Kernel Principal Component Analysis as Mathematical Tool In Processing Cryo-EM Images – A Suggestion Using Kernel Based Data Processing Techniques in a Java Virtual Machine(JVM) Environment.

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Abstract :

In this short communication,it was proposed to highlight some novel methodologies to probe,process and compute Cryo-EM Images in a unique way by using an open source Kernel-PCA and by interfacing the KERNEL-PCA via Java Matlab Interface(JMI) – JikesRVM system or any other Java Virtual Machine(JVM).The main reason to design and develop this kind of computing approach is to utilize the features of Java based technologies for futuristic applications in the promising and demanding domains of CRYO-EM Imaging in the nano-bio domains.This is one of the pioneering research topics in this domain with a lot of promise.Image de-noising and novelty detection paves the way and holds the key for better Cryo-EM image processing.

keywords:JikesRVM/JVM/Cryo-EM Imaging/Kernel PCA/Nano-bio systems.

Introduction :

In developing the informatics and computing architecture to test the mathematical algorithms,the following source was considered because of Hilbert Spaces concept in the processing of images.
A method was described which, like the kernel trick in support vector machines (SVMs), generalizes distance-based algorithms to operate in feature spaces, usually nonlinearly related to the input space. This was done by identifying a class of kernels which could be represented as norm-based distances in Hilbert Spaces. [1-5]

It could be observed that the common kernel algorithms, such as SVMs and kernel PCAs, are in fact termed as distance based algorithms and could be run with this class of kernels. Additionally these Kernel-PCA softwares provide a useful novel insight into how these algorithms work,the present work can form the basis for conceiving new algorithms and thus inspire others to propel this domain of Cryo-EM Imaging to newer heights.[2-9]

Ref: Advances in Neural Information Processing Systems, 2001 - /papers/upload_19728_msr-tr-2000-51.ps.gz ;The Kernel Trick for Distances - Microsoft Research, TR MSR(2000-51), Redmond, WA.USA.{Source : http://www.kernel-machines.org/publications/Scholkopf00}

As there is plenty of literature available online,the links to various references are mentioned here in this manuscript for the convenience of the readers.[1-17]

With the advent of Java based technologies and the Java™ Advanced Imaging API (JAI), sophisticated imaging functionality could be incorporated into Java™ applets and applications. This new capability facilitates the creation of cross-platform, Internet-enabled imaging software in an IoT Environment.[5-15] Please refer to the Figures shown in this paper: Figures [I-IV]

IoT – Internet of things.Developing Java based technologies have huge advantages.

Further it is useful to take a look at -

[i] JESSICA 2

[ii] JikesRVM

[iii] ImageJ/TomoJ/Fiji Software to develop or understand the approach presented in this paper.

[iv] http://eeweb.poly.edu/iselesni/DoubleSoftware/image.html {Simple MATLAB Files to perform de-noising of images}.It is however useful to download and play with these above mentioned software and their related publications.

[v].SCILAB/SCALALAB and MATLAB information is available on online.SCILAB/SCALALAB are free.MATLAB is a commerical product.

[vi] http://people.eecs.berkeley.edu/~wainwrig/stat241b/scholkopf_kernel.pdf

Implementation & Analysis :

