Analytical Study of Interrelation between Problem, Solution and Implementation Spaces from Computational Chemistry Compel to Develop Knowledge Management Framework

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Abstract - ***The problem space, which corresponds to well-defined computational problems, is the center of the computational chemistry problems in research domain chemistry. The lack of easily accessible problem specific information on the successful application of computational tools by others in the field is a critical barrier in this regard. This problem is faced by other domains in scientific computation also. In some of these domains knowledge management environments been developed to assist in this scenario***

I. COMPUTATIONAL CHEMISTRY DOMAIN – OVERVIEW

- The definition of computational chemistry offered by Lipkowitz and Boyd as "those aspects of chemical research that are expedited or rendered practical by computers" is perhaps the most inclusive. *Computational chemistry* is usually used when a mathematical method is sufficiently well developed that it can be automated for implementation on a computer.
- Computational studies can be used to predict the possibility of so far entirely unknown molecules or to explore reaction mechanisms that are not readily studied by experimental means. Computational chemists, in contrast, may simply apply existing computer programs and methodologies to specific chemical questions
- Branch of chemistry that uses principles of computer science to assist in solving chemical problems.
- It uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids.

It includes computational molecular science, empirical correlations and quantitative structure property relationships and aspects of process modeling and simulation.

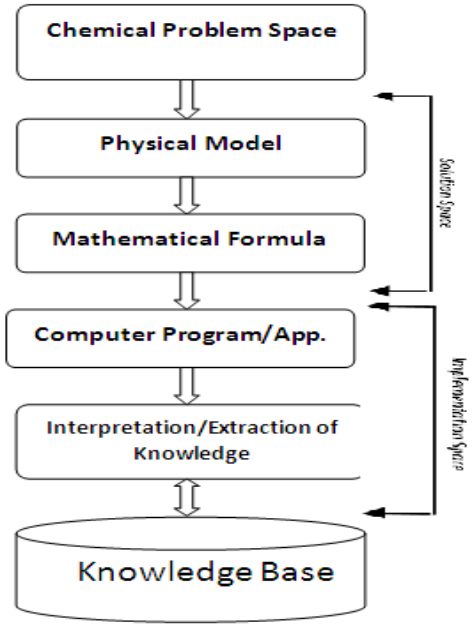
Aspects of computational chemistry include:

i. Molecular modeling.
ii. Computational methods.
iii. Computer-Aided Molecular Design (CAMD).
iv. Chemical databases.
v. Organic synthesis design.

***Examples for program suites*:**

i. GAUSSIAN
ii. NWCHEM ,
iii. GAMESS ,
iv. JMOL(IIT Bombay)
v. GchemPaint (IIT Bombay)
vi. TURBOMOLE ,
vii. ADF (DFT only) ,
viii. MOPAC (Semiempric and HF) ,
ix. TINKER (Molecular mechanics)

II. INVOLVED PROCESS FLOW



III. KNOWLEDGE MANAGEMENT IN COMPUTATIONAL CHEMISTRY

- A knowledge management environment focuses on capture, formalization and application of strong knowledge involved in a concerned domain. They formulate an exhaustive knowledge base and create a well-organized map of knowledge items and their relationships in it.
  - Computational chemistry requires such an environment to address the issues involving distribution and access of problem specific information in the domain.
  - Knowledge management comprises a range of practices used by organizations to identify, create, represent, and distribute knowledge for reuse, awareness, and learning across the organizations.
  - Knowledge Management through the objects –
    - Identify,Create,Represent,Distribute,Reuse,Codify, Awarness,Learning,Relate,Collect,Share,Capture,Organise,Transfer,Apply ,Use, Access,Map,Preserve

IV. PROBLEMS IDENTIFIED FROM COMPUTATIONAL CHEMISTRY DOMAIN

The problem space which corresponds to well defined computational problem is the heart of the ontology in this CC domain.

Based on literature review, primary and secondary datathere are 5major computational problems / methods which are taken for study as-

1. Reaction Mechanism
2. Molecular Modeling
3. Molecular Simulation
4. Geometry Optimization
5. Determination of Bond Energies

V. COMPUTATIONS AND ANALYSIS OF PROBLEM SPACE

Problem Category➔Reaction Mechanism

Formulation and Transformation of chemical reaction

Physical Model :

1. Combination Reaction
2. Decomposition Reaction
3. Displacement Reaction

Mathematical Formula➔ Chemical Interaction

Transformation

Element-1 + Element -2 -----→ Compound....Combination Reaction (A)

