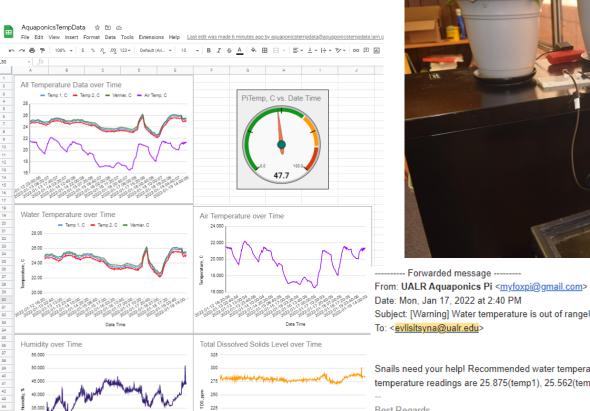
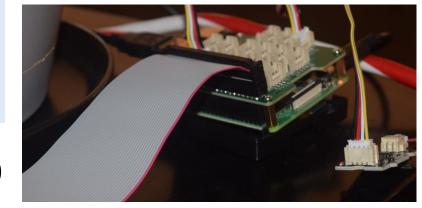
Introduction to IOST Internet of Science Things



Spring 2022: Chem 4399/5399

Dr. Robert E. Belford





From: UALR Aquaponics Pi <myfoxpi@gmail.com>

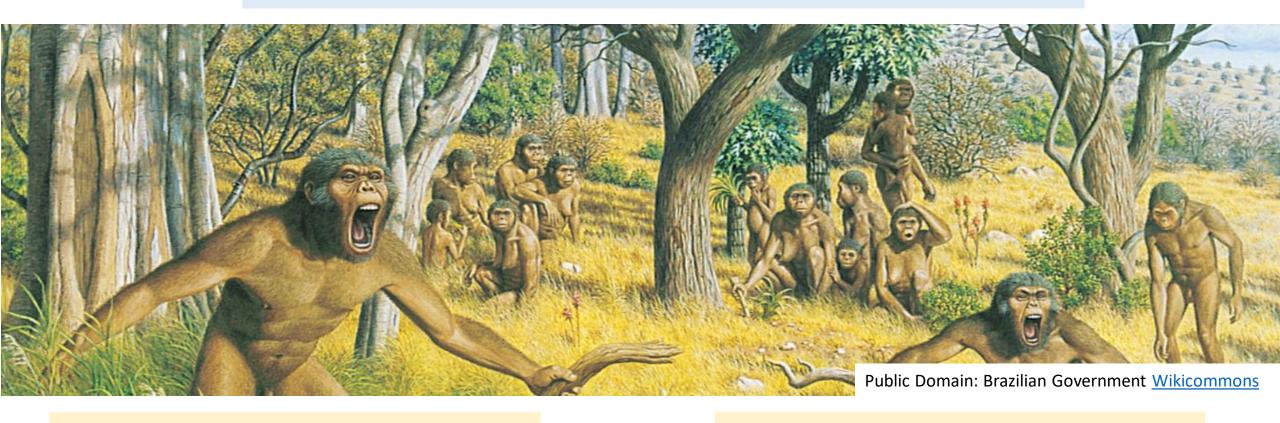
Snails need your help! Recommended water temperature for Mystery Snails is between 21C and 26C. Current water temperature readings are 25.875(temp1), 25.562(temp2) and 26.135(Vernier) degrees Celsius.

Best Regards, Elena Lisitsyna

What is the Internet of Science Things?

- The Internet is an **ICT**
 - Information and Communication Technology
- Science
 - A Philosophy of Knowledge
- IOT: (Internet of Things)
 - The Interconnected Digital Networking of Things
- IOST (Internet of Science Things)
 - Application of IOT Technologies to the Practice of the Philosophy of Science.

Pre-Technology Communication Primal Howls and Gestures



(Entity Based)

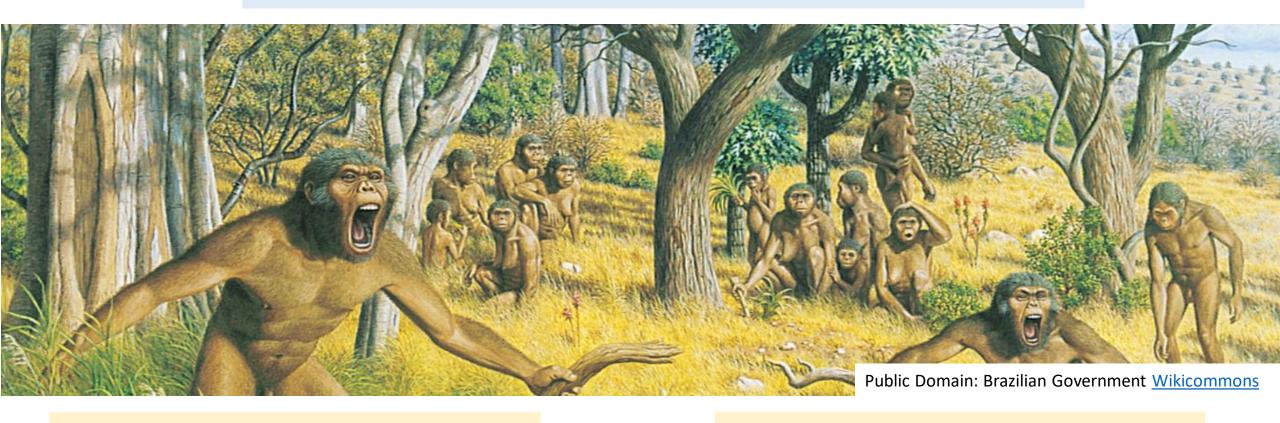
(Lions, Tigers and Bears)