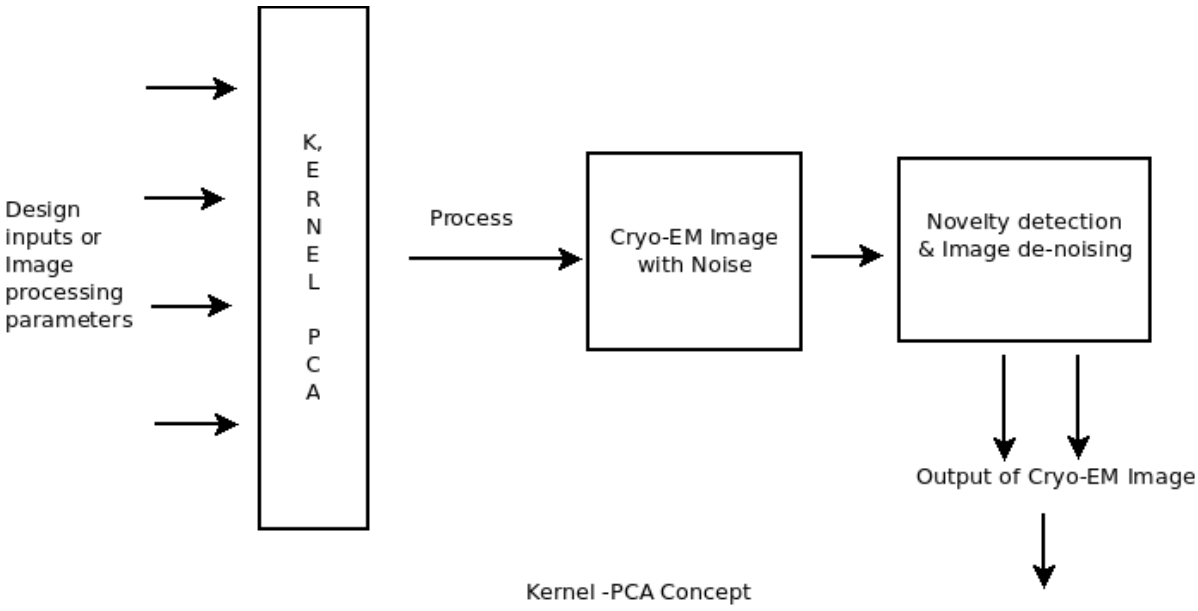

Figure I . Kernel – PCA concept and its software architecture

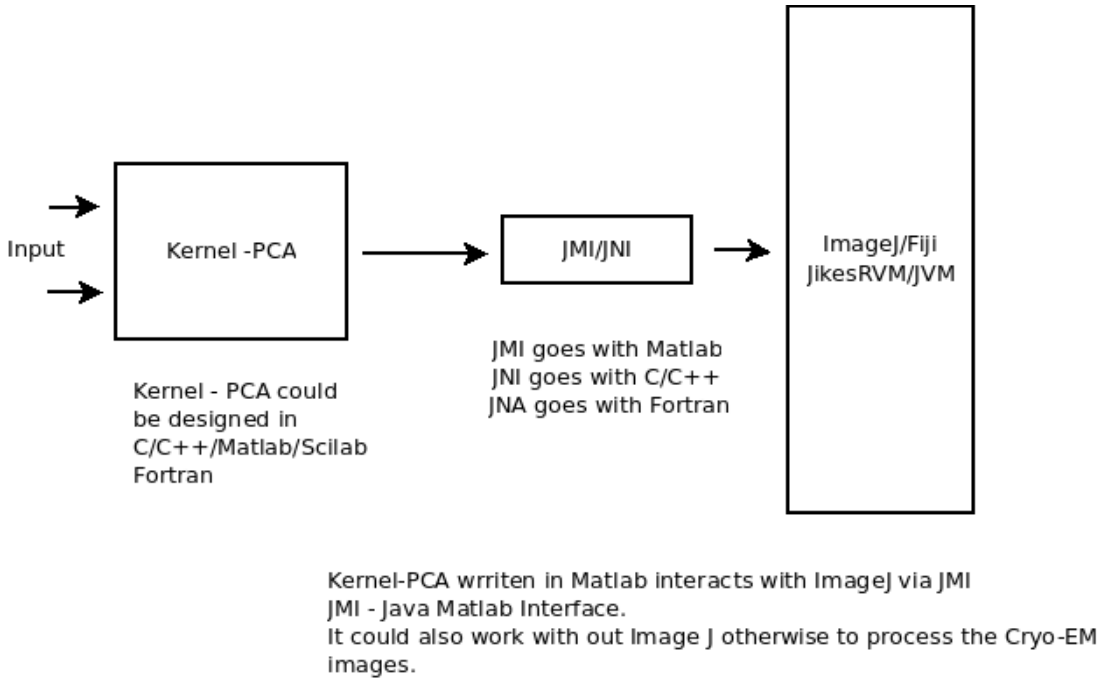

Figure II – Software Architecture to process Images

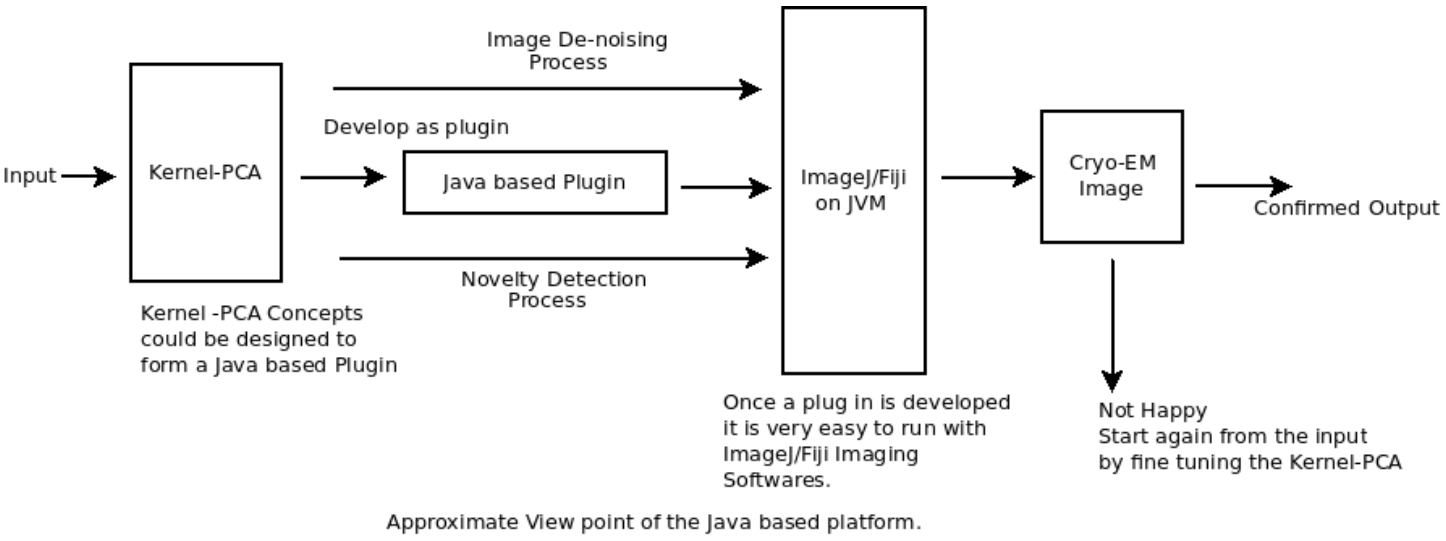

Figure III – Approximate viewpoint of the Java based platform for image processing

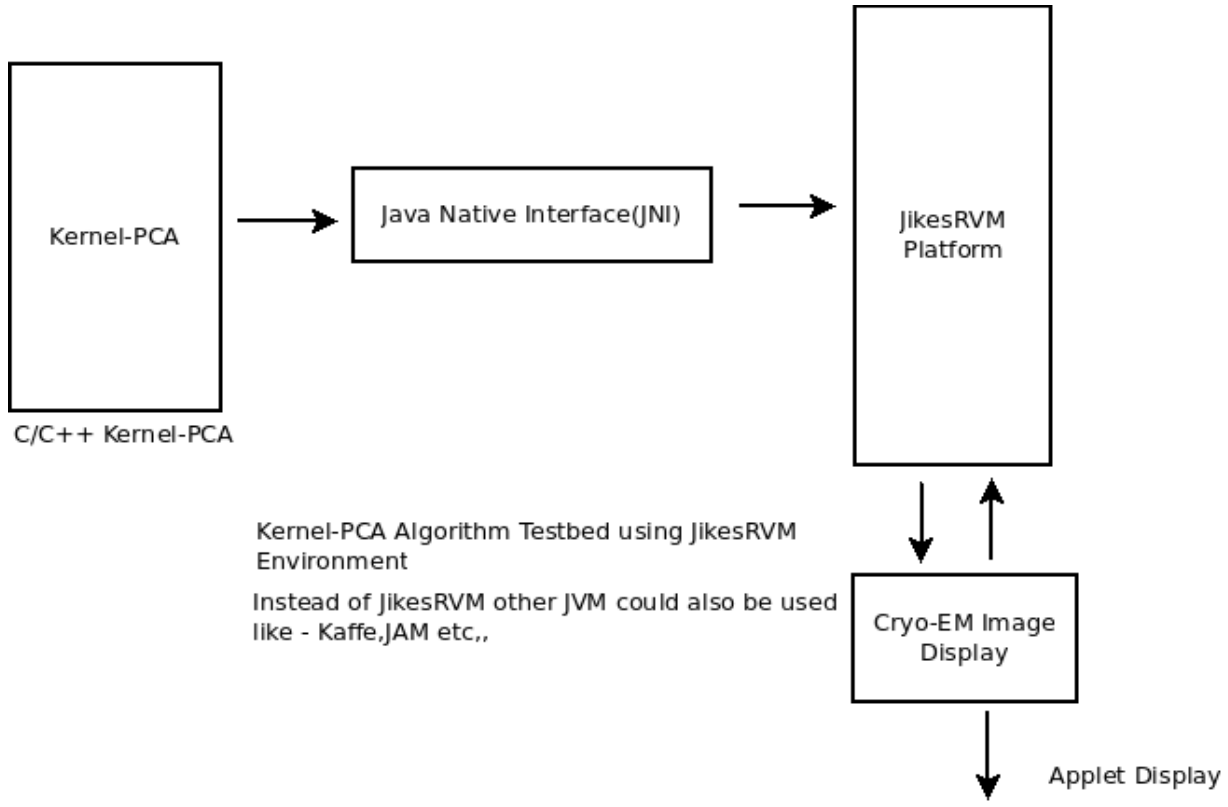

Figure IV – Kernel-PCA Algorithm Testbed Using JikesRVM or any other JVM(e.g.Kaffe/JAM)

Various methodologies and implementations were discussed using block diagrams from a simple view point.It is hoped that these architectures will certainly help in understanding the processing of Cryo-EM Images and their related processing[18-25].Kernel methods and applications are very wide spread in different areas of science and technology.

