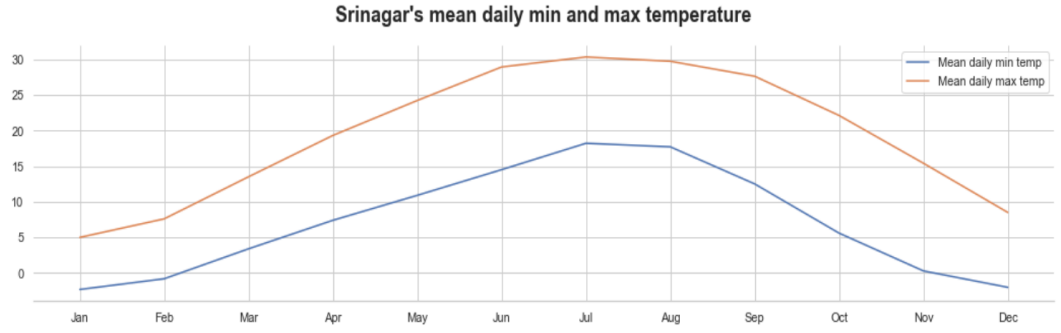
MTP Performance Report

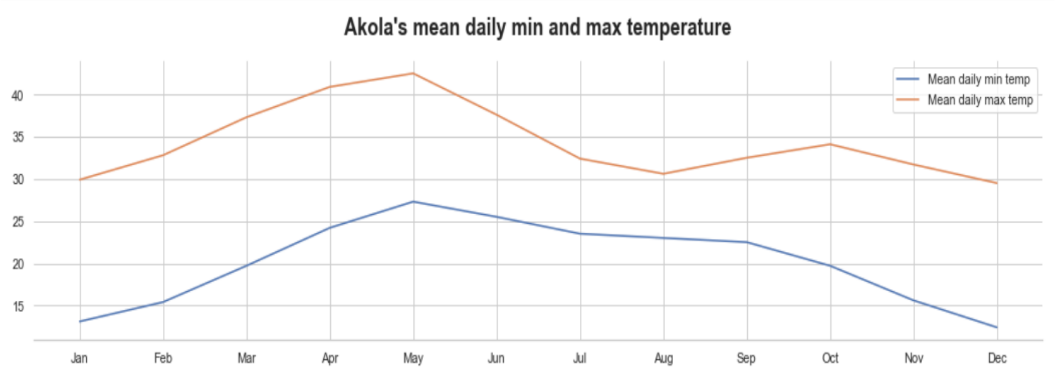
- Topic - Design aspects of lithium-ion batteries for electric vehicles.
- Supervisor - Dr Pattabhi Ramaiah

Data analysis on the temperatures of various Indian cities was done. The data was collected from the WORLD METEOROLOGICAL ORGANIZATION. Climatological information was based on monthly averages for the 48 years 1953-2000. Data analysis was done with the help of the programming language, Python.

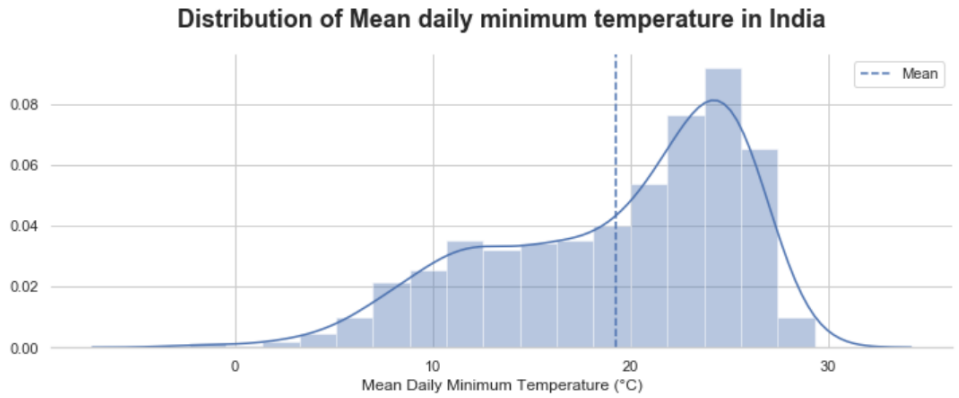
Some highlights from the analysis are presented below:

