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KNOWLEDGE MANAGEMENT: A MUST FOR QUALITY COMPUTATIONAL CHEMISTRY

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Abstract— As chemical product design and development issues become more complex, chemists and scientists will need to have instant and reliable access to technical information along with advanced calculators and modeling tools. A powerful knowledge management system gives users those tools and technology to access critical information. More access to this information gives users a better understanding and that often leads to greater innovation. Without a knowledge management system, you will be much more limited to what you can do during the early stages of product development. Chemists are now able to investigate the properties of chemical structures at the molecular level. The aim of the research described in this paper is to in light on how to determining KM Architecture & Measuring the Knowledge Flow in Computational Chemistry. This paper also explores the Problems Associated with Knowledge Sharing in Computational Chemistry &efficient way for conversion of chemical data into knowledge.

Keywords— Chemical Product, Knowlwdge Management System, Computational Chemistry.

I. INTRODUCTION

Chemistry in the computer instead of in the laboratory

Chemistry is the study of molecules and atoms for how they interact. Computational chemistry aims to do these using computers. There are various problems are tackled in computational chemistry like exactly how molecules &atoms interact is determined by quantum mechanics. The problem is, however, that for allbut a few very simple systems it is impossible to solve these equations analytically. Hence, by necessity, we are enforced first to make estimates and then to resort to numerical computation [1].

Not surprisingly the fewer the number of estimates made the greater the computational effort required, and the dilemma for every computational chemist is to weigh required accuracy with available computing resources.

Use computer calculations to predict the structures, reactivity's and other properties of molecules. Computational chemistry has become broadly used because of

- Design of efficient quantum chemical algorithms
- Dramatic increase in computer speed and the

The computer calculations permit us to

- explore new or unknown chemistry
- explain and rationalize known chemistry
- acquire fundamental information about isolated molecules without the complicating solvent effects
- acquire direct information whereas need to interpret experiments

II. COMPUTATIONAL CHEMISTRY CHALLENGES

There are various computational chemistry challenges being tackled here.First we are interested in the properties of so called ''ion channels'', while inthe second we are looking at one of the basic reactions that supports photosynthesis. The long-term challenges for the application of computing technology can be divided into four major zones:

- Conversion of data into knowledge
- Support tools for the process
- Support tools for the business
- Training methodologies

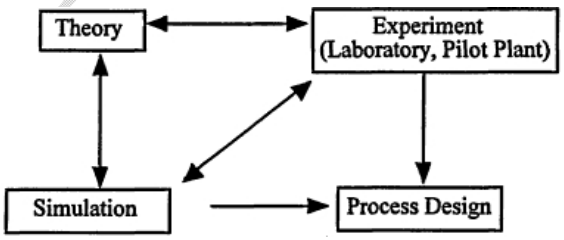

Fig 1 : Conversion of data into knowledge

2.1 Conversion of data into knowledge: The development of tools that would enable conversion of the wide-ranging data contained in enterprise information systems into actionable information and ultimately knowledge is of highest priority. Some of the capabilities that need to be pursued include soft-sensors, data rectification techniques, trend analysis and monitoring methods, and data visualization techniques [2]. Soft-sensors are critical to simplifying the detection of erroneous measurements by localizing the detection logic. Data rectification refers to the process of condensing and correcting redundant and inaccurate or erroneous process data so as to obtain the most likely status of the plant. Trend

analysis and monitoring refers to the process of using process knowledge and models to identify and characterize process trends so as to provide timely predictions of when and what corrective action needs to be taken. Data visualization is an essential element for facilitating understanding of process behavior and tendencies[3].

