An Insight into Commutative Algebra Based Informatics & Computational Architecture for Cryo-EM Image Processing involving Gröbner Bases Using C++/Java/HOL/Scala/Scalalab/ImageJ Software Environments – A Short Communication on Gröbner Bases With Applications in Signals and Systems Using JikesRVM/JVM.

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Abstract :

In this research communication on commutative algebra it was proposed to deal with Grobner Bases and its applications in signals and systems domain.This is one of the pioneering communications in dealing with Cryo-EM Image Processing application using multi-disciplinary concepts involving thermodynamics and electromagnetics based on first principles approach.

keywords: Commutative Algebra/HOL/Scala/JikesRVM/Cryo-EM Images/CoCoALib/JAS

Introduction & Inspiration :

Cryo-Electron Microscopy (Cryo-EM) is an expanding structural biology technique that has recently undergone a quantum leap progression in its applicability to the study of challenging nano-bio systems,because crystallization is not required,only small amounts of sample are needed, and because images can be classified using a computer, the technique has the promising potential to deal with compositional as well as conformational mixtures.Cryo-EM can be used to investigate the complete and fully functional macromolecular complexes in different functional states, providing a richness of nano-bio systems insight. In this short communication,pointing to some of the principles behind the Cryo-EM methodology of single particle analysis via references and discussing Grobner bases application to challenging systems of paramount nano-bio importance is interesting. Special emphasis is on new methodological developments that are leading to an explosion of new studies, many of which are reaching resolutions that could only be dreamed of just few years ago.[1-9][Figures I-IV]

There are two main challenges facing researchers in Cryo-EM Image Processing :

“(1) The first challenge is that the projection images are extremely noisy (due to the low electron dose that can interact with each molecule before it is destroyed).

(2) The second is that the orientations of the molecules that produced every image is unknown (unlike crystallography where the molecules are packed in a form of a crystal and therefore share the same known orientation).Overcoming these two challenges are very much principal in the science of Cryo-EM. “ - according to Prof. Hadani.

In the context of above mentioned challenges we intend to investigate and suggest Grobner bases to process Cryo-EM Images using Thermodynamics and Electromagnetics principles.The inspiration to write this short communication was derived mainly from the works of Prof.Buchberger and Dr.Rolf Landauer.

source : The physical nature of information Rolf Landauer - IBM T.J. Watson Research Center, P.O. Box - 218. Yorktown Heights, NY 10598, USA .

source : Gröbner Bases:A Short Introduction for Systems Theorists -Bruno Buchberger Research Institute for Symbolic Computation University of Linz,A4232 Schloss,Hagenberg,Austria.

Additional interesting facts are observed from an article by Jon Cohen :
“Structural Biology – Is HighTech View of HIV Too Good To Be True ?”.
(http://davidcrowe.ca/SciHealthEnv/papers/9599-IsHighTechViewOfHIVTooGoodToBeTrue.pdf)

Researchers are only interested in finding better software tools to refine the cryo-em image processing tasks on hand using all the mathematical tools at their disposal.Commutative Algebra is one such promising tool.Hence the justification for using Grobner Bases.

Informatics Framework Design,Implementation & Analysis :

