An Interesting Inspiration to Probe Protein Engineering & its Promising Applications Using Spin Glass Theory & Related Mathematical Concepts - Based on Higher Order Logic(HOL)/Haskell/Scala/Deep Learning(DL)/Java Virtual Machine/JikesRVM(Research Virtual Machine) as Future Informatics Platform in Protein Engineering Domains.

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### [I] Introduction & Inspiration:

MIT chemists hope manmade 'xenoproteins' can help battle diseases like Ebola:

## Request readers to read the following for an in-depth introduction & inspiration.

http://news.mit.edu/2018/chemists-synthesize-millions-proteins-not-found-nature-0521

http://www.pentelutelabmit.com/portfolio\_page/xenoprotein-engineering-via-synthetic-libraries/https://en.wikipedia.org/wiki/Xenobiology

https://www.bionity.com/en/publications/1179491/xenoprotein-engineering-via-synthetic-libraries-biophysics-and-computational-biology.html

https://www.darpa.mil/news-events/2016-06-21

https://www.biocompare.com/Life-Science-News/350167-Platform-Builds-and-Tests-New-Proteins-Not-Found-in-Nature/

http://www.cira.kyoto-u.ac.jp/e/pressrelease/news/170809-130000.html https://miami.pure.elsevier.com/en/publications/achievement-of-insulin-independence-in-three-consecutive-type-1-d

https://www.sbir.gov/sbirsearch/detail/268093

https://www.exphem.org/article/S0301-472X(03)00376-X/pdf

https://www.rosettacommons.org/ - Baker's LAB USA.[Protein Folding Mechanisms etc]

[David Baker @ University of Washington, USA]

https://foldingathome.org/ - Pande's Lab USA[Protein Folding Mechanisms etc]

[Vijay Pande @ Stanford University, USA]

https://physicstoday.scitation.org/doi/abs/10.1063/1.2811676 [Spin Glass Theory]

https://phy.princeton.edu/people/philip-anderson[Important]

https://tel.archives-ouvertes.fr/tel-00683603/document [Spin Glass theory & Interesting Applications]

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC49199/ [Spin Glass Theory/Protein folding Codes]

[Optimal protein-folding codes from spin-glass theory]

### [II] Informatics Framework & Implementation Using HOL/Haskell/Scala/DL/JVM:

Approximate Informatics Framework Only. Actual implementation could vary to a great extent. Readers are requested to satisfy themselves before using these algorithms/framework presented here. It is only a suggestion. Testing in progress at the time of submission. [This short technical communication is based on all the materials referred to in this paper.]

## Algorithm is presented in the form of a simple Block Diagram

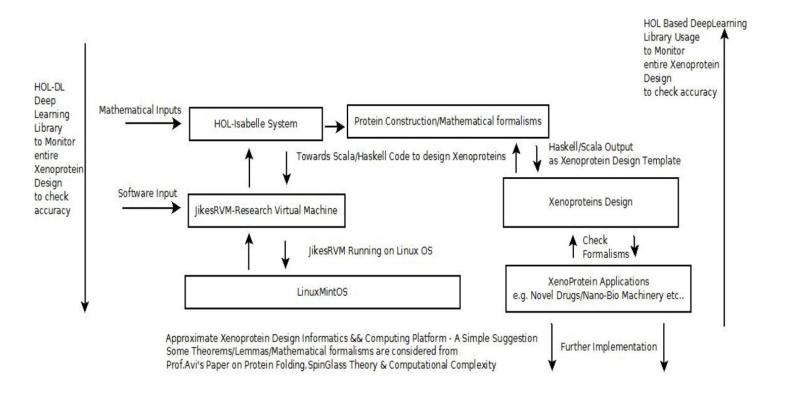


Figure I – Approximate Informatics & Computational Framework Simple Proteins or Xenoproteins could be considered to perform R&D further.

"MIT chemists have devised a way to rapidly synthesize and screen millions of novel proteins that could be used as drugs against Ebola and other viruses. All proteins produced by living cells are made from the 20 amino acids that are programmed by the genetic code. The MIT team came up with a way to assemble proteins from amino acids not used in nature, including many that are mirror images of natural amino acids. These proteins, which the researchers call "xenoproteins," offer many advantages over naturally occurring proteins. They are more stable, meaning that unlike most protein drugs, they don't require refrigeration, and may not provoke an immune response."