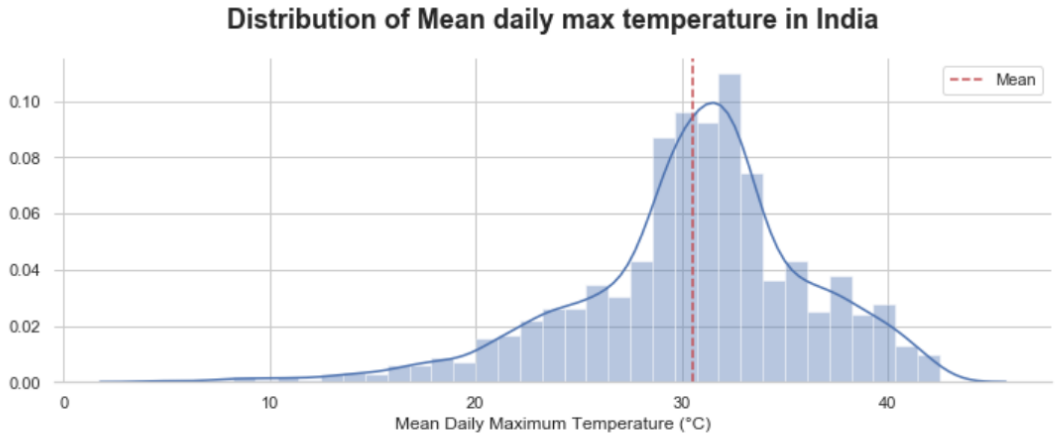


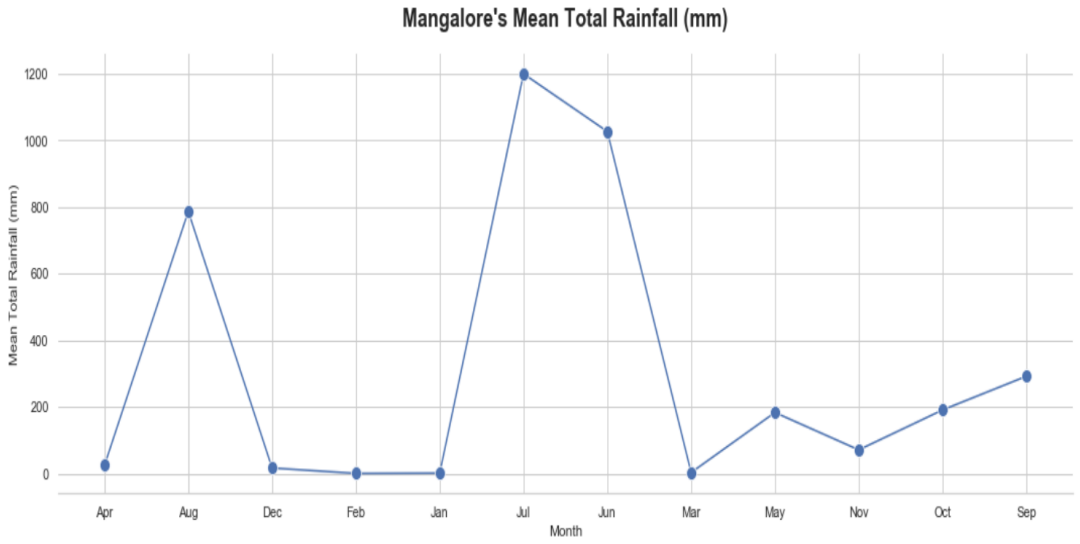
Therefore, the temperatures range from -2.5 to 31 degrees celcius throughout the year in Srinagar.



Therefore, the mean temperatures in Akola range from 13 degrees to 43 degrees.