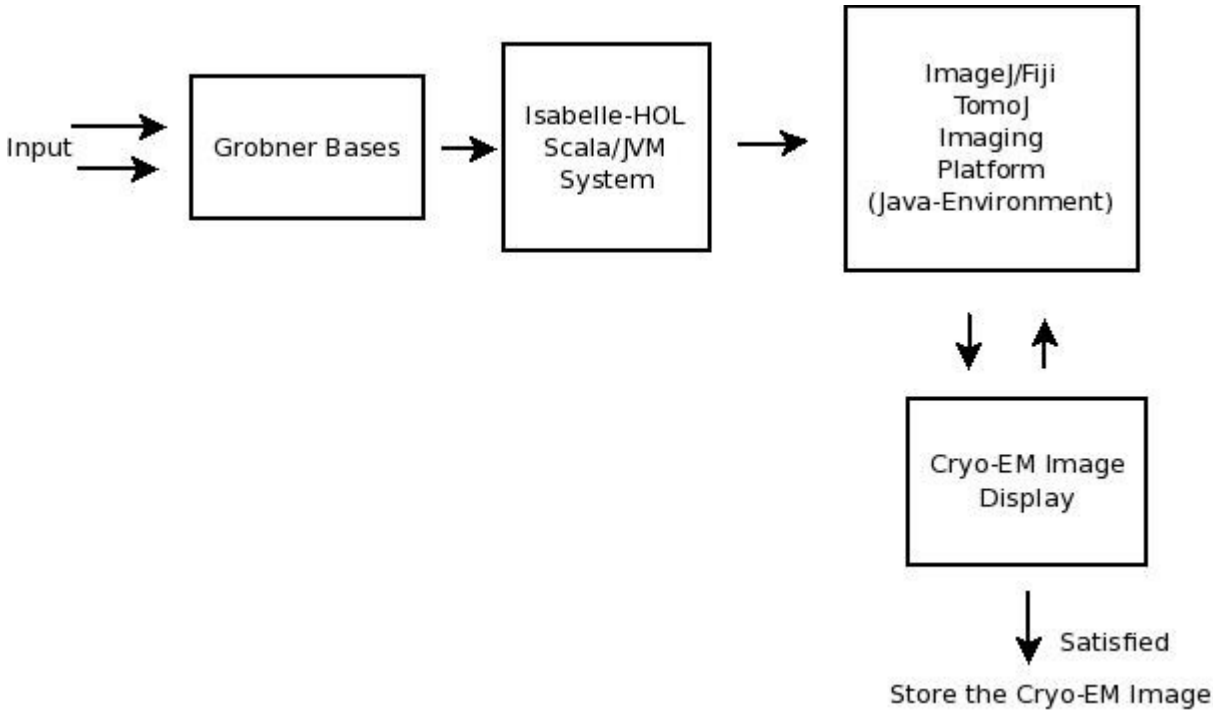

Figure I. Mathematical Algorithm Implementation and Software Architecture -Overall Idea presented in the paper.Self Explanatory Graphical Algorithm

Please Note : "Understanding JikesRVM in the Context of Cryo-EM/TEM/SEM Imaging Algorithms and Applications – A General Informatics Introduction from a Software Architecture View Point" by Nirmal & Gagik 2016 could be useful.

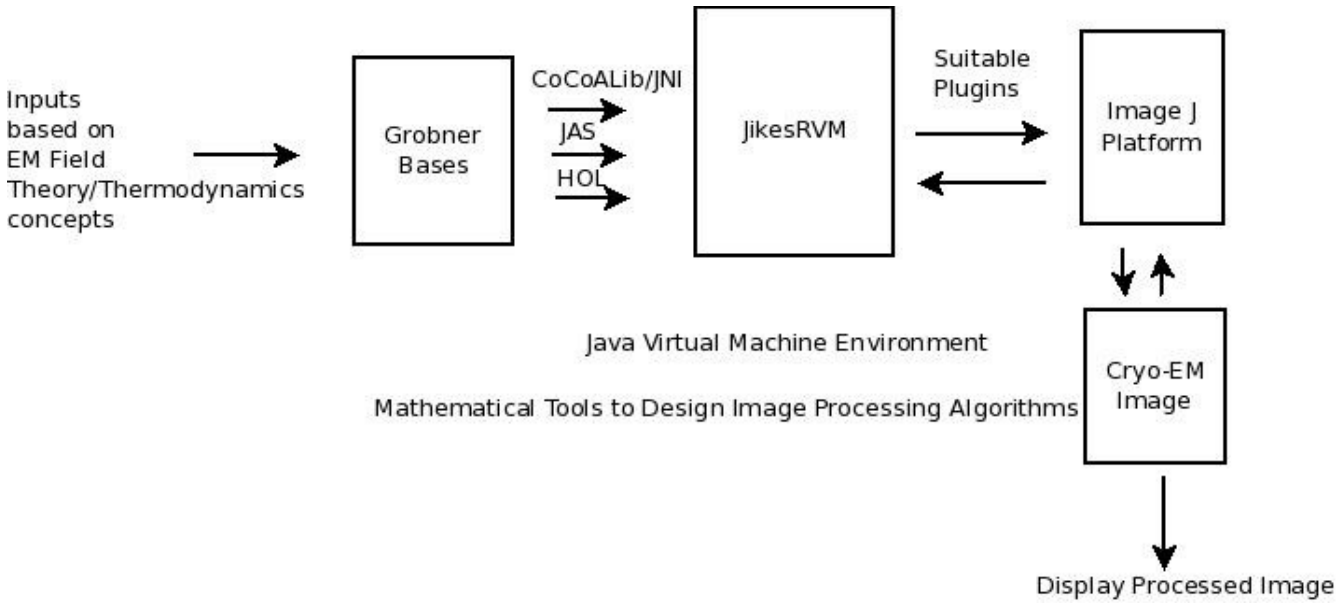

Figure II. Mathematical Algorithm with various Grobner Bases Mathematical Tools/Software.Self Explanatory Graphical Algorithm