2.2 Support tools for the process: The decision support tools for the process include streamlined modeling methodology, multi-view systems for abnormal situation management, nonlinear and adaptive model predictive control, and process optimization using dynamic, and especially hybrid, models. Model building is generally perceived to be a key stumbling block because of the level of expertise required both to formulate process models and to implement them using contemporary tools[4]. The goal is to make model building and management rapid and reliable and to create environments in which the models associated with the various levels of the operational decision hierarchy will be consistent and unified. The role of abnormal situation management systems is to identify plant trends, to diagnose likely causes and consequences, and to provide intelligent advice to plant personnel. While components that address portions of this entire process have been under investigation for the past decade, full integration of the various qualitative and quantitative support tools remains to be realized. Needed developments in process control have been discussed in an earlier session and hence will not be reiterated here, except to note that control of batch and other intentionally dynamic processes needs to be given considerably more attention. Finally, the optimization of models consisting of differential algebraic systems, and especially differential algebraic systems with discrete elements, is essential to the realization of the vision for process operations. The latter type of so-called hybrid systems is particularly relevant to processes that involve batch and semi continuous operations.

The overall goal of these decision support methodologies for the process is to realize the integrated model-centered paradigm for process operation [5]. Under this paradigm all of the decision levels of the operational hierarchy are fully integrated through the shared use of consistent, robust models. Models serve as the central repository of process knowledge. Information flows from the lower levels to the higher levels to ensure that decisions fully consistent with the status and capacity of the production resources are made.

2.3 Support tools for the business: Thenext area of need is in the development of tools to support the overall business decision processes. The objective is to expand the envelope beyond the process itself and to encompass the business processes that are essential to driving manufacturing and the entire supply chain.

2.4 Training methodologies: To identify a new potential drug a large number of training and jobs must be evaluated. This results in many hundreds of or even thousands of jobs being presented to the compute cluster for processing. Each job takes a finite time from perhaps a few hours up to many days .It may available in Parallel Processing, Symmetric multiprocessing & Compute Cluster Multiprocessing.

III. ROLE OF COMPUTATIONAL CHEMISTRY

Molecular Modeling & Simulation Issues in Computational chemistry is many role – as molecular modeling software allows the user to select atoms from the periodic table and to place them in a three dimensional workspace. In most modeling systems it is possible to build a three dimensional molecular structure by using a color graphics user interface (GUI).

Computational technologies are embodied in nearly every aspect of chemical research, development, design, and manufacture. They have a broad range of applications, from molecularmodeling to the simulation and control of chemical processes. The aspects of computationaltechnology that are most critical to the chemical industry include computational molecularscience, process modeling and simulation, optimization of operations, process control, and andcomputational fluid dynamics. The field of computational chemistry, broadly defined, includescomputational molecular science, empirical correlations such as linear free energy relationshipsand Quantitative Structure Property Relationships, and aspects of process modeling andsimulation.1 the focus of this report is on computational molecular science, sometimes calledmolecular modeling. This involves models of chemical systems at the molecular or atomisticlevel, as well as predictions of quantum effects, At the most basic molecular level, this involvesthe solution of the Schroedinger equation for electronic motion or the solution ofNewton's equations of motion.

Computational Chemistry covers the overall attempt to model physical and chemical properties of molecules, their associations, and their chemical reactions. Historically the chemical industry has used the following sequential steps to achieve commercialization:

1. Research and development
2. Scale-up
3. Design
4. Optimization

The development of mathematical models that afford a seamless transition from microscopic to macroscopic levels is a worthy goal, and much progress in this direction has occurred in the past 10 years in areas such as computational fluid dynamics. However, due to computational limitations and to some extent academic specializations, process engineering research has devolved into four more or less distinct areas:

1. Process design
2. Structure property relationships
3. Process control
4. Process operations

A molecular-level understanding of chemical manufacturing processes would greatly enhance the ability of chemical engineers to optimize process design and operations as well as ensure adequate protection of the environment and safe operating conditions [6]. Currently there is considerable uncertainty in thermodynamic and reaction models, so plants are normally overdesigned to allow for this uncertainty. Also plants are operated conservatively because of an inadequate understanding of dynamic process behavior and the dire consequences if an unsafe condition arises. Chemical reactors are at the heart of this issue, with uncertainties in kinetic mechanisms and rate constants and the effects of reactor geometry on heat and mass transfer. Clearly the availability of better microscopic mathematical models for macroscopic plant simulation will help the chemical industry operate more profitability and more reliably in the future.