(Action Based)

(Run, Hide and Fight)

Combined Entity and Action Based (Climb up Tree)

Howls and Gestures are Ephemeral



(Entity Based)

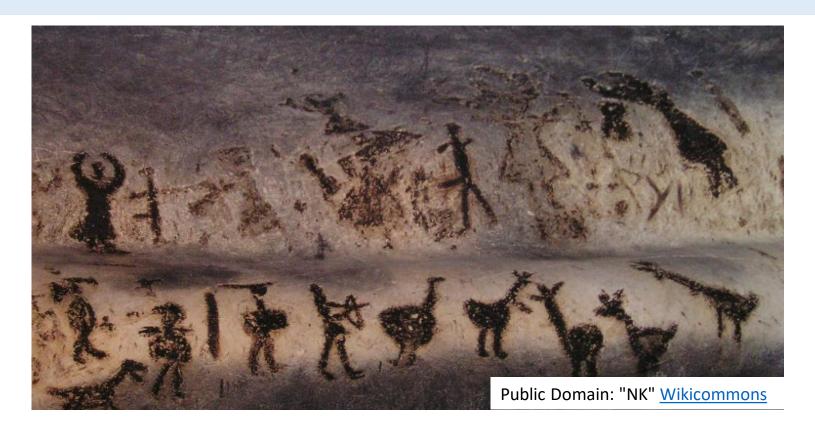
(Lions, Tigers and Bears)

(Action Based)

(Run, Hide and Fight)

Combined Entity and Action Based (Climb up Tree)

Early ICTs Enable Communication Beyond the Present

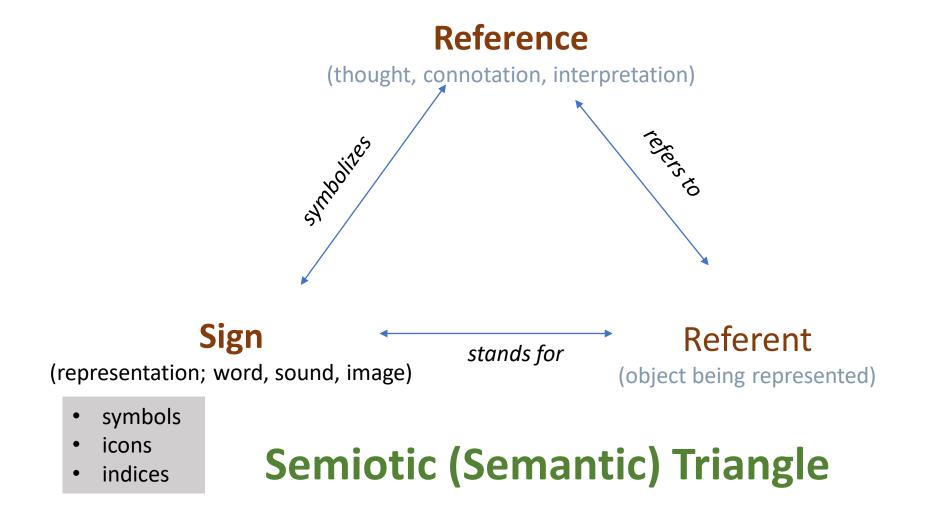


What is the story of this post-paleolithic cave drawing from the Magura cave in Bulgaria?

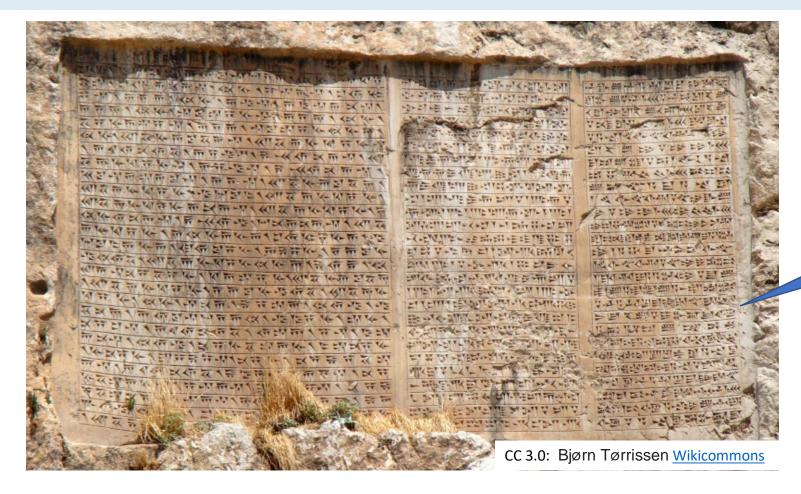
(ICT "Tools" were Used in its Generation)

