MD tutorial for electrochemists
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僕作る人，私食べるひと

MD code maker, MD code user

TV advertisement: (Boy)I cook, (Girl)I will have it.

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*「私作る人、僕食べる人」と言って男女同権論者から叩かれたことから広告はすぐに「**僕作る人**、私食べる人」になった。

In the first TV ad. it was reverse. [(Girl) I cook,...] Feminists complained about it and the ad. changed.

「僕作る人」の場合 : cook theorist and programmer

「僕作る人」の場合 : cook

theorist and programmer

急がば回れ！ to do a new thing, it is much better to make the code
but she/he should understand the theory completely
and make the code that has no error.

「僕作る人」の場合 : cook theorist and programmer

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熱力学・統計力学・量子力学
Thermodynamics, Stat. mechanics. , Q. mechanics

理論 Theory

定式化 Formulation

数値計算 Numerical cal.

プログラミング Programming

「私食べるひと」の場合: Eater / MD User

熱力学・統計力学・量子力学 / 理論 定式化 数値計算 プログラミング

→100%集中しないと卒業までにはむずかしい！

何してる？　何を用意する？

at least we should understand what's going on inside the code, what we should do prepare ?

Gaussainなどのプログラムを使ってab initio計算が誰にでも簡単に行えるようになった。使い方が簡単なだけに，基礎知識なしに誤用して，とんでもない間違いを犯すことになる。この本はab initio法の化学への応用に必要最低限の事柄をわかりやすく解説している。何はともあれ，ab initio法を使う前にこの本にあることぐらいは勉強してほしい。

エモリー大学　諸熊　「電子構造論による化学の探究」のあとがきより

Model Calculation is a kind of Risky Business!!

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Check GIGO or not

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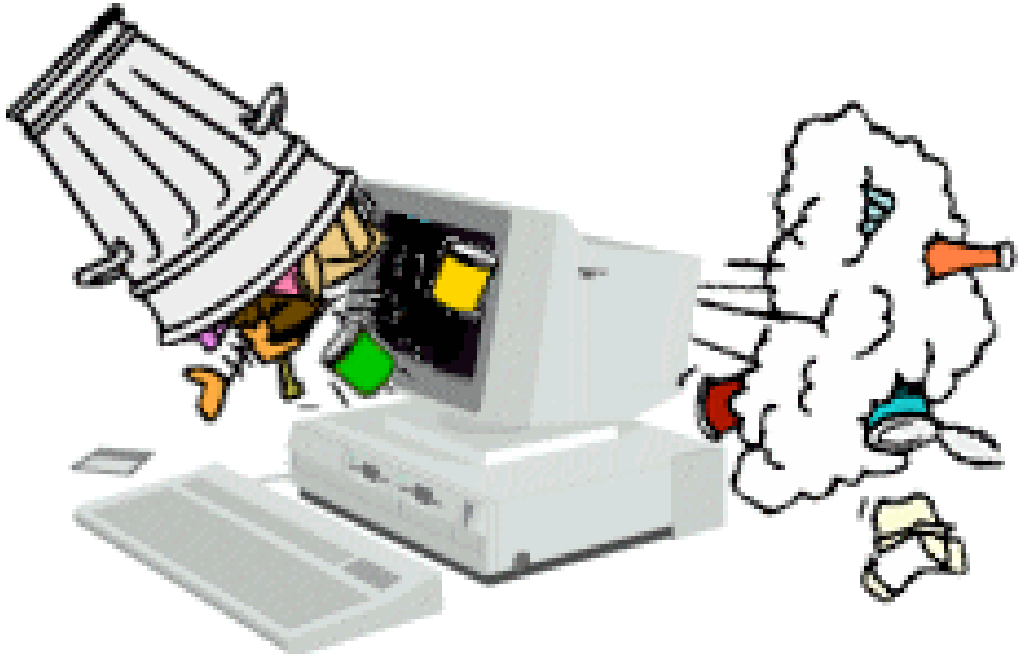
Check GIGO or not

Garbage in, Garbage out



D G Pettifor
Oxford 1997

Model Calculation is a kind of Risky Business!!