Knowledge Generated: Two reactant forms one product

Transformation

Reactant-1------→ Product-1 + Product-2....Decombination Reaction (B)

Knowledge Generated:

Electrolysis

Reverse of combination chemical interaction

No.of product is greater than no.of reactants

Displacement

Reactant-1+Reactant-2+....Reactant-n---→Product1+Product2+...Product-n---Displacement Reaction (C)

Knowledge Generated:

One molecule fragment another

New chemical fragmented may be harmful, waste product

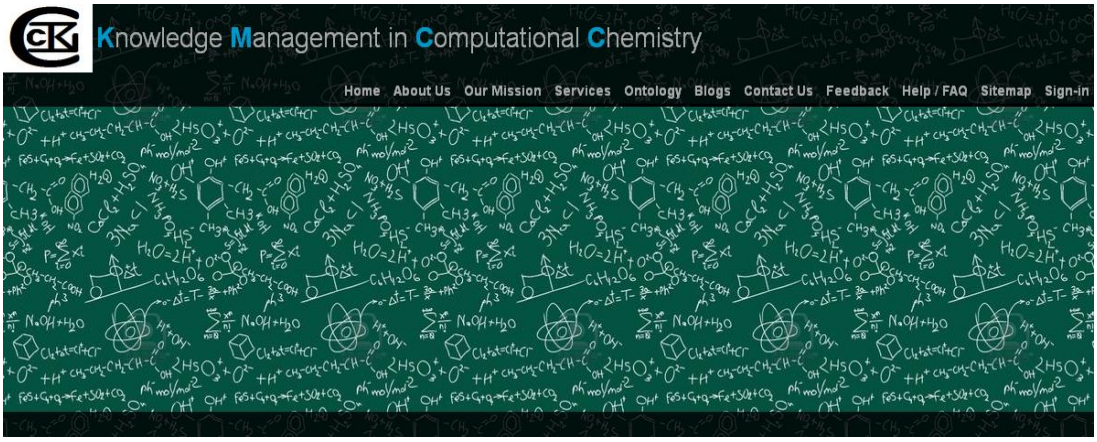
Catalytic converter required

VI. FORMULIZED SOLUTION SPACE

The solution space, which corresponds to existing algorithmic solutions, provides an up-to-date theoretical view of problem solving effort made by this framework.

VII. FORMULIZED IMPLEMENTATION SPACES

The implementation space is a practical view of the KMinCC domain that corresponds to existing implementation.



ICT (software) - based chemical computation will make computational chemistry more accessible in terms of the entry point in chemical domain.

All the study may further apply to describe the discovery of novel reaction mechanism and molecular modeling knowledge of which might help to build powerful chemical software knowledge-base in the future.Effective knowledge management supports the iteration and advancement of product and process understanding as knowledge flows, grows and evolves across the lifecycle in chemical domain. Your knowledge is an asset to your organization, and approaches exist to help manage as such KMinCC has been predominantly useful to handle challenges via relevant Computational Spaces.

A successful implementation of KMinCC would provide; set of application program as well as expertise required reaching higher level of knowledge base for productivity, individually and in workspace. This would facilitate quick, effective decisions in support of enterprise business objectives in Computational Chemistry domain.