Therefore, the city with maximum Mean Total Rainfall is Mangalore. The mean total rainfall ranges from 0mm to 1200mm.

Afterwards, a thorough literature survey is being done. Some of the highlights have been presented below.

Li-ion is considered to be one of the most sophisticated pieces of technology in energy storage right now. It is also the most commercialized technology for its cost to performance ratio.

What we call Li-ion is a family of chemistries. They differ by Cathode material (mostly) or by Anode material. There are major variations that should be included in the Li-ion family or not is debatable, and then there are minor or very custom variations made for very specific purposes. The most common chemistries which are well known and commercialized by multiple companies are:

1. NMC (Nickel Manganese Cobalt)
2. LFP (Lithium Ferro Phosphate or Lithium Iron Phosphate)
3. NCA (Nickel Cobalt Aluminium Oxide)
4. LMO (Lithium Manganese Oxide)
5. LCO (Lithium Cobalt Oxide)

Li-ion cell is made of:
Cathode: NMC, LFP, LMO, NCA, or LCO
Anode: Carbon (In Graphite form) or LTO
Separator: Ceramic or similar material
Electrolyte: Lithium salt (e.g. LiPF6), in organic solvent (e.g. Ethylene Carbonate)
Current Collectors: Aluminium and Copper.

A summary of all the common chemistries has been presented below in a tabular and pictorial form.

Battery	Energy Density (Wh/kg)	Cyclability (Cycles)	Advantages	Disadvantages
LCO	150–190	500–1000	Technological maturity, Low-self discharge,	High cost, low inherent safety

			High discharge voltage	
LMO	100–140	1000–1500	High inherent safety, Cobalt-free	Low energy density
LFP	90–140	up to 2000	High inherent safety	Low energy density
NCA	200–250	1000–1500	Low cobalt content	Capacity fade at elevated temperature
NMC	140–200	1000–2000	Low cobalt content	Safety issues in Ni-rich batteries