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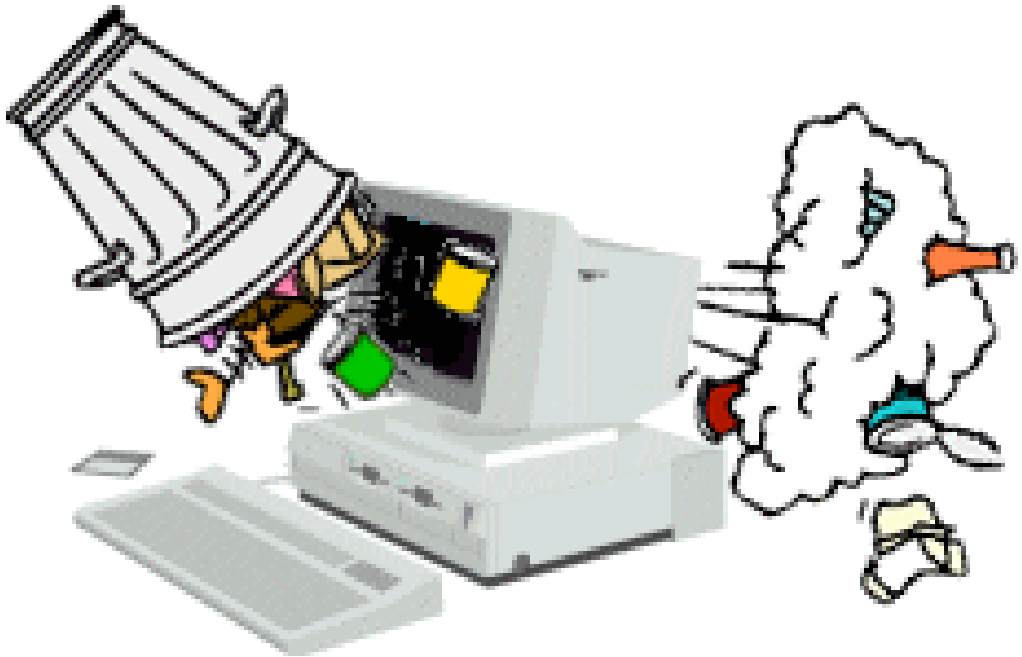


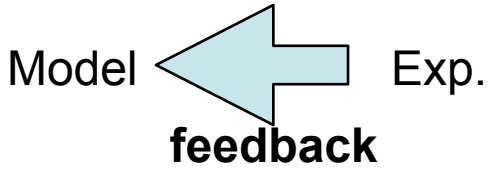
D G Pettifor
Oxford 1997

Model ← Exp.

feedback

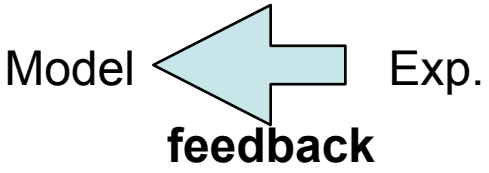
Garbage In → Garbage Out

Garbage In → Garbage Out



Junk In → Junk Out

junk: objects that have little value



Something In → Something Out

Userとして: tool

- Amber — Dr. Sokolov once tried, but ... 
- Insight — Dr. Sokolov once tried, but ... 
- DL-POLY 2 — user friendly, free, update frequently 

Userとして: tool

- Amber — Dr. Sokolov once tried, but ... 
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- ☞ The DL_POLY Molecular Simulation Package by W. Smith, CSE Department, CCLRC Daresbury Laboratory
- http://www.cse.scitech.ac.uk/ccg/software/DL_POLY/index.shtml

- Please download the manual (300 pages) from there and check it out

- DL_POLY is supplied to individuals under an **academic licence**, which is free of cost to academic scientists pursuing scientific research of a non-commercial nature.

Molecular Simulation

- 分子の集団の世界について
  (例えば溶液系，自己組織化膜，タンパク)
  for molecular ensembles such as liquid, SAM, and protein
- 見てきたような絵を描く
  have a virtual image
- 最も簡単な方法で正確に！
  using one of the simplest method with a high accuracy
- 最終的に熱力学量を求める。
  final goal: evaluate the thermodynamic properties.

Molecular dynamics　分子動力学法

１）原子iに働く力$\vec{F}_i$を計算する。 cal. the force on atom i

古典的　結合＝バネ，点電荷間のクーロン相互作用

Classical: bond=spring, Coulomb interaction between point charges

量子力学的　結合=電子，原子核，密度汎関数理論

Quantum mechanical: bond=electron, nucleus, DFT

２）原子iの運動方程式を解く。 solve the eq. of motion

$$\vec{F}_i = m_i \frac{d^2\vec{r}_i}{dt^2}$$

３）座標・速度（運動量）・力についての数値解を得る。 $\{\vec{r}_i(t)\}, \{\vec{v}_i(t)\}, \{\vec{F}_i(t)\}$

obtain the numerical solution of the time dependence of the atomic position, velocity(momentum), and force.

Molecular dynamics　分子動力学法

４）座標・速度（運動量）・力について時間平均・時間相関・空間相関を計算し，熱力学量・物性値を求める。cal. the time average, space-time correlation and get thermodynamic properties.

５）内部エネルギー，エンタルピーについては簡単にもとめられるが，エントロピーや自由エネルギーについては工夫が必要でありかつ計算時間が必要である。

It is easy to cal. inner potential and enthalpy but we need some trick to cal. free energy and entropy and it is time consuming.