VIII. ANALYSIS OF INTER-RELATION BETWEEN PROBLEM, SOLUTION AND IMPLEMENTATION SPACES

SrNo	Problem Category	Usage	Maths Formual	Algorithic Solution	ICT Tool	Open Source/License	OS	Language	Source
1	Reaction Mechanism	Two dimensional chemical structure editor for Linux Operating System,FOSS developed in 'C'.It allows to draw and display two dimensional chemical structure	$L_2 = \frac{1}{2}(\mathbf{z}-\mathbf{Hs})^T \mathbf{R}^{-1}(\mathbf{z}-\mathbf{Hs}) + \frac{1}{2}(\mathbf{s}-\mathbf{s}_p)^T \mathbf{Q}^{-1}(\mathbf{s}-\mathbf{s}_p)$	ab initio Algorithm	Schempain	Open Source	Linux	Dot.Net	http://www.nongnu.org/gchempaint/
2	Molecular Simulation/	Three dimensional viewer for chemical struoture and macro molecules.We can create and edit 3D model structure,FOSS developed in Java.Run on Win,MacOS,Linus,Android	$f_\Phi \leftarrow \max\{f(X_1), \ldots, f(X_m)\}.$	Aoocierated Random Soarch (ARS) Algorithm	Jmol	License	Windows	Java	http://jmol.sourceforge.net/
3	Geometry Optimizatio	To find total enery,charge density and elcotronic struoture of systems of electronics and nuclei within the Density Functional Theory(DFT)	$CRF \triangleq a_1 R_1 + a_2 R_2 + \ldots + a_m R_m = b_0 (b_1 P_1 + b_2 P_2 + \ldots + b_{m_p} P_{m_p}) \triangleq \sum_{i=1}^{m} a_i R_i = b_0 \sum_{j=1}^{m_p} b_j P_j$	ACRB algorithm	ABINT	License	Windows	Java	http://www.abinit.org/
4	Ab initio methods	Amsterdam Density Functional program system for high quality computational chemistry research.ADF	$ACR_4^n(t) = ACR_4^n(\Delta) + \frac{BW \, RIF_n \, PCR}{N_{VC} \, N_{RM_n}}(t-\Delta)$	ACRN Algorithm	ADF	Open Source	DOS	Dot.Net	https://www.scm.com/
5	Semi-empirical and o	EMAX offers a variety of programs, including EMAX Reagent Manager and EMAX Substance Manager. The Substance Manager program is designed to aid in tracking the entire life cycle of potential drug candidates, while the Reagent Manager is targeted at maintaining a chemical inventory.	$F = \sum_{i=1}^{m} \frac{f(j) - f_{\min}(j)}{f_{\max}(j) - f_{\min}(j)}$	AHM Algorithm	EMAX	License	DOS	Clipper	http://www.fuseschool.org/communities/113?qclid=CLnS5qzTgcdCFdcGwAodwJgAIA
6	Methods for solids	tracking the chemical inventory	$Max\{S_{Dice/Jaccard}(i,j), S_{MZE}(i,j)\}$	Arvis-Patrick Algor	TemboCher	Open Source	Linux	cobol	http://www.mkchow.com/tembochem.html
7	Reaction Mechanism	The technology uses the customer's choice of bar coding and tracks chemicals and containers as well as newly made compounds.	$\phi_j^{n+1} = \phi_j^n - \frac{\Delta t}{\Delta x_j}\left(F_{j-1/2}^n - F_{j-1/2}^n\right)$	ASD Algorithm	ChemCore	Open Source	Unix	Dot.Net	http://cmidd.northwestern.edu/chemcore/
8	Molecular Modeling	chemical inventory, programs are available to track fixed assets and equipment.	$\mathbf{v}(t) = \frac{1}{2}[\mathbf{v}(t+\frac{1}{2}\delta t) - \mathbf{v}(t-\frac{1}{2}\delta t)]$	Beeman's Algorithm	ChIM 5.0	Open Source	Linux	Fortran	http://pubs.acs.org/subscribe/archive/tcaw/10/i11/html/11comp.html
9	Molcoular Simulation/	eMolecules discovers sources of chemical data by searching the Internet, and receives submissions from data providers such as chemical suppliers and academic research institutions	$H_{tot} = (T_n + V_n) + T_e + V_{ne} + V_e = (H_n) + H_e$	Berny Algorithm	eMolecule	Open Source	DOS	PHP	https://www.emolecules.com/
10	Geometry Optimizatio	provides thermochemical, thermophysical, and ion energetics data compiled by NIST under the Standard Reference Data Program	$f_{\Omega}(x) := \begin{cases} f(x) & \text{if } x \in \Omega, \\ \infty \end{cases}$	Black Box Algorithm	NIST Chemistry WebBook	Open Source	DOS	Dot.Net	http://webbook.nist.gov/chemistry/
11	Determination of Bon	This database contains chemicals with their physical characteristics. Everybody can submit chemical information and retrieve information with a Web browser	$(A + UCV^T)^{-1} = A^{-1} - A^{-1}U(C^{-1} + V^T A^{-1} U)^{-1} V^T A^{-1}$	BLTF Algorithm	ChemExpo	License	Windows	Dot.Net	https://www.chemexper.com/advanced_search.shtml

IX. CONCLUSION

There is a need to characterize a chemical knowledge resources in a more comprehensive and integrated manner for example- reaction mechanism.

- In order to promote a common understanding of Knowledge Management in Computational Chemistry (KMinCC), it is essential to organize and unite knowledge manipulation activities in a way that not only describes each activity clearly and completely, but also identifies their inter-relationships.
- Framework designed and described here can serve as a starting point for creating a generic framework that unifies KMinCC concepts for reaction mechanism computational problem from chemistry domain.
- Creating a generic expressive framework of knowledge management would benefit from a synthesis of the descriptive framework obtainable here, favorable and direct inputs from KMinCC experts and scholars.

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