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Review

Activity of the Computer Chemistry Society of Japan and Future Prospects Regarding Chemical Software

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Interdisciplinary activities involving chemistry and computers have been underway in Japan since 1982, and a lot of chemistry software were collected and distributed free to our members. In the age of the Internet, CAI was renamed as E-learning. The media have changed from floppy diskettes into mobile phone. Development of chemistry software will be more and more important in the future.
Key words: Computer chemistry, Chemical software, Chemistry education, CAI, E-learning

The Chemical Society of Japan (CSJ) is the largest of academic type in Japan. Since organizations such as the American Chemical Society do not exist in Japan, various societies have been formed for each professional field. In computer chemistry, we established the Society of Computer Chemistry of Japan (SCCJ) in 2002 to engage in interdisciplinary studies of chemistry and computer science. The society started in 1982 as the Japanese Association of Personal Computers for Chemists (JAPC). In 1992, the Chemical Software Society of Japan (CSSJ) was founded. The CSSJ and the Japan Chemistry Program Exchange (JCPE) merged to form the SCCJ in 2002. After the foundation of the JAPC in Japan, science groups combining the use of computers and chemistry were formed in Japan. One such group was the Division of Chemical Information and Computer Science in the CSJ, the CBI Society, the Theoretical Chemistry Workshop, and the CAC forum. To increase the strength and influence of the organizations, an effort was made to integrate the groups [1].

The present society (SCCJ) has a membership of approximately 1,000 persons, and symposia are held twice a year. Electronic and paper versions of the *Journal of Computer Chemistry of Japan* are published annually. The Internet version is available free of charge at http://www.sccj.net/publications/JCCJ/.

E-Learning Chemistry Education

The educational terms, CAI (computer-aided instruction) and CAL (computer-assisted learning), were novel in the initial stage of computers. The use of computers and the teaching of chemistry have developed in conjunction from the time of the primitive 8-bit computers and have continued to become more sophisticated. Eight-bit computers lacked the computing power to display Chinese characters and Kanji and were, therefore, unsatisfactory for many applications. A computer language, called BASIC, was used to develop resources for chemical dry labs. Graphic resources in the BASIC language were useful for chemistry education in the 1980s. The expansion of computer memory made it possible to use larger programs, especially when the shift from floppy diskettes to hard disk drives became common. Video learning was especially useful for studying chemical experiments.

E-learning is currently quite common. The use of local area networks (LANs) is also common in

teaching chemistry over the Internet. E-learning is presently used in Japan to teach chemistry. Japanese educators also make use of the Internet and LANs. A pool of educational resources using the Internet is currently available. A number of devices, such as personal computers, CD-ROMs, digital televisions, personal digital assistants, and mobile phones, are used for E-learning. Mobile telephones with Internet connections are commonly used in today's classroom by most students. In this manner, students have access to vast dictionaries available on the Internet that give them convenient portability.

Utility Computer Chemistry Software

The various chemistry societies assumed the responsibility for collecting and distributing chemical software to their members. Since 1986, when JAPC was in operation, an annual report on chemical software for PCs has been published. Free chemical software is distributed with a copyright. The software collection report in 1997 [2] included serials ISSN0919-4894 and ISBN4-906620-01-9, and the software was distributed on floppy diskettes (FD). In the next generation, the memory also increased, and it was downloaded from the network (SIG in PC-VAN). Thus, FD distribution ended. With the publication in 1997, the annual report of chemical software was terminated.

Software is now distributed on the Internet. There was no annual report on chemistry software in 1998. The JCPE registration list before 2002 is shown in Figure 1 with the present home page of the SCCJ. The current software can be used with existing computer systems. The utility software is listed in *Chemistry and the Chemical Industry*, a publication of the Chemical Society of Japan [3].