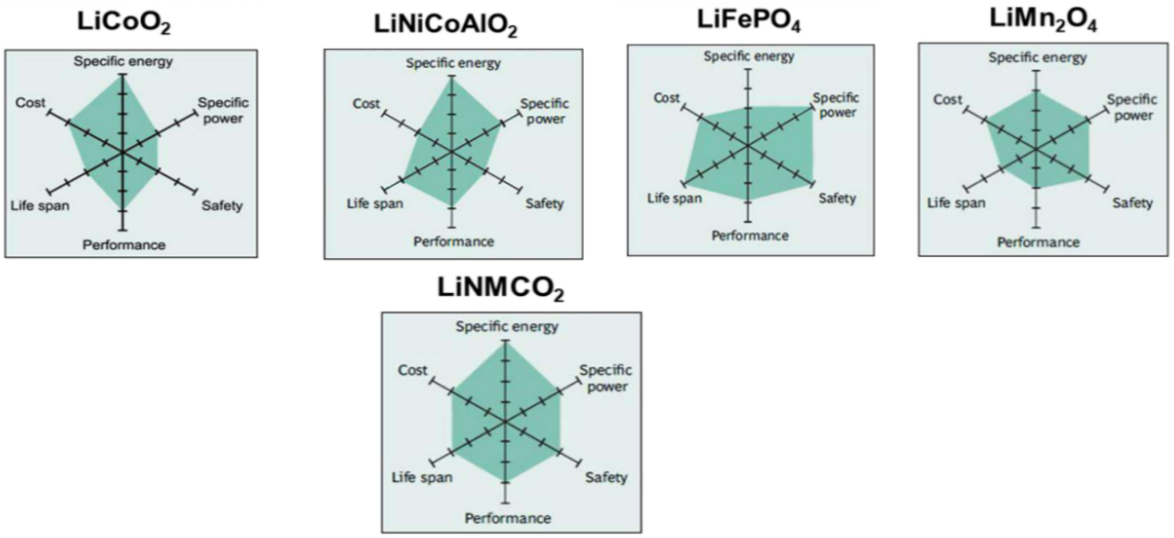


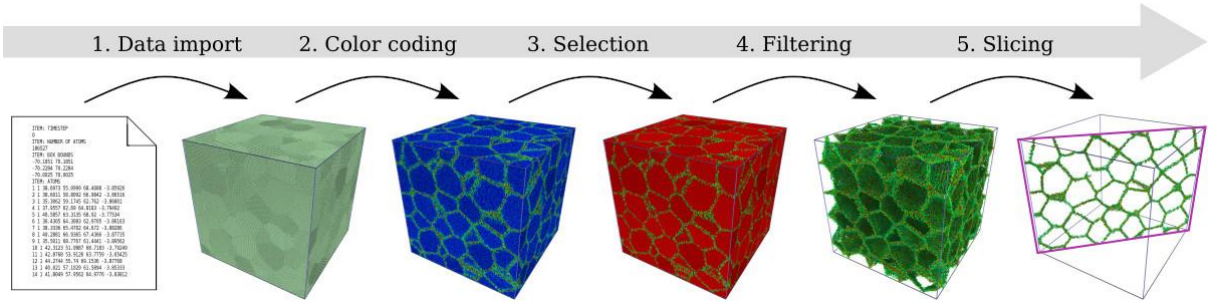
Figure: Comparisons of different types of Li-ion batteries used in EVs.

Lithium Nickel Manganese Cobalt Oxide (NMC), Lithium Iron Phosphate (LiFePO4) and Lithium Manganese Oxide (LMO) stand out as being superior among these candidates.

Now I am working towards estimating the influence of cathode materials on the power output characteristics of Lithium-ion batteries. The factors influencing

the crack formation and growth in Lithium ions, as well as the cathode material. The simulation of crack growth and hence the performance characteristics will be estimated through molecular dynamics simulations using Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).

I am familiarizing myself with LAMMPS by running example scripts and running the simulations in software called OVITO. OVITO makes molecular dynamics simulations visual. It offers a wide range of basic visualization and analysis functions (building blocks), which you can assemble into a sequence of processing steps. These operations, which are all configurable, will then be applied to the simulation data in real-time by the software. The outcome of the data pipeline is finally displayed on the screen.



Running example script of Cu compression and visualizing it in OVITO:

Five images at seconds 1, 8, 9, 14 and 16 are shown below respectively.
Colour coding was set to colour based on the centre symmetry and then adjusted this range to go from zero to five. What the centre symmetry does is, indicates how close to a perfect lattice structure each atom is in so the dark purple atoms have a centre of symmetry very near zero and that essentially means that it's nearly in a perfect crystal structure so all the atoms around it are in the right places. The atoms with lighter colours have a relatively high centre symmetry which means they're vibrating or are somewhat out of their perfect crystal structure and their vibrations are why we see this variation in colours even before we started deforming it.

