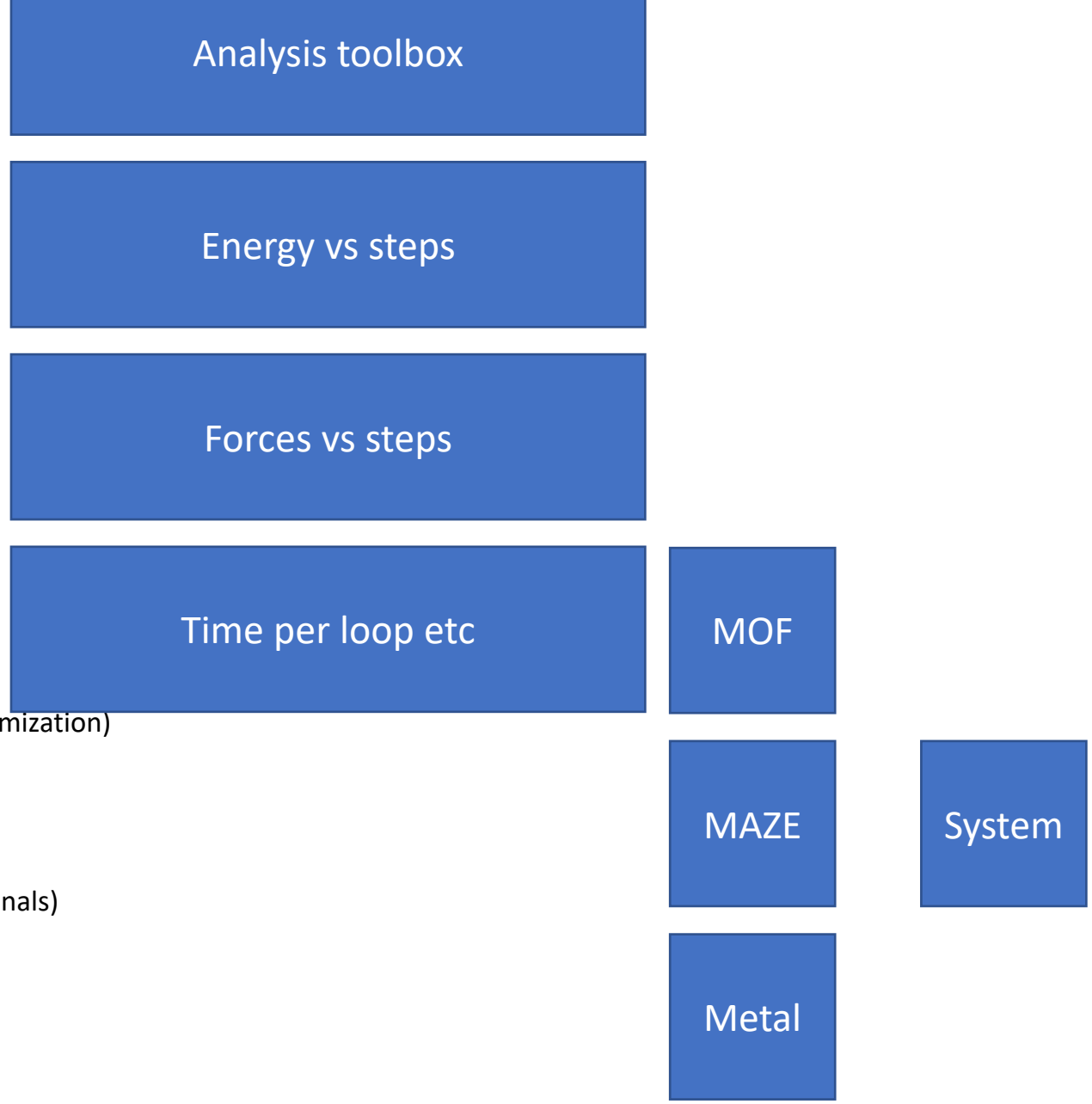
- What is my system? What does my traj fine contain?
  - Zeotype (“insulators”) + MOFs
  - Metals (“conductors, metallic oxides)
  - Isolated molec > LREAL = True
  - to set system defaults (this needs defaults.py file)
- Cluster specific parameters
  - This needs to be separate file
- How to move ions?
  - Optimization
    - Staged optimization  (300, 400, 500 eV)
    - Staged layers (2 layers, 3 layers, 4 layers etc)
  - MD
  - Vib
    - Isolated molec
    - Bulk
    - Ads
  - Hybrids (starting w a GGA)
  - Charges Bader and DDEC (these should just follow an optimization)
  - Solvation runs (starting w a GGA)
- Calculation checker?
- Convergence check
  - kt “convergence” functional TiO2 bulk (w different functionals)
  - kt k points, encut
  - Differnet nodes
- ~/.ktrc (“MgO project”)



- Calculation_type = “convergence”