Semiotics

Semiotics: Study of Signs, Symbols, their Interpretation and Communication



Beyond the Ephemeral: Written Words

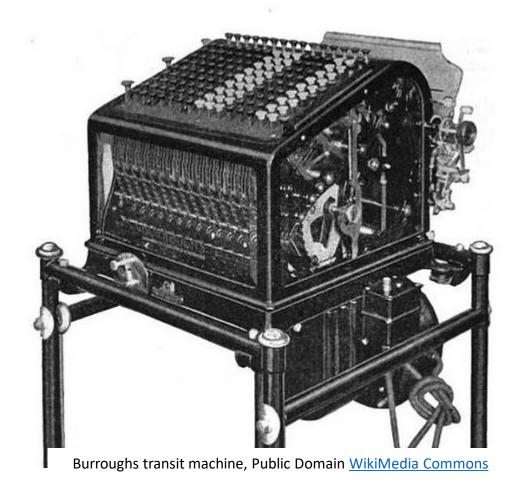


Early writing was often developed to track agricultural productivity and commerce

Two types of words

- entities & actions
- numbers (amenable to arithmetic operations)

Printed Words: Mechanical Devices





Mechanical Devices Evolved to Print and Perform Computations

Printed Words: Gutenberg Era ICTS



The Printed Press Enabled Mass Communication through Printed Texts

Printed Words: Gutenberg Era ICTS



Education

UNESCO » Education » Literacy



United Nations Literacy Decade (2003 - 2012)



UNESCO leads the United Nations Literacy
Decade (UNLD) under the slogan of "Literacy as
Freedom". Launched at UN Headquarters in
2003, the Decade aims to increase literacy
levels and to empower all people everywhere. In
declaring this Decade, the international
community recognised that the promotion of
literacy is in the interest of all, as part of efforts
towards peace, respect and exchange in a
globalizing world. At the request of the UN
General Assembly, UNESCO is coordinating the
Decade and its international activities. UNESCO
launched the Literacy Initiative for Empowerment

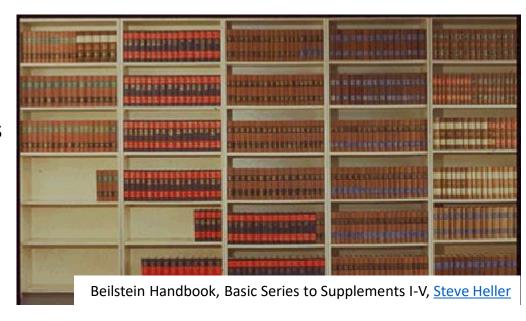
(LIFE) in 2005 as a framework for achieving the Decade's goals.

Literacy Became a Fundamental Human Right by the 21st Century

Printed Words: Gutenberg Era Legacy Databases

Gmelin Handbook

- 400 vol (1998)
- 1.5 Million Compounds
- 1.3 Million Reactions
- 85,000 Keywords and abstracts
- >800 data fields



Beilstein Handbook

- 1st Edition (1881)
 - 15,000 Organic Molecules
 - 2 vol (2,200 pages)
- 4th Edition (1918-1998)
 - 503 Volumes
 - >440,000 Pages
 - 1.5 Million Organic Compounds

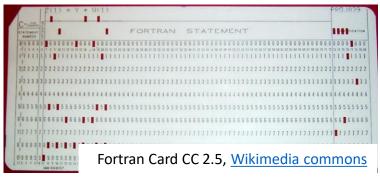
Gutenberg Era ICTs are Inadequate to Handle the Flow of Information but are Firmly Entrenched in the Practice of Science

Digital Words: Beyond Gutenberg



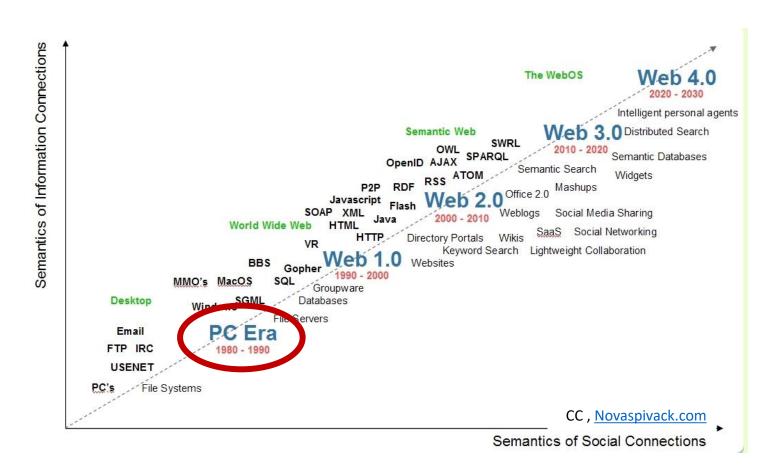
IBM Type 604 (1957). Public Domain, Wikimedia commons