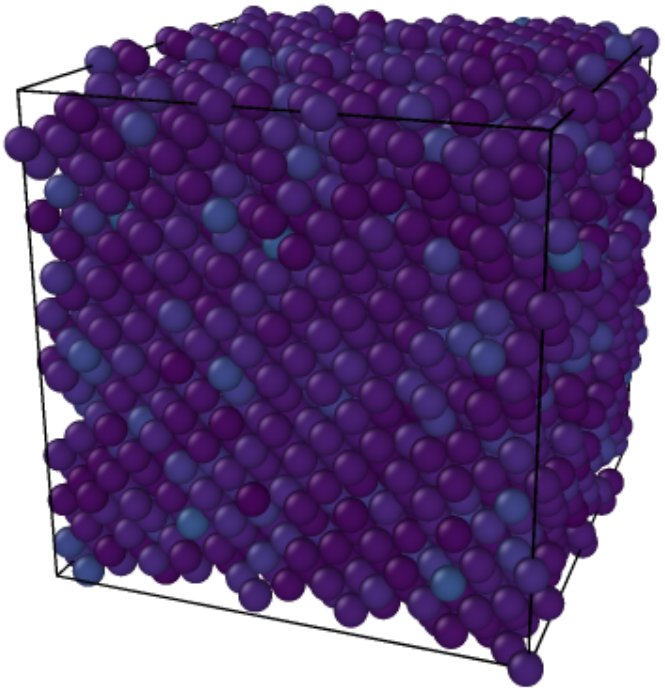


Fig 1. Simulation at 1 second

As we simulate by clicking the play button and we see it compress. We start to see some very high Center symmetry values and this indicates a dislocation and they happen in these very specific planes. So those are the dislocations forming and then we can see it just gets squashed and squashed and then comes back a little bit.

