

AI Based Catalysis Informatics Framework Using JI Prolog/jCompound Mapper/JikesRVM/IoT Computing Environments – A Novel Insight into the Chemical Informatics World of Catalysis.

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Abstract :

As explained in the TITLE mentioned above,we intend to explore the informatics aspects of Catalysis using Java related technologies.

index words: AI/Catalysis/Java/IoT/JI Prolog/jCompoundMapper/Nanotechnology.

Introduction/Inspiration :

“Catalysis is the increase in the rate of a chemical reaction by the addition of a reagent — the catalyst — that is not itself consumed. The catalyst works by opening up a route between starting material and product with a lower activation barrier than the uncatalyzed process.” -

Source/s :

[a] <https://www.nature.com/subjects/catalysis> ;

[b] <https://www.nature.com/news/can-artificial-intelligence-create-the-next-wonder-material-1.19850>

[c] <http://www.digitalistmag.com/digital-supply-networks/2018/02/27/iot-machine-learning-boost-chemical-companies-to-next-level-05921363>

AI Based Catalysis Informatics Framework & Implementation :

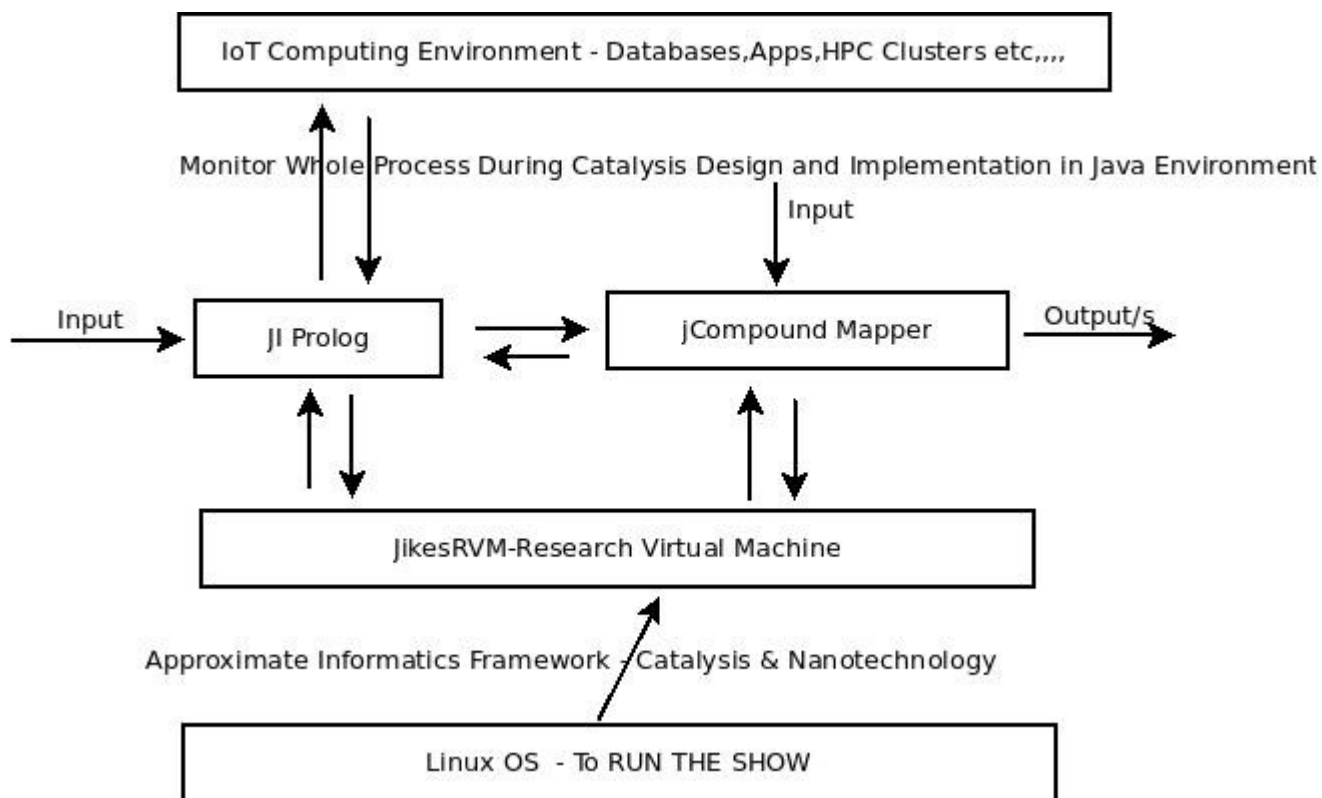


Figure I : Approximate Informatics Framework Using Java and Other Technologies.

R&D Analysis & Conclusion/s :

We have shown a simple informatics framework to probe the frontiers of Catalysis & Nanotechnology domains. This is one of the pioneering technical notes using these aspects of Software and Concepts.

Additional Information on Mathematics & Software Used :

[i] <http://www.jiprolog.com/> - JI Prolog

[ii] <http://www.jikesrvm.org/> - JikesRVM

[iii] <http://jcompoundmapper.sourceforge.net/> - jCompoundMapper: An Open Source Java Library and Command-Line Tool for Chemical Fingerprints.

Acknowledgement/s :

Thanks to all who helped me with this technical note meant for NON-PROFIT ACADEMIC R&D Purpose/s. This is only an approximate framework to encourage others to explore the interesting computational domains of nanotechnology. We do not vouch for any specific application in any way.

References :

[1] <https://en.wikipedia.org/wiki/Cheminformatics>

[2] <https://en.wikipedia.org/wiki/Catalysis>

[3] <https://en.wikipedia.org/wiki/Prolog>

[4] <https://en.wikipedia.org/wiki/IOT>

[5] <http://www.iotsworldcongress.com/wp-content/uploads/2016/01/document.pdf>