The Late 20th Century Saw the Introduction of Digital Words

Evolution of Digital ICT Systems



Let's start with the PC Era

PC Era: Navigating a Document





1968 Douglas Englebart Demonstrated the First Mouse and the Ability to Navigate within a Document. Google "Mother of All Demos"

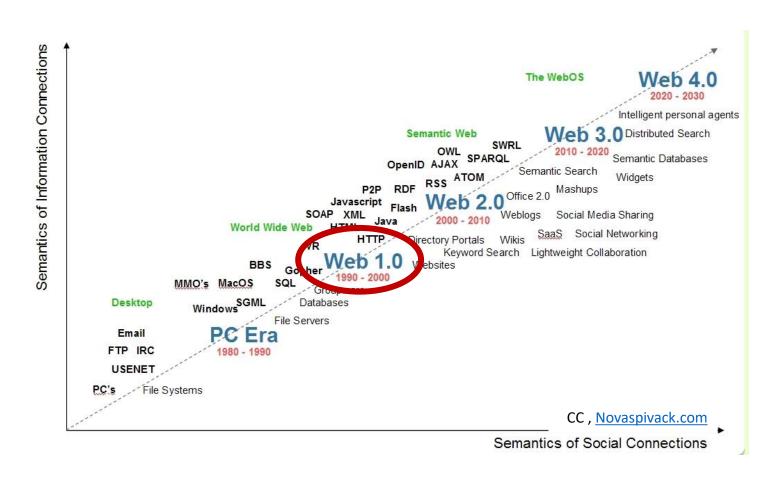
PC Era: Computer as Cognitive Artifact





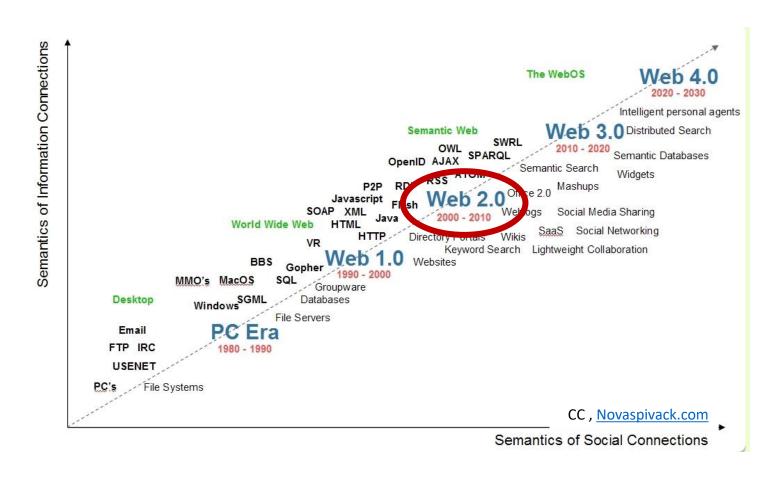
Cognitive Artifact: "Those artificial devices that maintain, display, or operate upon information in order to serve a representational function and that affect human cognitive performance." (Norman, 1991)

Web 1.0: Static Web



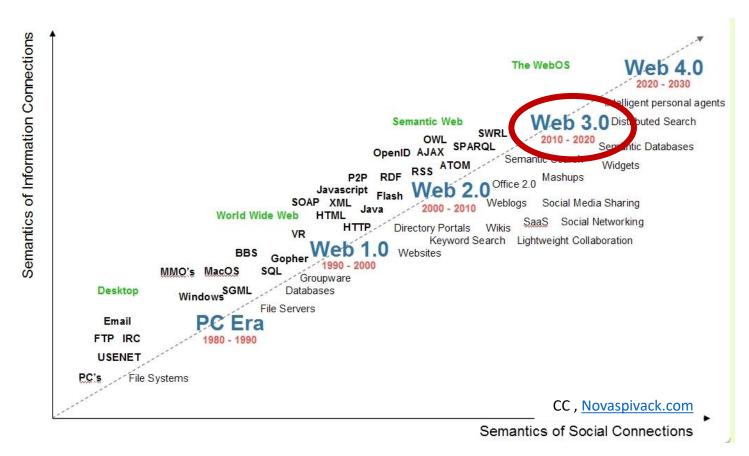
The Ability to Navigate Between Documents (Surfing from Webpage to Webpage)