DL-POLY 2：現状 current status

- すでにFortranソースコードは入手済み We got Fortran source code.
- いくつかのUnixマシーン上でコンパイル終了 The source code is already compiled on some Unix machines.
- [数種のUnixコマンド（通信関係，ファイルのコピー等々，実行ファイルをバックグランウンド走らせるコマンド等）とファイルのUnix上での編集(結局，vi が良いように思うが，個人の好みによる。）が必要である。分子の初期配置をするプログラミング（Fortran, C, C++)も場合によっては必要かもしれない。] Some Unix commands and the program to make the initial atomic positions may be necessary.
- Dr. V. Sokolovさんが，水バルク相・自己組織化膜・イオン性液体・イオン性液体｜水界面の計算を既に行った実績あり。 Dr. V. Sokolov used the MD code and cal. water, SAM, IL, IL|W interface.

Programming のおすすめ

- 非常に普遍的・マシーンによらない・Free of charge
- Fortran or C　どちらもGNU(http://gcc.gnu.org/)により提供されている.

- おすすめ本・サイト (これ一冊でOK)
- JIS FORTRAN入門(上) 森口 繁一 東大出版
- FORTRANが生き残っているのには理由がある。:特に数値計算分野
- http://www.komoto.org/fortran/
- http://members.at.infoseek.co.jp/kitaurawa/fortran.html

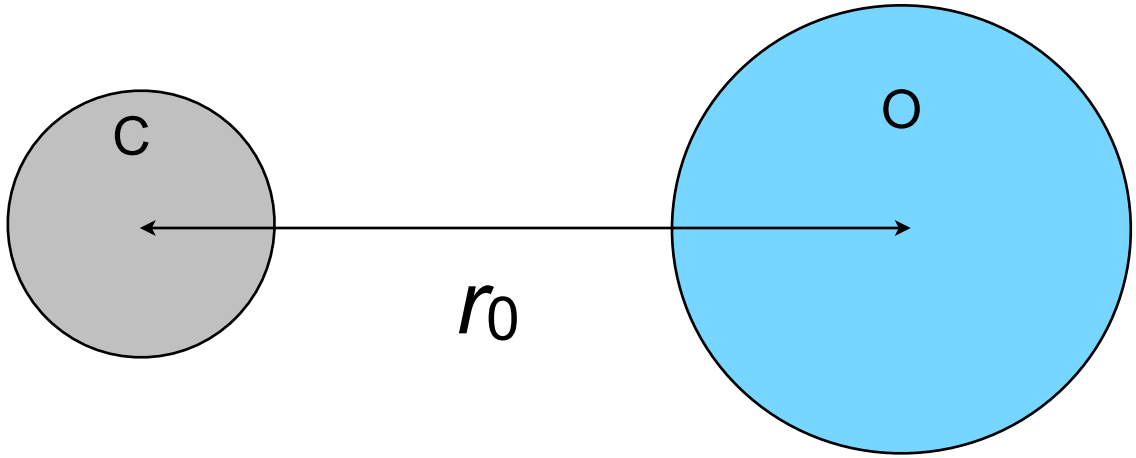
- 標準的なC言語でもよい。 http://www9.plala.or.jp/sgwr-t/index.html
- **or**　速習C言語入門—脳に定着する新メソッドで必ず身につく (単行本) 菅原 朋子 (著)

Problem 1

- Now we consider the system which contains *N* argon (Ar) atoms.
- 1) How many degree of freedom does the system has? The degree of freedom is equal to the number of the coupled equation of motion that we should solve.
- 2) We assume that the interaction between two Ar atoms depends on the interatomic distance. Then an Ar atom feels the force from the remaining *N*-1 Ar atoms. How many atom pairs we should consider for this system? The computation time strongly depends on the number of the interatomic potential!
- 3) How can we define the temperature of this system?