Source: [http://news.mit.edu/2018/chemists-synthesize-millions-proteins-not-found-nature-0521]

"There is no other technological platform that can be used to create these xenoproteins because people haven't worked through the ability to use completely nonnatural sets of amino acids throughout the entire shape of the molecule," says Brad Pentelute, an MIT associate professor of chemistry and the senior author of the paper, which appears in the *Proceedings of the National Academy of Sciences* the week of May 21."

Source: [http://news.mit.edu/2018/chemists-synthesize-millions-proteins-not-found-nature-0521] [https://www.nature.com/scitable/topicpage/protein-structure-14122136] — Important.

#### [III] Additional Information on Mathematics & Software Used :

### [a] Spin Glass theory & Protein Folding Mechanisms

http://guava.physics.uiuc.edu/~nigel/courses/563/essays2000/ricci.pdf

http://www.wisdom.weizmann.ac.il/~fraenkel/Papers/pfs.ps

https://dl.acm.org/citation.cfm?id=1013647.1013655

https://www.worldscientific.com/doi/abs/10.1142/9789814415743\_0008

https://www.annualreviews.org/toc/biophys.3/34/1?topicUri=ATYPON-AUTO-URI-cluster-3219

https://www.brandeis.edu/igert/pdfs/dasguptanotes.pdf

https://arxiv.org/abs/cond-mat/0505032

https://www.imsc.res.in/~menon/disorder\_chapter.pdf

http://people.fas.harvard.edu/~lsci1a/10-12.pdf

https://biology.stackex change.com/questions/51295/thermodynamics-of-spontaneous-protein-folding-role-of-enthalpy-changes

https://www.brown.edu/Research/Istrail\_Lab/papers/2001/2001\_newman\_chapter.pdf https://www.ncbi.nlm.nih.gov/pubmed/8281132

https://physicstoday.scitation.org/doi/10.1063/1.2811268

http://www.physics.rutgers.edu/~pchandra/physics681/sglass3.pdf

http://www.physics.rutgers.edu/~pchandra/physics681/sglass6.pdf

https://books.google.co.in/books?id=OMKpCAAAQBAJ&printsec=frontcover#v=onepage&q&f=false [Important Notes] - **DNA Computing: 6th International Workshop on DNA-Based Computers, DNA 2000, Leiden, The Netherlands, June 13-17, 2000**. Revised Papers – by Anne Condon,Grzegorz Rozenberg,Springer,29-Jun-2003-Computers-278 pages.

#### [b] HOL Software/Haskell/Scala/JikesRVM/JavaVirtual Machine

https://isabelle.in.tum.de/ &&

http://www.cse.chalmers.se/research/group/logic/TypesSS05/Extra/nipkow\_sl\_4lan.pdf

https://isabelle.in.tum.de/doc/tutorial.pdf

https://www.cl.cam.ac.uk/research/hvg/Isabelle/dist/library/HOL/HOL/document.pdf

https://www.isa-afp.org/

https://www.isa-afp.org/entries/Deep\_Learning.html

[The Archive of Formal Proofs is a collection of proof libraries, examples, and larger scientific developments, mechanically checked in the theorem prover <u>Isabelle</u>.]

https://www.jikesrvm.org/ && http://dmakarov.github.io/work/guide/

https://www.java.com/en/download/ && https://www.scala-lang.org/

https://www.tutorialspoint.com/scala/

https://github.com/tyrcho/scala-ai

https://bigdl-project.github.io/0.7.0/

https://ai.google/research/pubs/pub36605

https://www.haskell.org/ && https://mmhaskell.com/blog/2017/8/7/the-future-is-functional-haskell-and-the-ai-native-world

https://www.springboard.com/blog/best-programming-language-for-ai/

https://github.com/HuwCampbell/grenade; https://github.com/austinvhuang/awesome-haskell-deep-learning; http://hackage.haskell.org/package/haskell-ml

https://news.ycombinator.com/item?id=14411067

https://crypto.stanford.edu/~blynn/haskell/brain.html

https://towardsdatascience.com/starting-out-with-haskell-tensor-flow-49ec8aa7697f

#### [IV] Acknowledgment:

Thanks to all who made this happen. Non-profit Academic R&D.

This Short Technical Notes is Written & Presented in Free Style.

#### THE END