Besides providing fundamental data for process simulations, computational chemistry plays an important role in the molecular design process beginning at the basic research level. By predicting accurate thermochemistry, one can quickly scope out the feasibility of reaction pathways as to whether a reaction is allowed or not [7]. Computational chemistry can also reliably predict a wide range of spectroscopic properties to aid in the identification of chemical species, especially important reaction intermediates. Electronic structure calculations can also provide quantitative insights into bonding, orbital energies, and form, facilitating the design of new molecules with the appropriate reactivity.

IV. GOALS FOR COMPUTATIONAL CHEMISTRY

Computational chemistry can assist in the design and optimization of new and existing processesand products. It can be used to reduce the costs of development, improve energy efficiency andenvironmental performance, and increase productivity and profitability [8],[9]. Although computationalchemistry is currently being applied in the chemical industry to some degree, it is difficult, costly, and could see much greater use. There are significant limits to the type and size ofproblems that can be modeled, as well as the validation and reliability of the results. There are considerable barriers to entry for development of commercial software packages available to thebroad user community, and many codes that are available are difficult or impossible for no expertsto use.

Contributing to these limitations is the lack of people qualified or willing to workin the field, and the lack of published information and education about the benefits and use of Computational tools.Ideally, computational chemistry tools for the chemical industry need to be:

- ***Applicable to a wider range of systems*** — larger systems, liquid orsolid-state systems
- ***Flexible*** — inter-operable between various computing platforms and software, graphical userinterfaces, scalable
- ***Affordable*** — capable of running on desktops or lower-cost parallel computing platforms
- ***User Friendly*** — technical support mechanisms, expert systems for non-experts and experts
- ***Experimentally-validated*** — computations validated through experimentation
- ***Included in the educational curricula*** — undergraduate and graduate level software, coursework

V. CHEMICAL ANALYSIS: PROPERTIES CALCULATIONS

Chemical analysis is ananalytically important enabling technology essential to every phase of chemical science, product and process development, and manufacturing control.

- Equilibrium structures
- Transition State structures
- Reaction energies
- Reaction barriers
- Charge distributions
- Reaction Rates
- Reaction Free Energies
- Solvent Effects
- Density matrix methods
- Linear Scaling
- Crystal structures
- Melting points
- Molecular dynamics
- Solvent dynamics

Computational chemistry can be used to describe a diversity of chemical systems with a widerange of complexity. At the quantum molecular level, chemical systems of hundreds of atomscan be modeled today, and highly accurate calculations are possible for up to 10 atoms. Moreapproximate classical atomistic methods canhandle systems up to millions of atoms,

depending on the time scale. At the upper end, the mesoscale involves systems of billions ortrillions of atoms which still manifestmolecular effects.

There are many potential applications ofcomputational chemistry in chemical processes. Where predicting the characteristics andbehavior of a system may be beneficial. Bypredicting a system's behavior, computationalchemistry can potentially be used to improvethe efficiency of existing operating systems aswell as the design of new systems. It can helpto shorten product and process developmentcycles; optimize processes to improve energyefficiency and environmental performance, andsolve problems as they arise in plant operations.

VI. KNOWLEDGE MANAGEMENT IN COMPUTATIONAL CHEMISTRY

Knowledge Management: 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 Systems (KMS) focus on formalization and application of high domain knowledge. It is possible to measure the KMS's strength using the collaboration levels. In addition to adding a certain level of automation to the organization of the global knowledge structure, can assist in problem solving efforts by providing a greater amount of advanced device Intelligence. Seven steps to implement Knowledge Management, asfollows:

Step 1: Identify the Business Problem
Step 2: Prepare for Change
Step 3: Create the KM Team
Step 4: Perform the Knowledge Audit and Analysis
Step 5: Define the Key Features of the Solution
Step6: Implement the Building Blocks for Knowledge Management
Step 7: Link Knowledge to People

If we were to find molecules with the correct shape to fit to our binding site but would place regions of high electron density in contact with one another, Coulomb's Law dictates that the two molecules would repel and thus binding would not be able to take place. Similarly, repulsion would take place between molecules with a significant degree of electrostatically positive contact. Productive binding can thus only take place when the drug and drug target display regions of opposite charge on the electrostatic surfaces that would be in contact with one another when the drug docks into the target binding site.