Web 2.0: Social Web



Collaborative Authoring (Wikis, Blogs and Sites Like Facebook) where the "Webpage" is not a Static Document but Rendered from a Database

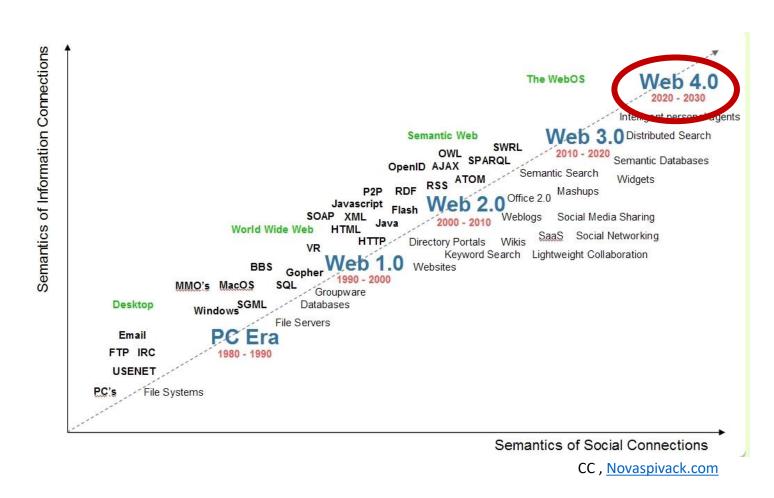
Web 3.0: Semantic Web



Linked Frameworks Not Generate by Authors

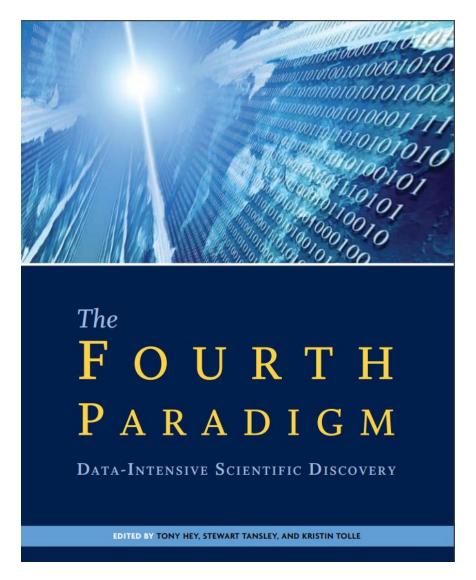
- RDF Triplet (Subject, Predicate, Object) Frameworks
- Tag-Base Ontological Frameworks (Folksonomies)

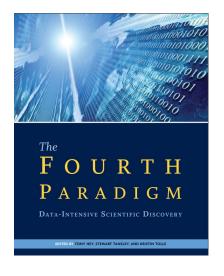
Web 4.0: Symbiotic Web



Living Data – The Internet of Things

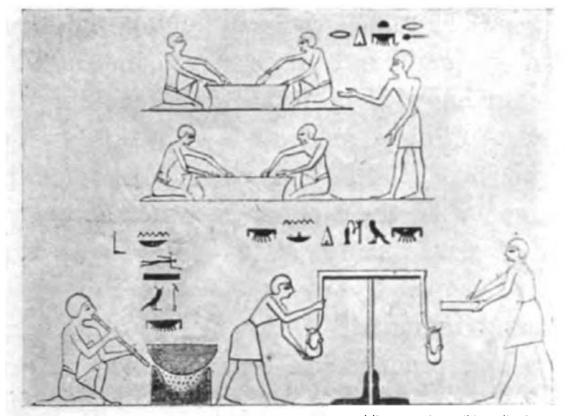
Paradigms of Science





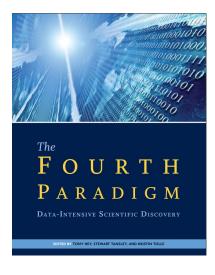
1st Paradigm: Empirical Science

- Thousands of Years Old
- Science Based on Measurements and Experiments Involving the Physical World



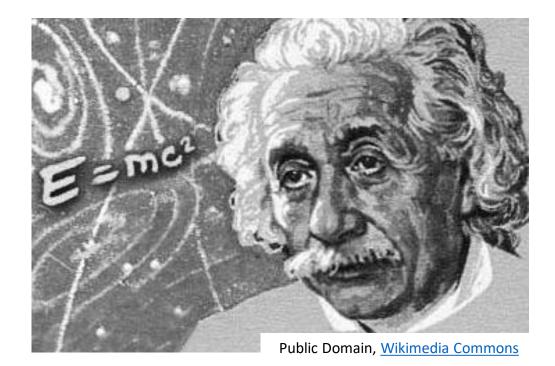
Public Domain, Wikimedia Commons

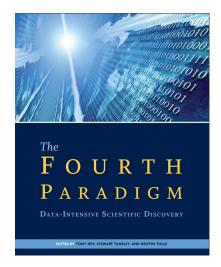
Public Domain, Wikimedia Commons



2nd Paradigm: Theoretical Science

- Centuries Old
- Science Based on Theoretical Models





3rd Paradigm: Computational Science

- Decades Old
- Science Based on Complex Computations

Guess Wavefunction Calculate Charge Density

- \hat{F} is called the **Fock operator** and
- $\{|\varphi_i\rangle\}$ are the Hatree-Fock orbitals with corresponding energies ϵ_i .

