics and Hydrodynamics

Murashima et al.[\[51\]](#page-16-9) utilized the Smoothed Particle Hydrodynamics (SPH) method in 3D to simulate icy moon ocean dynamics considering the tidal heating specifically. The problems of unphysical rotation-hindering forces from the conventional viscosity formulations and artificial internal energy partitioning from the SPH were mitigated by a modified viscosity formulation and density-independent SPH approach. Introduced methods were marginally slower in computation, but similar while mitigating the issues above.

Wu and Chen[\[33\]](#page-15-6) performed a 2D simulation of protoplanetary disks to check the impact of magnetohydrodynamic disc winds on planetary accretion. They built upon the previous work with 2D hydrodynamics simulations for giant planet migrations by extending the parameter space to smaller planets.

Calcino et al.[\[34\]](#page-15-7) utilized 3D smoothed particle hydrodynamics (SPH) to simulate the streamer-disc interactions of a prograde streamer among protoplanetary discs. They examined their streamer pattern speeds, interactions, disc interactions, and mode persistences. Their representative was a T Tauri-like protoplanetary disc. They used PHANTOM code for this simulation, one disc, and infall initialisation. They reported potential sudden pitch angle changes for spiral arms, lasting time for these spiral arms, and azimuthal mode persistence.

Shah[\[52\]](#page-16-10) investigated marginal stability in stars with low Prandtl number^{[1](#page-6-8)}. Shah worked

¹The ratio of momentum diffusivity to thermal diffusivity

with different Prandtl, Peclet, Froude numbers, and Reynold number value cases. Specifically, the study examined low-Pr equations in low and high buoyancy Peclet numbers in the strong stratification limit.

Lim et al.[\[53\]](#page-16-11) examined the clumping and disk thickness according to the planetesimal formation in the streaming instability (SI). They used ATHENA code, and x-z axisymmetric 2D simulations. For numerically solving the shearing box's hydrodynamic fluid equations they used the following integrators: unsplit Cornet Transport Upwind integrator, third-order spatial reconstruction, and HLLC Riemann solver. Then, they reported the clumping and thickness states with specific stopping times and the critical dust-togas surface density ratio (Z).

Nail et al.[\[54\]](#page-16-12) modeled the large-scale asymmetric outflows from the HAT-P-67 b and HAT-P-32 b exoplanets with a 3D hydrodynamical model and focused on the metastable helium tripled λ =1083 nanometers using Athena++.

N-body Works

Dittmann[\[55\]](#page-16-13) studied multi-point Hermite interpolation for N-body problem works. The results outperformed the standard comparatively lower order 2 and 4th Hermite schemes computationally and accurately in most cases. The methodology has concepts from both Hermite methods and the Adams-Bashforth-Moulton ones. The example scripts for this paper were stated to be provided [here.](https://github.com/ajdittmann/HermiteScripts) They mention libration timescale, U-turn timescale, and radial advection timescale across the horseshoe region. They simulated the disc wind effects with the modified grid-based hydrodynamic code FARGO3D. They provided the results and under which conditions planets were estimated to migrate inwardly and outwardly.

Xing et al.[\[56\]](#page-16-14) combined 1D binary stellar evolution code MESA and N-body simulation code REBOUND to see the dynamic evolution of circumbinary planets around interacting binary systems. They began to construct a reference binary star and planet model (one star with a2.21 solar mass, the other with a 1.76 solar mass, with a 6-day circular orbit representing an sdB (subdwarf B)-forming binary), then changed the parameters to see the impacts. They provided the mass evolution of accretor and donor stars, semimajor axis changes of the planet with changing the rate of mass change from donor to accretor in a million years (zooming in 530 to 540 Myrs). Moreover, they considered potential tidal effects for a Jupiter-like planet.

Siraj et al.[\[57\]](#page-16-15) studied the potential of an unseen Planet X in the solar system with orbital stability calculations and 300 N-body simulations and stated that the presence of such a planet is statistically significant, followed by predicted orbital and planetary characteristics.

Eatson et al.[\[58\]](#page-16-16) conducted N-body simulations to model short-lived radioisotope enhancement in the star-forming regions using massive star's stellar winds and supernovae with ^{26}Al and $60Fe$ foci and reported that Al-enhancement was at the upper end of the distribution, while Fe was very highly enhanced in the Solar system, which originates from the supernovae.