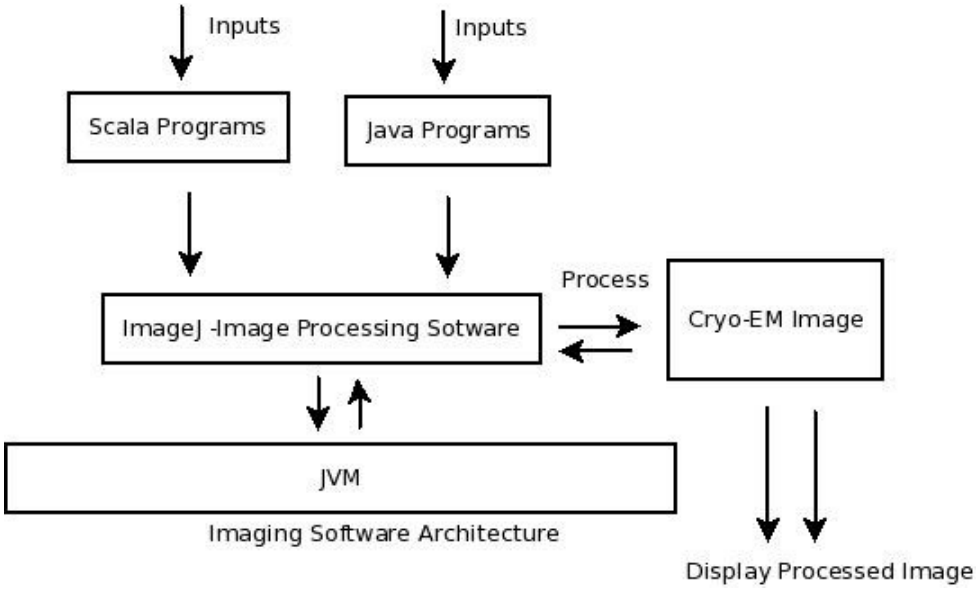

Figure III.Scala and Java based Software Architecture Flow Self Explanatory Graphical Algorithm

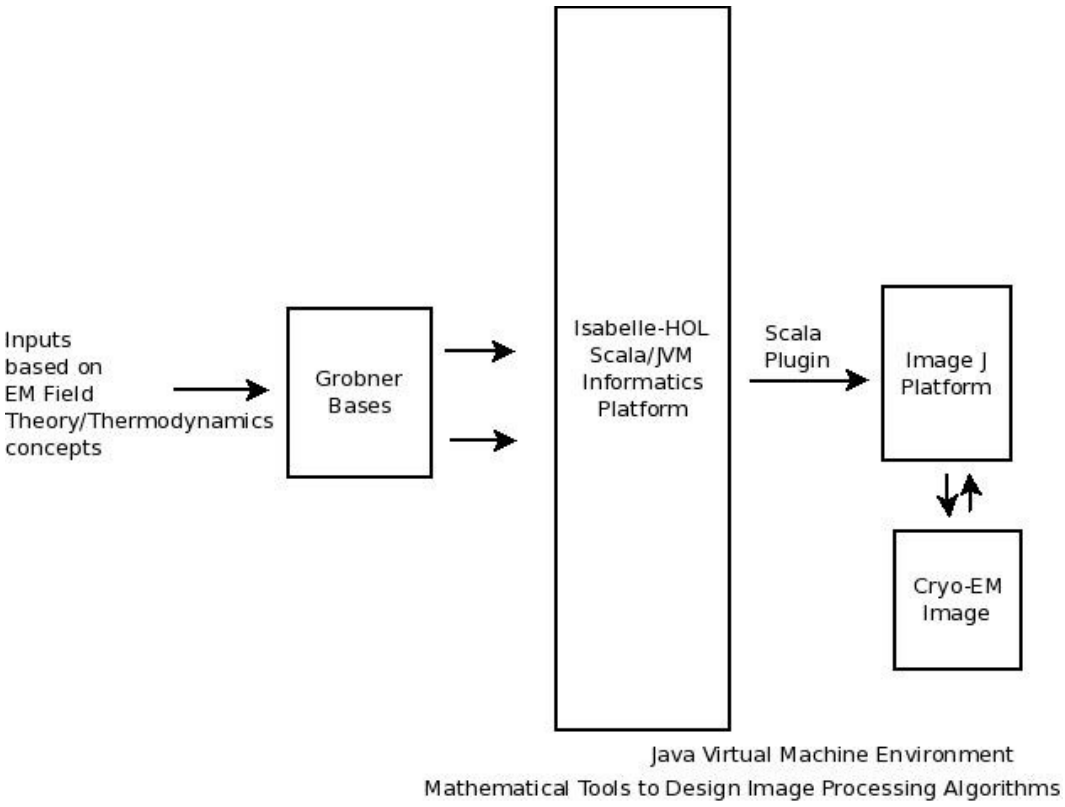

Figure IV. Mathematical Algorithm involving EM Field Theory & Thermodynamics Self Explanatory Graphical Algorithm