Concluding Remarks :

In this short communication,the author has highlighted and shown how to design and implement a simple imaging architecture by establishing communications between programs written in MATLAB/SCILAB/C/C++/Fortran via JNI/JMI/JNA in a Java Virtual Machine(JVM) software Environment.As the importance of Cryo-EM Imaging is growing in the nano-bio domains it is sincerely hoped that the readers would be inspired and create more advanced architecture based on novel methodologies for future computing platforms involving Cryo-EM Image Processing Application.

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Sincerely thank every one who made this happen in my life.No competing financial interest/s are declared in preparing this manuscript.This manuscript is meant to inspire others to develop more advanced Cryo-EM Software in this demanding area using novel methodologies.The Author strictly abides by all copyright agreements in using open source software or other such technologies used in this paper.Purpose - NON-PROFIT ACADEMIC R&D only.

Additional Information on Software & Mathematical Concepts :

[a].https://en.wikipedia.org/wiki/Fisher_kernel

/Graph_kernel ; /Kernel_smoother ; /Polynomial_kernel ; /Radial_basis_function_kernel

/String_kernel { Information is available from the same link }

[b].https://en.wikipedia.org/wiki/Kernel_principal_component_analysis#cite_note-4

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

[d].https://www.ebi.ac.uk/pdbe/emdb/empiar/entry/10060/

[e].http://imagej.net/Fiji ; http://www.jikesrvm.org/ ; http://cmib.curie.fr/en/download/softwares/TomoJ

[f].http://ei.is.tuebingen.mpg.de/person/bs
{ Kernel PCA. RBF Toy Example by Bernhard Schölkopf (in MATLAB). In this research paper some algorithms were tested using this software for pure academic purpose only }

[g] http://i.cs.hku.hk/~clwang/papers/cluster2002-FNL-jessica2.pdf

[h] http://spr.math.princeton.edu/ - Since ASPIRE CRYO-EM Software is in MATLAB -readers could try this option also additionally to test and see their MATLAB-JMI interfacing in a JVM environment.

References :

[1]. http://www.kernel-machines.org/

[2].http://www.kernel-machines.org/publications

[3].https://en.wikipedia.org/wiki/Support_vector_machine

[4].http://www.support-vector.net/

[5].Schölkopf, Bernhard; and Smola, Alexander J.; *Learning with Kernels*, MIT Press, Cambridge, MA,USA. 2002. ISBN 0-262-19475-9.

[6].Ivanciuc, Ovidiu; *Applications of Support Vector Machines in Chemistry*, in *Reviews in Computational Chemistry*, Volume 23, 2007, pp.291–400

[7].Ben-Hur, Asa, Horn, David, Siegelmann, Hava, and Vapnik, Vladimir; "Support vector clustering" (2001) Journal of Machine Learning Research, 2: 125–137.

[8].hawe-Taylor, John; and Cristianini, Nello; *Kernel Methods for Pattern Analysis*, Cambridge University Press, 2004. ISBN 0-521-81397-2.

[9].http://rsb.info.nih.gov/ij/

[10].https://imagingbook.com/links/

[11].https://yunhokim.wordpress.com/research/cryogenic-electron-microscopy/

[12].http://cryoem.berkeley.edu/cryoem

[13].http://www.drdobbs.com/jvm/a-long-look-at-jvm-languages/240007765

[14].https://www.ma.utexas.edu/users/hadani/publications.htm

[15].http://www.math.tau.ac.il/~bernstei/Publication_list/Publication_list.html

[16].http://www.cs.virginia.edu/~whitehouse/matlab/JavaMatlab.html

[17].https://code.google.com/archive/p/matlabcontrol/downloads

[18].http://www.cs.haifa.ac.il/~rita/uml_course/lectures/KPCA.pdf

[19].https://www.lri.fr/~gcharpia/chapter_kernels_CHS.pdf

[20]. http://research.cs.tamu.edu/prism/lectures/pr/pr_l28.pdf

[21]. http://www.face-rec.org/algorithms/Kernel/kernelPCA_scholkopf.pdf

[22].https://www.computer.org/csdl/proceedings/avss/2006/2688/00/26880041.pdf

[23].https://www.microsoft.com/en-us/research/publication/spectral-clustering-and-kernel-pca-are-learning-eigenfunctions/

[24].http://jmlr.org/papers/volume8/guenter07a/guenter07a.pdf

[25]. http://www.stat.wisc.edu/~xdeng/rkpca-rev2.pdf