Problem 2

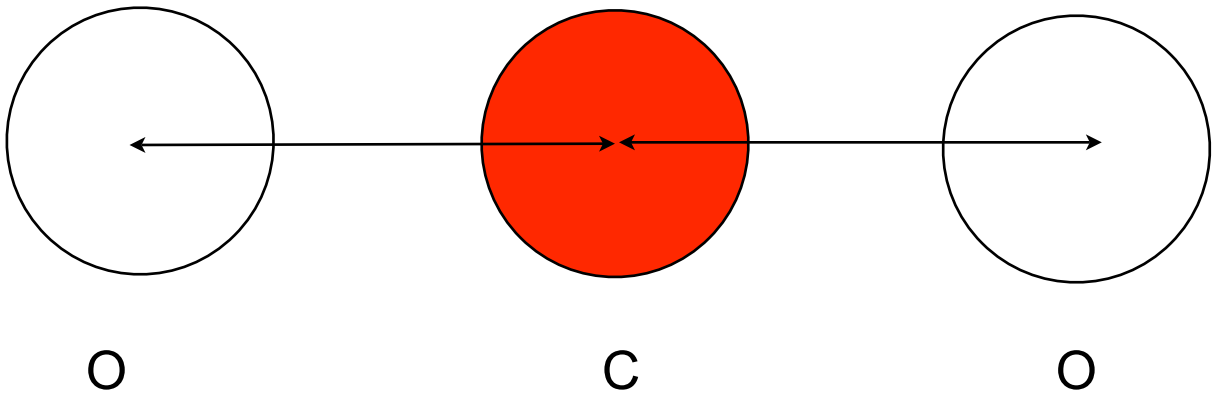
- Consider the vibrational motion of carbon monoxide CO molecule. Solve the equation of motion when the force constant(バネ定数) of C-O is given by k, mass of carbon and oxygen is given by m_1 and m_2. respectively. The equilibrium distance between C and O is r_0. The vibrational frequency of CO is 2170 cm^{-1}. Determine the value of k / Nm^{-1}.



Get the potential energy V of the vibration. $F = -dV/dr$

Problem 3

- Next we consider linear CO_2 molecule. How many does this molecule has the degree of freedom for vibration? (Hint: translation:3, rotation:2) Show the vibrational frequencies of the mode that the vibrational motion is confined in the molecular axis. The force constant of CO is *k'* and the atomic mass is the same as problem 2. The equilibrium distance between C and O is r'_0. Using this model can we get the experimental vib. frequencies 1333, 2349 cm^{-1}?



Answer

- 1. 3N, N(N-1)/2, the velocity is Maxwell-Boltzman distribution
- 2. $x(O) = x_0(O)+Aexp(-i\omega t)$, $x(C) = x_0(C) + Bexp(-i\omega t)$, $m_2 A + m_1 B = 0$, $\omega^2=k(m_1 + m_2)/(m_1m_2)$, $x_0(O) - x_0(C) = r_0$, $k=1900\ Nm^{-1}$ $V= (1/2)k(x-x_0)^2$, $x = [x(O) - x(C)]$, $F(O) = -k[x(O) - x(C) - x_0]$
- 3. 4 degree of freedom, $\omega^2=k'/m_2$ (symm.), $\omega^2=k'(m_1+2m_2)/(m_1m_2)$ (anti-symm), $2349/1333=1.76$, $[(m_1+2m_2)/(m_1m_2)]^{0.5} / [1/m_2]^{0.5} = 1.91$

学習プラン:Proposed Study Plan

http://www.users.kudpc.kyoto-u.ac.jp/~d54649/web_material/selfstudy.html
にあります　**「大学院授業資料１へ」**　**「大学院授業資料２へ」**　**「 大学院授業資料３へ」**
をまずはざっとお読みください。次回からDL-POLY2のmanualに従って進行しますので，少々の基本知識を各自仕込んでおいて頂ければ幸いです。

- **§古典的分 子シミュレーション　Classical　Molecular　Simulation**
- 2. 分子動力学シミュレーション　MD (Molacular Dynamics)
- MD self-study note 自習ノート(pdf more than 70 pages by MY)　→作る人用かもしれない
- 関連資料 by MY　大学院授業資料１へ　大学院授業資料２へ　大学院授業資料３へ
- LJ-Potential MD program (Fortran)　LJ-Potential MD input data: liquid case
- LJ-Potential MD input data: solid case
- radial distribution function G(r) for LJ solid and liquid
- mean square displacement of LJ- solid and liquid
- movie of LJ-liquid
- Link: The DL_POLY Molecular Simulation Package by W. Smith
- Amber Home Page
- VMD(visual molecular dynamics)

Please download the some files from http://www.users.kudpc.kyoto-u.ac.jp/~D54649/web_material/MD2006_04.pdf, http://www.users.kudpc.kyoto-u.ac.jp/~D54649/ web_material/func_sol_chem1.pdf, http://www.users.kudpc.kyoto-u.ac.jp/~D54649/web_material/fun_liq_2.pdf, http://www.users.kudpc.kyoto-u.ac.jp/~D54649/web_material/fun_liq_3.pdf . We will have a seminar using the DL-POLY manual next, so it is my great pleasure if you will learn something from them.

I will send the second correspondence on request.

three examples for DL-POLY

1) Argon gas, liquid, solid (LJ)
2) Water (O-H, H-H rigid) (LJ + charge)
3) Water (flexible) (LJ + charge, bond distance and angle)
4) 1,2-dichloroethane (flexible) (LJ + charge, bond distance ,angle and torsion)