Conclusion :

In this paper, a brief overview on Gröbner bases theory,was addressed to novices without prior knowledge in the field but experienced readers would find it useful to apply these frameworks to the challenging aspects of Cryo-EM Image Processing. After explaining the general strategy for solving Cryo-EM Informatics and Image Processing problems via “Gröbner approach”, it was possible to develop some interesting concepts of Gröbner bases by studying the uniqueness of their nature in signals and systems domain. The algorithms are applied to Cryo-EM image processing examples.

Additional Information on Mathematics & Software Used :

[a]. Mathematical inspiration obtained from the following:

Hadani R, Singer A. Representation theoretic patterns in three dimensional Cryo-Electron Microscopy II – The class averaging problem. Found Comput Math (FoCM) 2011;11(5):589–616.

Hadani R, Singer A. Representation theoretic patterns in three dimensional Cryo-Electron Microscopy I – The intrinsic reconstitution algorithm. Ann Math 2011;174(2):1219–41.

https://www.ma.utexas.edu/users/hadani/research_statement2014.pdf

http://www.eigenvector.com/Docs/MIA_Intro.pdf

[b]. Cryo-EM Image Processing/HOL Software/Mathematical Software :

https://www.cl.cam.ac.uk/research/hvg/Isabelle/ ;

http://blake.bcm.edu/emanwiki/EMAN2

http://simple.stanford.edu/ ; http://bsoft.ws/ ; https://imagej.nih.gov/ij/

[c]. Scala/Scalalab/JVM/JikesRVM/JAS/CoCoALib :

http://www.jikesrvm.org/ ; https://docs.oracle.com/javase/specs/jvms/se7/html/

https://www.scala-lang.org/ ; https://github.com/sterglee/scalalab; http://krum.rz.uni-mannheim.de/jas/

http://cocoa.dima.unige.it/cocoalib/ ; https://arxiv.org/pdf/1611.07306.pdf {Grobner Bases for Everyone }

http://cocoa.dima.unige.it/cocoalib/examples/

https://mattpap.github.io/masters-thesis/html/src/groebner.html

[d]. Grobner Bases & Other Concepts :

http://www.risc.jku.at/people/buchberger/

http://www.risc.jku.at/publications/download/risc_2211/2001-02-19-A.pdf

Zhiping Lin et al : IEEE TRANSACTIONS ON CIRCUITS AND SYSTEMS—I: REGULAR PAPERS, VOL. 55, NO. 1, FEBRUARY 2008.

http://cqi.inf.usi.ch/qic/64_Landauer_The_physical_nature_of_information.pdf – **{** The physical nature of information Rolf Landauer - IBM T.J. Watson Research Center, P.O. Box - 218. Yorktown Heights, NY 10598, USA .}

http://philipball.blogspot.in/2013/01/the-thermodynamics-of-images.html

http://web.mit.edu/18.705/www/12Nts-2up.pdf – Text Book on Commutative Algebra

https://www.singular.uni-kl.de/

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[1].Tang G, et al. EMAN2: An extensible image processing suite for electron microscopy. J Struct Biol 2007;157(1):38–46.

[2]. https://www.researchgate.net/profile/Gs_Shmavonyan - Article: Understanding JikesRVM in the Context of Cryo-EM/TEM/SEM Imaging Algorithms and Applications – A General Informatics Introduction from a Software Architecture View Point by Nirmal & Gagik 2016.

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[4]. http://www.ncbi.nlm.nih.gov/pmc/articles/PMC3537914/

[5]. https://web.math.princeton.edu/~amits/publications.html

[6]. https://commons.wikimedia.org/wiki/File:Cryoem_groel.jpg

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[8].https://www.researchgate.net/publication/242023480_Presentation_CoCoALib_a_C_library_for_Computations_in_Commutative_Algebra [CoCoALib Information]

[9].https://www.researchgate.net/publication/307852987_CoCoALib_a_C_library_from_Algebra_to_Applications [CoCoALib Information]