Many programmes have been developed that are able to assign surface electrostatic potentials of molecules based upon a qualitative knowledge of the properties of their constituent atoms and then attempt to dock them together, and many new compounds in the clinic have been designed with the aid of these techniques. However, the ability of the computer to assign these charges and other properties of the molecules in question is entirely dictated by parameter sets stored within the computer.

In reality, it is known that when two molecules come into contact with one another they perturb the electron distribution within one another. This interplay between the electrostatic potentials of the two molecules in many instances is rather subtle but in some cases can lead to unexpected effects when the two molecules are allowed to bind to one another in real life. Moreover, many drugs that have long been on the market, such as aspirin and penicillin, operate by causing a chemical reaction between themselves and their target molecules alongside the initial binding event. These effects are much more difficult to anticipate and are often impossible to predict using the standard software in the industry based upon the traditional parameterized molecular mechanics (MM) approaches.

VII. DETERMINING KM ARCHITECTURE

7.1 Molecular Knowledge Bases

The molecular knowledge base design requires client and server interfaces. Both ofthese must be able to store and retrieve multiple conformations associated with integeridentifiers. The client contracts methods to retrieve entries from and record them backto the knowledge base, calculating them upon request if they are not available. It alsocollects recently-loaded entries for quick access should they be requested again. Theserver only has to process new data: it must identify newly-committed entries and store them in the knowledge base, resolving any clashing updates if necessary.

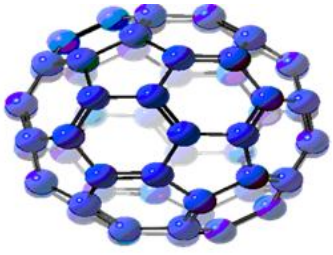

Fig 2 : Atom Model

MKB entries are accessed by name and conformation number (zero if they apply tothe ligand in general, not any particular shape). They also have an internal revisionnumber, incremented by the server whenever a new version is

committed, to identifyany clashes between multiple clients' edits. The standard base class, MKBEntry, handles allthe semantics of interacting with the client or server. Each possible entry type (molecularproperties, scoring function LUTs, etc.) must complete four additional functions: *IsPersistent* returns a Boolean indicating whether the value should be recorded in theMKB, or recalculated whenever it is requested.

Calc is the calculation function which should retrieve the molecule conformation andgenerate the appropriate data for the entry.

Load-Save should read-write the entry's value from/to the provided data stream fortransfer with the data repository. These may do nothing if IsPersistent returns false.

Following guidelines for running a KM project or creating a KM portal as describedby and, we propose a KM architecture that consistsof the following four parts-

1. People, specifically those who produce and use knowledge objects. Memberroles include administrator, knowledge author, knowledge reviewer, andtechnology designer. If no active knowledge authors can be found, it shouldbe considered a warning sign that the KM initiative in question is failing.

2. Knowledge objects, meaning sharable information based on extractedknowledge structures. The three knowledge object types in OpenCPS arecomputational problems, algorithmic solutions, and implementations. Here awarning sign of KM initiative failure is the lack of understanding of corecontent.

3. Technical infrastructure. Technology enables the capture, storage, anddelivery of content at the user's discretion. The costs associated withconstructing, maintaining, and improving technological interfaces are a keyissue for enablers. To ensure a quick launch of our KM project, we leveragedthe technology layer with existing content management systems (CMSs) thataddress the processes of creating, managing, and deploying content, but keptcontent separate from its presentation. A thorough description of what to consider when choosing a CMS can be found in.

4. Knowledge management processes. The KM life cycle modelscan is simplified for our proposed KM architecturefor two reasons: we already extracted the well-formed CPS knowledgestructure, and content management was delegated to the workflow-enabledCMS. When investigating the essential components of human interaction andcreativity, we discovered that has proposed four coreconcepts:-

a) New knowledge is built on previous knowledge
b) Powerfultools can support creativity
c) Refinement is a social process
d) Creativework is not complete until it is disseminated

The resulting four-phase"generate excellence (Genex)" framework—collect, relate, create, anddonate—provides a perspective that can be applied in the form of non-linearknowledge management processes in our work.