Last week in Analytical Chemistry

Author: Yasin Güray Hatipoğlu

The preprints summarized here were published between October 22 - October 28, 2024. They are more in nature of spectroscopy alone, and hence several studies regarding biochemistry, chromatography, and several other disciplines might be missed here.

Mass Spectroscopy

Shi et al.[\[59\]](#page-16-17) utilised the Gas Chromatography-Atmospheric Pressure Chemical Ionization coupled to ion mobility-high resolution mass spectrometry (GC-APCI to IM-HRMS) to be able to detect novel substances absent in the electron ionization databases while working with hydrophobic contaminants in the sediment medium. They used both standard reference sediment and sediments from the Baltic Sea, from an Arctic shelf, and from a Norweigan lake. Besides the target identifications, several novel fluorotelomer thiols, disulfides, and alkyl sulfones were also determined.

Another ion mobility spectra study was done by Graham et al.[\[60\]](#page-17-0) in analysing intact protein ions. They improved upon the collision-induced dissociation/trapped ion mobility spectrometry (CIDtims) method in several different ion dynamics control, optimized bioinformatic approach, and with a better instrument, timsTOF Pro2. They also worked on internal ion assignments to increase the signal-to-noise ratio in eventually detect more product ions.

Spesyvyi et al.[\[61\]](#page-17-1) developed a surrogate to synthetically produce large unilamellar lipid vesicles to simulate extracellular vesicles and worked on its separation for the subsequent mass spectrometry analysis. One of the important details was using the frequency-scanned quadrupole in m/z separation. They found the approach successful.

Vuppala et al.[\[62\]](#page-17-2) employed the Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) to study phosphorylation, normally indistinguishable by the collision-induced dissociation, such as the RNAPII C-terminal domain heptads YSPTSPS. Solvent modifier modulation of the carrier gas and the compensation voltage scan improved the differentiation of the gas-phase metal-peptide adducts.

Benabou et al.[\[63\]](#page-17-3) studied the collisioninduced unfolding in native mass spectrometry and presented the caveats arising after examining the voltage conditions, pH responses, and different structures.

Electrochemiluminescence

Wang et al.[\[64\]](#page-17-4) worked on oxygen evolution reactions' proton evolution and its qualitative and quantitative monitoring via electrochemiluminescent species with a hybrid electrochemiluminescence-pH sensor. They theoretically predicted such a dye, then, synthesized it by grafting fluorescent dyes onto carbon nitride nanosheets, presenting one of them, CN-FITC (carbon nanosheet-fluorescein isothiocyanate).

High-Performance Liquid Chromatography

Ambroso et al.[\[65\]](#page-17-5) developed a reverse-phase liquid chromatography from cellulose acetate butyrate, and characterized it with $1H\text{-NMR}$ and FTIR. The acetate/butyrate and cellulosic hydroxyl groups enhanced the selective separations of the Tanaka mixtures and found the material generally more successful and a green technology without the adverse toxic residues of the available reverse-phase columns.

Last week in Remote Sensing

Author: Yasin Güray Hatipoğlu

The preprints summarized here were published between October 22 - October 28, 2024. These are generally based on the preprints retrieved when "remote sensing" words are given between quotation marks within the entire arXiv.

Reviews

Xiao et al.[\[66\]](#page-17-6) reviewed the use of foundation models for earth observation remote sensing, presenting different training methods, model structures, common tasks, and metrics encountered in the relevant literature.

Modelling-Forecast

Garg et al.^{[\[67\]](#page-17-7)} presented the advancement in image resolution for the enhanced EOS-06 Ocean Color Monitor-3 Data over different sceneries with a newly-developed neural network architecture that constructs a super-resolution image from a sequence of low-resolution ones.

Luo et al.[\[68\]](#page-17-8) presented the MMM-RS, the multi-modal, multi-ground sample distance, multi-scene remote sensing dataset for benchmarking text-to-image generation models^{[2](#page-9-5)}. BLIP-2, the large-scale vision-language model generated text prompts and trained the crossmodal ControlNet models with these from the 9 publicly available remote sensing datasets.