The software is the same despite the fact that it is 10 years old. The following software is listed: Spartan'04, WinMOPAC, ChemOffice, and CAChe. They are utilized worldwide because of their excellence for solving chemistry problems. The four types of software are briefly described below. Spartan'04 is a graphic utility software based on nonempirical and semiempirical molecular orbital calculations. WinMOPAC is a Window's version based on MOPAC, the semiempirical molecular orbital calculations. ChemOffice is a set product of ChemDraw, Chem3D, and ChemFinder, which are types of integrative software for a chemical aspect solution. CAChe is a molecular modeling system for a three-dimensional molecular calculation. The Japanese topic was MOLDA, a molecular modeling program developed by Hiroshi Yoshida et al. (1984) [4].


アドレス(D) http://www.sccj.net/download/JCPE/ 移動 リンク

日本コンピュータ化学会
Society of Computer Chemistry, Japan
http://www.SCCJ.net/

Home	SCCJについて	入会案内	ダウンロード
事務局からのお知らせ	発刊物・論文誌	イベント情報	化学の学校
会員エリア	賛助会員		リンク集

HOME -> ダウンロード -> JCPE登録プログラム

JCPE 登録プログラム一覧

JCPE Registered Program Information List

ID No.	プログラム名	用　途
No.124	Structure Model-Assembly Program Ver.1.10	粉末X線回折データ解析をモンテカルロ法とR因子法にて計算
No.123 頒布中止	cntmap2D & 3D: contour map CG creation program using Mesa	Contour map CG creation program using Mesa
No.122	MOLCAT ver.2.5.2(Gaussian98対応版)	分子構造・分子振動表示プログラム
No.121	ABINIT/GB	拡張ボルンの式(Generalized Born Formula)によって溶媒効果を取り込んだab initio分子軌道計算プログラム
No.120	ABINIT	ab initio分子軌道計算プログラム
No.119	F77-QB	FORTRAN77のプログラムをQuick-Basicプログラムへ変換
No.118	MOPAC Ver.6.03	溶媒効果を計算できるように改良されたMOPAC Ver.6.0(SOLPAC)
No.117	PiMO98	Huckel MO法の計算

Figure 1　The JCPE registration list before 2002

Table 1 The number of themes discussed in the symposia of the last 5 years

Year	2006	2005	2004	2003	2002
Simulation	6	12	11	18	13
Data analysis	52	70	44	74	50
Software	41	57	49	58	49
Apparatus	11	2	8	7	11
Database	2	6	6	5	7
Summation	112	147	118	162	130

Future Prospects of Chemical Software

Computer chemistry is likely to become a major discipline with the chemistry field. The four types of software listed above are likely to become even more popular and will most likely be enhanced as their use in research continues. ChemOffice is typical and widely used.

Interdisciplinary activities involving chemistry and computers have been underway in Japan since 1982. The number of themes discussed in the symposia of the last 5 years is shown in Table 1. The discussions are divided into the following categories: simulation, data analysis, software development, apparatus development, and database. The majority of the entries were in the disciplines of data analysis and software development. The discipline of computer chemistry will become more prominent as technology advances.

The development of E-learning chemistry resources is very important. Emphasis will be placed on the promotion and development of teaching resources and E-learning systems over the Internet. Video teleconferencing over the Internet is also being used. In addition, video-on-demand is available and makes it possible to use LANs for teaching. In addition to the many technological advances, facilities are being improved that all add to a better environment for education in the relatively new discipline of computer chemistry. Most chemistry teachers are able to teach students with several E-learning methods.

References

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日本コンピュータ化学会の活動と化学ソフトウェアに関する今後の展望

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我々は日本においてコンピュータ化学に関する学術活動を行い、化学ソフトウェアをたくさん集めて会員に無償で配布してきた。インターネット時代になると、CAI は e-ラーニングと呼ばれるようになった。コンピュータのメディアもフロッピーから携帯電話に至るまでいろいろと変化した。化学ソフトウェアの開発は今後ますます重要になるでしょう。
キーワード: コンピュータ化学、化学ソフトウェア、化学教育、CAI、e-ラーニング