The Fock operator is a one-electron operator and solving a Hartree-Fock equation gives the energy and Hartree-Fock orbital for one electron.

The nature of the Fock operator reveals how the Hartree-Fock (HF) or Self-Consistent Field (SCF) Method accounts for the electron-electron interaction in atoms and molecules while preserving the idea of **independent atomic orbitals**. The wavefunction written as a Slater determinant of spin-orbitals is necessary to derive the form of the Fock operator, which is

$$\hat{F} = \hat{H}^0 + \sum_{j=1}^{N} (2\hat{J}_j - \hat{K}_j) = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} + \sum_{j=1}^{N} (2\hat{J}_j - \hat{K}_j)$$
 (Lecture Extra.20)

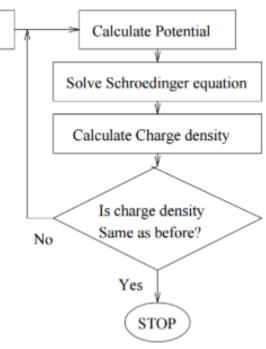
- \hat{J} is the **Coulomb operator**, defining the electron-electron repulsion energy due to each of the two electrons in the jth orbital.
- \hat{K} is the **exchange operator**, defining the electron exchange energy due to the antisymmetry of the total n-electron wave function. This (so called) "exchange energy" operator, K, is simply an artifact of the Slater determinant.

The Hartree-Fock equations $h_e\phi_i=\epsilon_i\phi_i$ imply that the orbital energies ϵ_i can be written as:

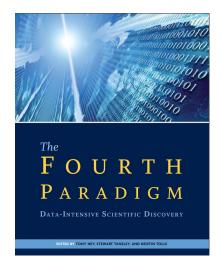
$$\epsilon_i = \langle \phi_i | h_e | \phi_i \rangle = \langle \phi_i | T + V | \phi_i \rangle + \sum_{j \text{(occupled)}} \langle \phi_i | J_j - K_j | \phi_i \rangle$$
 (Lecture Extra.21)

$$= \langle \phi_i | T + V | \phi_i \rangle + \sum_{j \text{(occupied)}} [J_{i,j} - K_{i,j}], \qquad \text{(Lecture Extra.22)}$$

where T+V represents the kinetic (T) and nuclear attraction (V) energies, respectively. Thus, ϵ_i is the average value of the kinetic energy plus Coulombic attraction to the nuclei for an electron in ϕ_i plus the sum over all of the spin-orbitals occupied in ψ of Coulomb minus Exchange interactions of these electrons with the electron in ϕ_i .



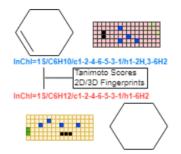
Hartree Fock CC 3.0: Libretexts



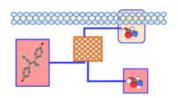
4th Paradigm: Data Intensive Discovery

- Emerging
- Scientific Discovery Based on Data Relationships

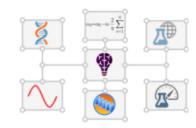
6: Molecular Similarity



7: Computer-Aided Drug Discovery and Design



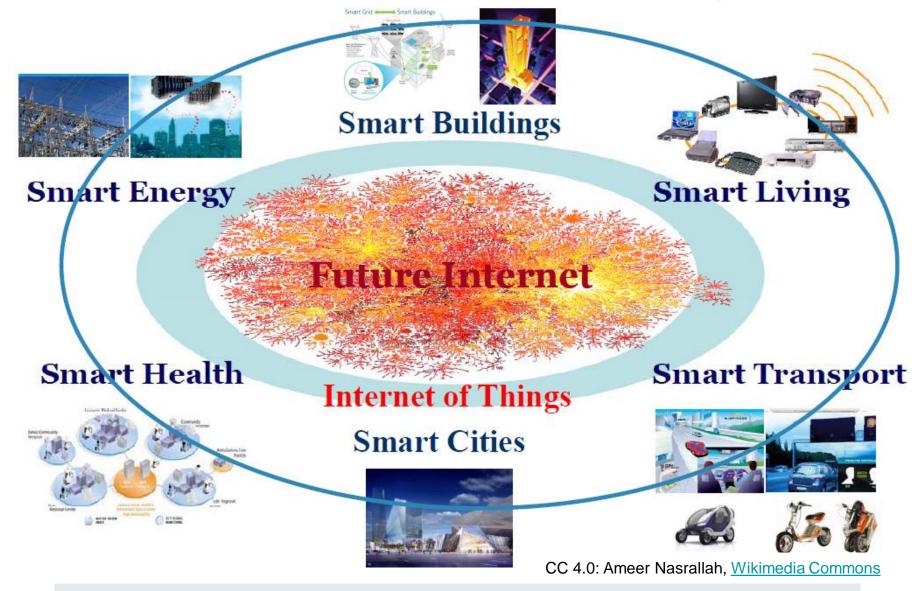
8: Machine-learning Basics



Cheminformatics OLCC CC 3.0: Libretexts

Is Science Evolving From Causations to Correlations?