7.2 Measuring the Knowledge Flow

To support research of large scale or hard-core problem solving over a long timeperiod, we can highlight important CPS objects to attract the attention of researchersand new participants. By adopting the commonly accepted axiom— the morevaluable the information, the greater its access rate, we established a means ofmeasuring knowledge flow—that is, the process of sharing knowledge among peopleor knowledge processing mechanisms.

Knowledge flow measurement can help identify important topics within acollaborative knowledge portal. Some simple measures are provided by associatingthe actions of knowledge workers according to the four knowledge managementprocesses—collect, relate, create and donate, which are highly related to humancreativity. Tracking these measures with OpenCPS helps in the identification of activesubjects, which may take the form of problems, solutions, implementations, andaccessible resources within the OpenCPS knowledge portal.

7.3 KM Process- Brief Information about Problems in Computational Chemistry

Problem solving environments are platforms that provide all of the computational facilities required to solve a target class of problems. In Computational Chemistry large knowledge base is built on the formalization of a computational problem, and creates a well-organized map of knowledge items and their relationships in chemistry. Effective knowledge structures and collaboration facilities that are required to become useful knowledge base for computational chemistry problem solving. The problem space, which corresponds to well-defined computational problems, is the center of the computational chemistry problems in research domain chemistry. The solution space, which corresponds to existing algorithmic solutions, provides an up-to-date theoretical view of problem solving efforts made by computational chemistry problem solving research. Finally, the implementation space is a practical view of the computational chemistry research in chemical domain that corresponds to existing implementations. In this computational chemistry problem solving in chemical research, researchers can search a problem

space to see if a computational problem is well-defined, if algorithmic solutions are available, or if there is a need for a new computational problem object and the potential for a collaborative effort to create it.

In general, the greatest barrier to the application of computational chemistry is the limited ability to obtain results that are quantitative enough for practical problem resolution. Both non-expert and expert users often have difficulty linking the computational methodology with real applications, and in deriving meaningful knowledge from the results. This problem is exacerbated by a lack of good accessible benchmarks that could be used for comparison. The lack of published information on the successful application of computational tools by others in the field is also constitutes a critical barrier without some proven past success, many engineers are reluctant to expend the considerable cost and effort needed to apply these complex tools to their real problems

Table No.1: Critical Problem Areas in Computation Chemistry

Sr. No	Practical Usability For Non-Experts	Practical Usability By Experts	Applicability To Real Problems	Commercial Software Development
1	Lack of expert for running computations	Molecular simulation codes are not easy to use	Lack of sufficient quantitative accuracy	Small market size/insufficient funding
2	Lack of familiarity about computational Tools	Current training tools are not comprehensive enough	Lack of force fields for problems of interest	Commercial codes do not keep up with science
3	Lack of readily accessible database	Lack of framework for implementing results	Lack of many demonstrated successes	Lack of understanding of the software Development.
4	Start-up time for new model users	Realistic solution behavior is not routinely accounted for calculations	Lack of good accessible benchmarks	Too much of the software is UNIX based

The limited availability of input data such as general purpose, reliable force fields as well as easy-to-use methodologies is a major barrier to the application of computational chemistry to practical problems. One major issue is the lack of force fields (intermolecular potentials) that can be applied to solving problems of industrial interest. Many industrial problems require the ability to deal with liquids and solutions — a situation that is not routinely accounted for in currently available computational tools at the quantum scale. Current models also lack the capability to integrate time and length scales, and most simulations are limited by time, size, and number of units that can be handled. To solve real problems or design new materials, it is often important to be able to link and/or compare computational results with experimental data. This capability is quite limited at the present time. There is also little ability to link the results of molecular simulations with engineering correlations and process models. Developing this capability would greatly extend the utility of computational results for problems arising in chemical plants.

VIII. CONCLUSION

Computational problem solving researchers can search a problem space to see if a computational problem is well-defined, if computational chemistry solutions are available, or if there is a need for a new computational problem object and the potential for a collaborative effort to create it. The problem space, which corresponds to well-defined computational problems, is the heart of the computational problem solving research domain. The solution space, which corresponds to existing algorithmic solutions, provides an up-to-date theoretical view of problem solving efforts made by computational problem solving researchers.

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