Xu et al.[\[69\]](#page-17-9) worked on generating a realistic and diverse set of clouds to ameliorate remote sensing algorithms on cloud-related challenges (Physical Law Embedded Generative Cloud Syn-thesis - PGCS^{[3](#page-9-6)} from the StyleGAN and cloud scattering law-related information combination).

Ghaboura et al.[\[70\]](#page-17-10)'s comprehensive Arabic LLM Benchmark CAMEL-Bench included remote sensing-based land-use understanding within 8 diverse domains.

Change Detection

Elgendy et al. [\[71\]](#page-17-11) presented the GeoLLaVA^{[4](#page-9-7)}, which is a modification from the vision language models trained on videos on detecting changes, action and complementing them with the textual annotation. They used the fMoW RGB dataset, temporal annotations from the GPT-4o mini, model fine-tunings, low rank adaptation and evaluated the results in ROUGE-1 -2 -L, BLEU, and BERT, optimized the models with pruning, and reported significant improvements.

Object Detection

Dias et al.[\[72\]](#page-17-12) scaled the foundation model use with up to several hundred million parameters for the high-resolution satellite imagery to billion parameter pretrained foundation models (OReole-MR and OReole-HR) for image classification, semantic segmentation, and object detection benchmarks with the ORBITaL-Net and TIU pretraining datasets.

 $\rm{^2The}$ data was provided [here.](https://github.com/ljl5261/MMM-RS)

³The code was stated to be provided [here.](https://github.com/Liying-Xu/PGCS)

⁴The annotated data and code was stated to be [here.](https://github.com/HosamGen/GeoLLaVA)

Last week in Environmental **Chemistry**

Author: Yasin Güray Hatipoğlu

The preprints summarized here were published between October 22 - October 28, 2024 in chemRxiv's Earth, Space, and Environmental chemistry preprints are being surveyed, and unfortunately, not many preprints are published under environmental topics in this field.

Nguyen and Kumar[\[73\]](#page-17-13) assessed the formulation and evaluation of a nanocream with a targeted increase in its performance, stability, and sustainability. This is a mixture of surfactants, bioactive oil compounds, and vitamins forming nanoemulsions. Their optimum material had the mean droplet size of 121.3 ± 1.19 nm and 0.094 ± 0.001 polydispersity index with high uniformity and stability and an in vitro membrane permeation ratio of 97.15%.

Rzemieniecki et al.[\[74\]](#page-18-0) worked on an Lasparagine and L-alanine aminoacid originating quinine cation and anion-based quaternary ammonium salts. They identified the structure of these materials precisely with $1H - NMR$ method, water solubility with the OECD 105 Guidelines flask method, the Octanol-Water partition with the OECD Test No. 107 guidelines, and the antimicrobial toxicity against several gram-positive bacteria, yeasts, and filamentous Fungi. They further checked the biopesticide property (adult granary weevil beetles, larvae of the confused flour beetle, and khapra beetle), phytotoxicity (OECD 208 guidelines), and aquatic toxicity (algae and Daphnia magna). They reported a strong antifeedant activity and an increased disinfectant potential with an elongated alkyl substituent in the alkylquininium cation side. They performed well in terms of phytotoxicity absence and lower aquatic toxicity.

Blanco et al.[\[75\]](#page-18-1) focused on ultrafine particles and late-life neuro-cognitive function relation from the Adult Changes in Thought cohort (with a sample count of 5283). One of the main purposes of their study was to find the minimum required number of ultrafine particle measurement to accurately monitor the relationship. Nevertheless, they did not find a link between ultrafine particle exposure and late-life cognition.

Kumar and Yoshida[\[76\]](#page-18-2) investigated the "sustainability" in the plastic industry and provided the actual numbers from 2023, and what should be done to achieve sustainable growth.

Young et al.[\[77\]](#page-18-3) provided very high-temporal resolution of C2-C6 perfluoroalkyl carboxylic acids (PFCA, 1-minute resolution for trifluoroacetic acid - TFA, and 10-minute resolution for C3-C6 compounds) over 6 weeks in winter and summer in 2022, Toronto, CANADA.

Last week in Data Decomposition/Transformation

Author: Yasin Güray Hatipoğlu

The preprints summarized here were published between October 22 - October 28, 2024. This is generally from arXiv's stat.ML or stat.ME cross-list. The section focuses on preprints heavily worked with or developed data decomposition/transformation techniques, such as principal component analysis (PCA) or Fourier Transformation.