What is the Internet of Things?

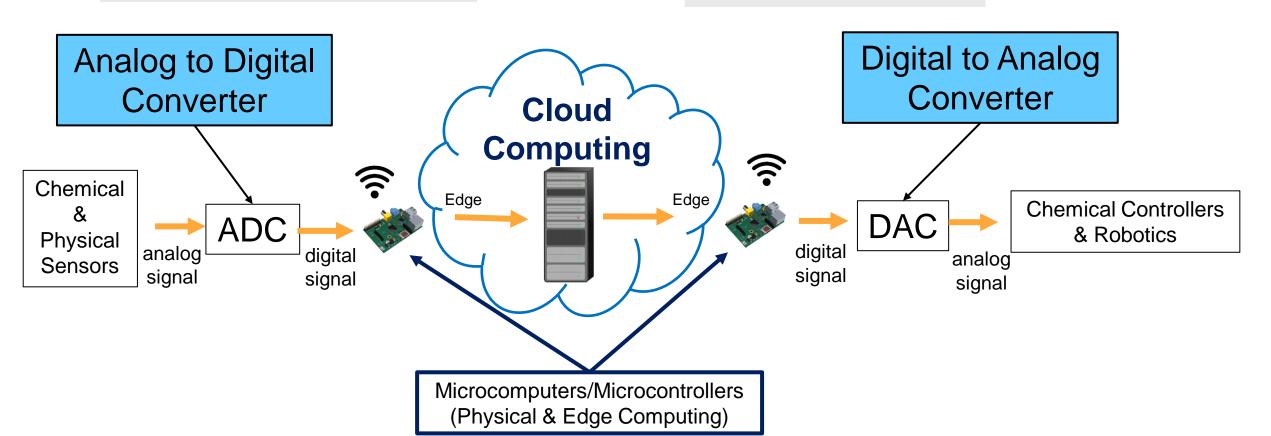


Interconnected Digital Networking of Physical Objects

What is the Internet of Science Things?

Interconnected
Digital Networking
of
Physical Objects

Connecting
Empirical Science
to
Data Science



Prior Course Projects

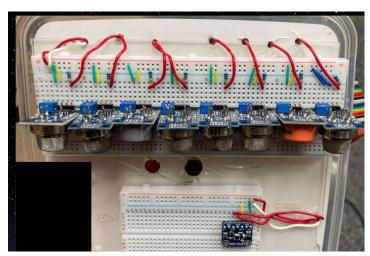


Set up in chemical storage lab.

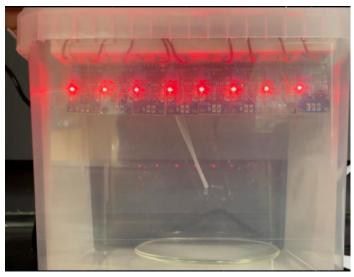
Multi-Variable Sensor Array for Air Quality Machine Leaning

Prior Course Projects









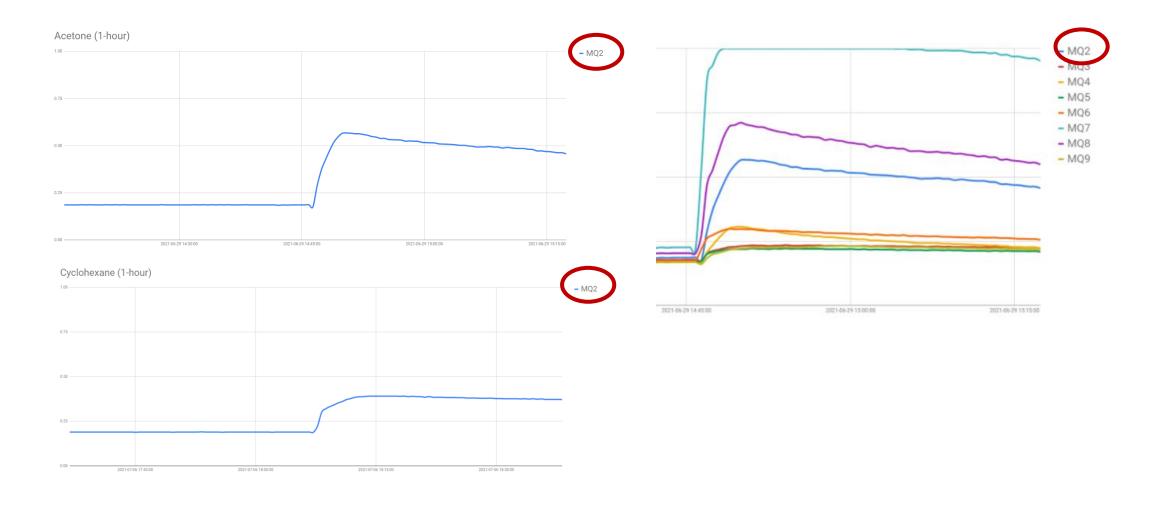
Multi-Variable Sensor Array for Air Quality Machine Leaning