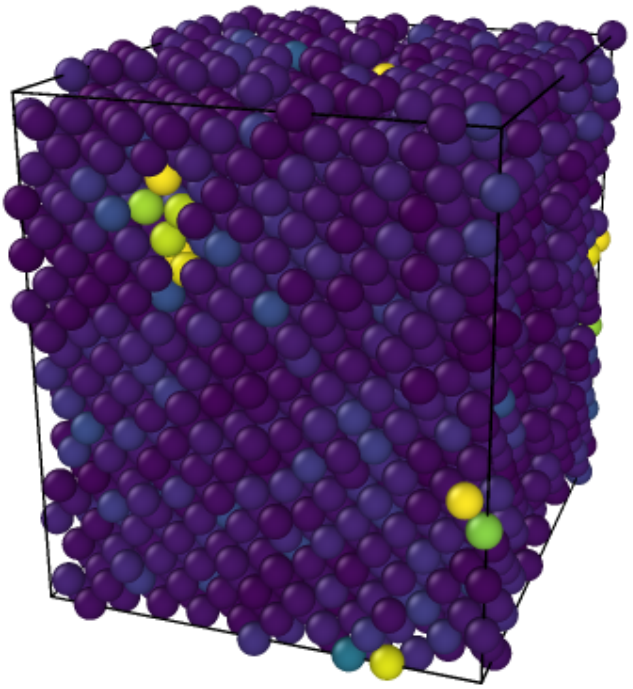


Fig 2. Simulation at 8 seconds

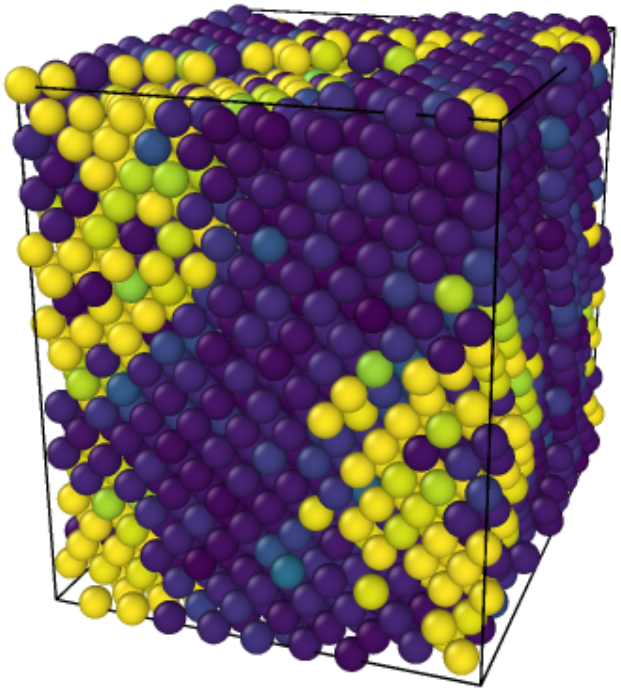


Fig 3. Simulation at 9 seconds

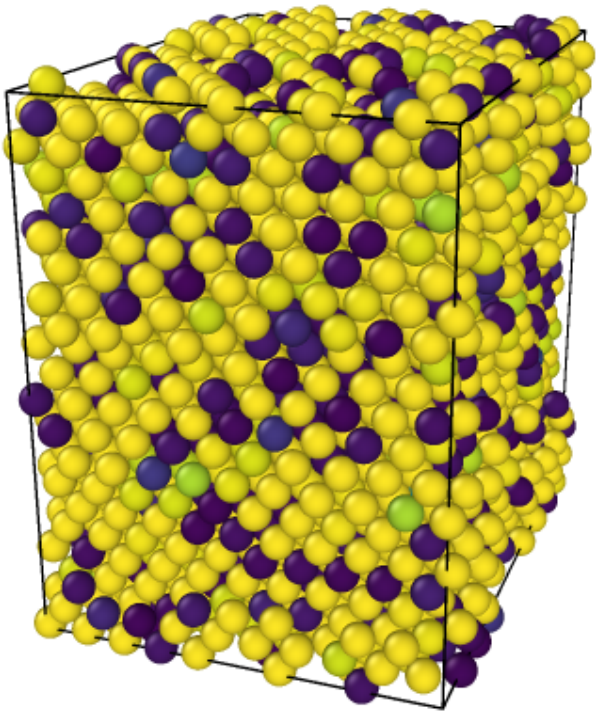


Fig 4. Simulation at 14 seconds

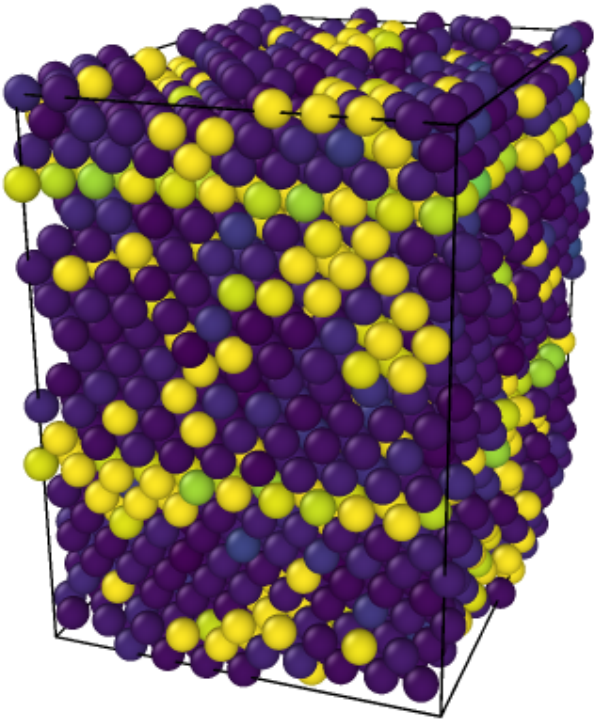


Fig 5. Simulation at 16 seconds

Now, I am working on the simulation of Lithium Manganese Oxide cathode. For that, I am trying to build the LMO structure for the same. A literature survey of its structural properties is being done. Some of the highlights have been presented below:

- LiMn2O4 unit cell contains eight lithium ions, eight trivalent manganese ions, eight tetravalent manganese ions, and 32 oxygen ions.
- The movement of lithium ions within the cathode material is dictated by the diffusion coefficient of the electrode material. The value of the diffusion coefficient will vary with state of charge (SOC) values, as the availability of the vacant sites changes.
- It is very difficult to perform precise experiments at the molecular level because there is a wide range of diffusion coefficients values at room temperature (10−8 cm2/s to 10−15 cm2/s) that have been reported in the literature using the different experimental methods.
- This is because the transport and other properties depend strongly on the initial procedures used, which influence the microstructure, defects, and atomic structure of the LiMn2O4.

- Interactions between various ions determine the potential, which is responsible for atomic movement, that will eventually govern the mechanical and chemical properties.
- In LAMMPS, pair potentials are defined between pairs of atoms that are within a cutoff distance and the set of active interactions typically changes over time.
- A unit cell of LiMn2O4 contains 56 ions (eight Li+, eight Mn3+, eight Mn4+, and 32 O2−), and these ions are in a cubical structure in the Fd3m space group.

References:

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