Dimensional Reduction

Lie et al.[\[78\]](#page-18-4) presented the Leave-One-Out mapping (LOO-map) to mitigate the challenges in neighboring embedding from high-dimensional data to two-dimensional visualization. They worked on diagnosing the overconfidence-inducing discontinuity in well-separated clusters coming from the overlapping clusters in the input dataset, and the fracture-inducing discontinuity, formed locally, comparatively small and random spurious $\mathrm{clusters}^5$ $\mathrm{clusters}^5$.

Sort et al.[\[79\]](#page-18-5) presented a novel tensor decomposition CANDECOMP/PARAFAC (a.k.a Canonical Polyadic Decomposition, but now extended for the probabilistic and functional tensors) to assist in investigating time-continuous longitudinal data. They applied this to the Alzheimer's Disease Neuroimaging Initiative study (ADNI)'s multiple neurocognitive scores.

Beyaztas et al.[\[80\]](#page-18-6) presented the functional PCA and functional partial least squares (FPLS) for a robust spatial functional linear regression estimation (can be found under the rfsac R library). They built upon the spatial scalar-onfunction regression model (SSoFRM) and applied the approach to the U.S. COVID-19 dataset with reported success.

Das et al.[\[81\]](#page-18-7) presented the novel algorithm Parsimonious Dynamic Mode Decomposition (parsDMD), suitable for both spatiotemporal and temporal-only data. They successfully applied this method to the standing wave signals, hidden dynamic identification, fluid dynamic simulations (flow past a cylinder), and atmospheric science-related sea surface temperature data.

Engelke et al. $[82]$ focused on Lévy processes and worked with decomposing them using the Lévy-Ito decomposition to a Brownian motion part and an independent jump process. They applied this to model the stock returns from the U.S. companies successfully.

Modelling

Beyaztas et al.[\[83\]](#page-18-9) studied the function-onfunction regression models, their robustness against outliers and attempted to improve them using a functional principal component decomposition of the function-valued variables and τ estimator. The optimum truncation constant was determined with the Bayesian information criterion and the method's empirical performance was investigated with a U.S. COVID-19 dataset.

Chattopadhyay et al.[\[84\]](#page-18-10) studied the causal effect estimation in event studies, and offered a novel decomposition (exact decomposition) and a robust weighting approach. Their exact decomposition features the subtraction of the control cases from the treatment cases with a τ_l parameter from the two-way fixed effects dynamic estimator.

Fu[\[85\]](#page-18-11) studied the Qualitative Comparative Analysis (QCA) techniques, typically seen in sociology, political science, public administration, and business management, and addressed the limitations of the QCA applications. After working with random data and specific datasets, they considered that $scpQCA^6$ $scpQCA^6$ as a more robust alternative among them with its rigorous simplification method and the necessity analysis (more causal oriented perspective).

Capezza et al.[\[86\]](#page-18-12) constructed the functional mixture regression control chart (FMRCC) to monitor the quality in industrial settings without encountering the multimode profile monitoring problem. They used an extensive Monte Carlo simulation test study and a real case study of the resistance spot welding process in the automotive industry and found superior in both examinations.

Bortolato and Canale[\[87\]](#page-18-13) presented the Adap-tive Partition Factor Analysis (APAFA^{[7](#page-11-6)}) to overcome study-specific variations in identifying latent factors in similar cases. They used a shrinkageprior assignment for latent factors and built upon the Bayesian multi-study factor analysis (MFSA).

Missing Data Imputation

Cui and Gorodetsky[\[88\]](#page-18-14) worked on the Bayesian low-rank matrix completion with a new prior model using the singular value decomposition and designed a geodesic Hamiltonian Monte Carlo algorithm (within Gibbs) for the posterior generation to SVD factor matrices and reported that

 5 They provided the R code for their methodology in the following GitHub [repository.](https://github.com/zhexuandliu/NE-Reliability-MapContinuity)

 6 The algorithm is both in PyPI and in the following GitHub [repository.](https://github.com/Kim-Q/scpQCA)

⁷The code to reproduce this study was stated to be available [here.](https://github.com/elenabortolato/APAFA)

this approach resolves the standard Gibbs samplers sampling difficulties. They applied this to the mice protein dataset and MovieLens recommendation problem and reported success.

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