Thesis Project

Volatile Organic Compound Identification
Using Metal Oxide Sensors and Machine Learning
Hunter Tiner

Multi-Variable Sensor Array for Air Quality Machine Leaning

Thesis Project



Multi-Variable Sensor Array for Air Quality Machine Leaning

Thesis Project

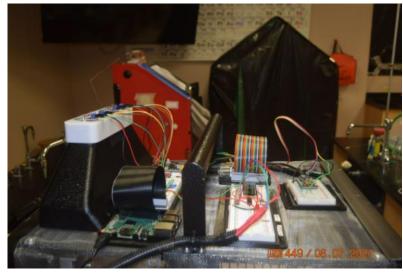
Chemical Prediction									
	25			50			100		
Learner	Acc	Prec	Recall	Acc	Prec	Recall	Acc	Prec	Recall
GNB	93.5%	93.5%	95.4%	94.5%	94.5%	95.7%	96.5%	96.5%	97.4%
KNN	94.5%	94.5%	96.1%	94.5%	94.5%	96%	96%	96%	97%
RF	100%	100%	100%	98%	98%	98%	96%	96%	97.3%
SVM	97%	97%	97.9%	98%	98%	98.6%	96%	96%	97.2%
					A. () []	M 200			

- Scores are averaged of the 10 splits

Multi-Variable Sensor Array for Air Quality Machine Leaning

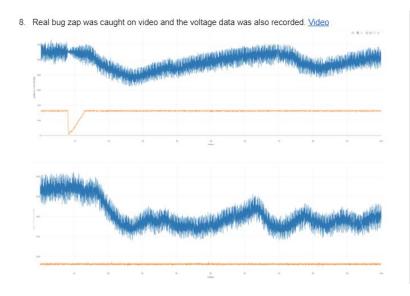


SolaRid













GAN:

GARDEN AREA NETWORK PROJECT

Capstone Project Report

Prepared for

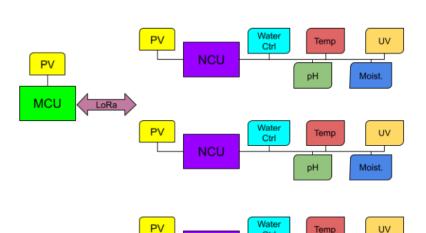
Capstone II, SYEN 4385

Dr. Jing Zhang

Capstone Advising Professor Associate Professor, Systems Engineering University of Arkansas at Little Rock

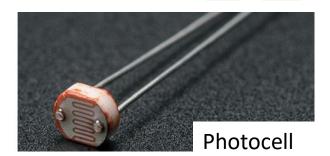
Ву

Joshua Mitchell, Electrical and Computer Systems Engineering, Project Lead Abdulaziz Alotaibi, Electrical and Computer Systems Engineering John Harty, Electrical and Computer Systems Engineering Samuel Jordan, Electrical and Computer Systems Engineering Elizabeth Rivera, Electrical and Computer Systems Engineering



NCU

NCU







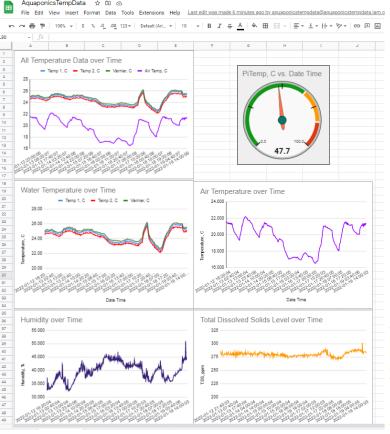






Heifer Aquaponics

AquaponicsTempDataSheet







----- Forwarded message ------

From: UALR Aquaponics Pi < myfoxpi@gmail.com>

Date: Mon, Jan 17, 2022 at 2:40 PM

Subject: [Warning] Water temperature is out of range!

To: <evlisitsyna@ualr.edu>

Snails need your help! Recommended water temperature for Mystery Snails is between 21C and 26C. Current water temperature readings are 25.875(temp1), 25.562(temp2) and 26.135(Vernier) degrees Celsius.

Best Regards, Elena Lisitsyna