Computational Materials Science (計算材料学特論)

http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/D2MatE_programs.html?page=cms

COMPUTATIONAL MATERIALS SCIENCE 2026 Q2
2026年度Q2 計算材料学特論 (資料: 英語＋日本語版)

Lecture materials for numerical analyses (by Kamiya)
数値解析に関する講義資料・pythonプログラム (神谷担当分)

Update News:

- **June 16, 7:52, 2026:** Lecture materials for June 16 has been updated: course_materials.zip
- **June 15, 12:40, 2026:** Lecture materials for June 16 has been uploaded
- **June 12, 17:17, 2026:** Final version: Lecture materials for June 12 has been updated: course_m

We would wait for five minuities (i.e., till 8:55).
In meantime
- **download the latest lecture materials (updated this morning)**
- **hear the short audio guide. English and Japanese versions available**

FY2026

#02 June 16, 2026: Numerical differentiation (数値微分), N integration(数値積分), Differential equation (微分方程式)

Course materials (Lecture slides and python programs):

- course_materials.zip

5-8min audio guide:

- 日本語: 0:00 / 5:26 (VOICEVOX 四国めたん&ずんだもん)
- English: 0:00 / 6:09

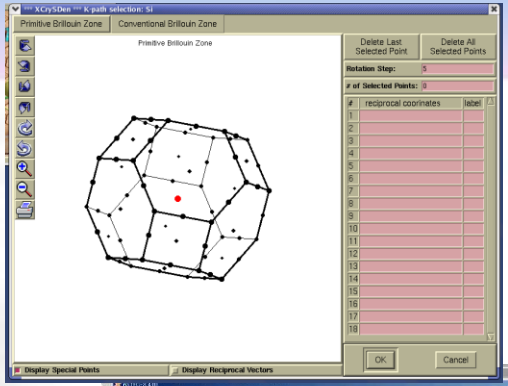
Slide files and Videos (monologue):

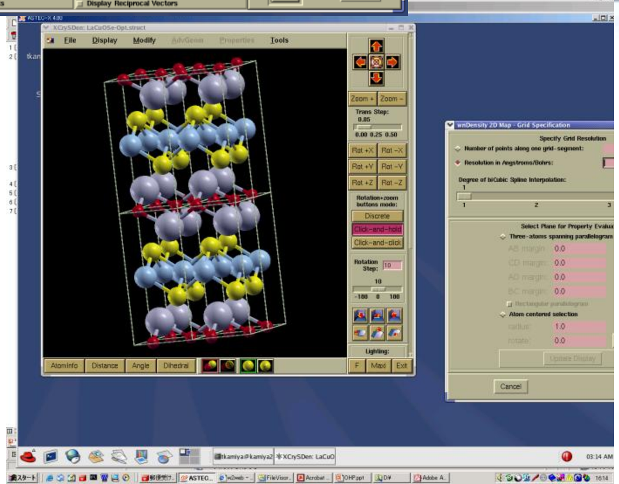
1. **Introduction:** 20260616-01-1.pptx
2. **Numerical differentiation:** 20260616-02-1Differentiate.pptx

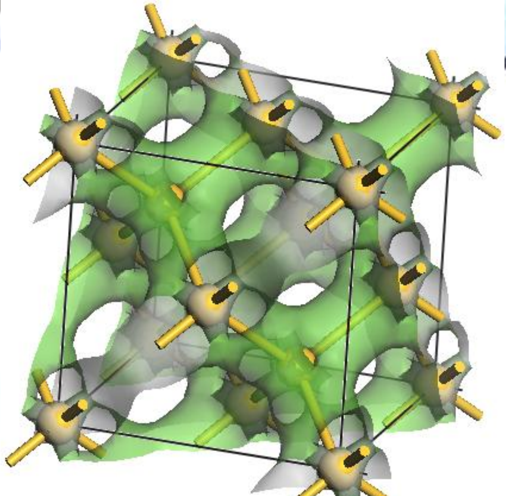
MAT.C505

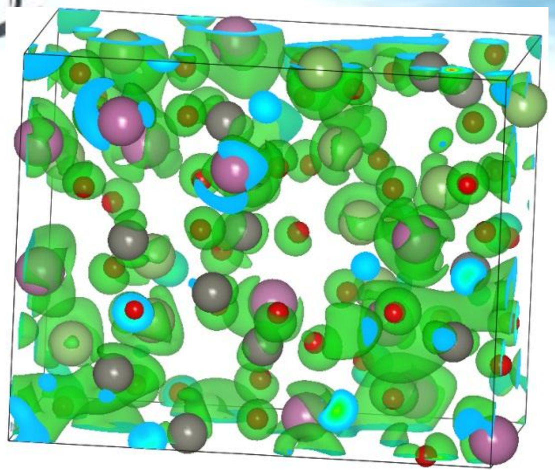
Computational Materials Science
計算材料学特論

Toshio Kamiya
神谷利夫









Class Schedule

Lecture materials (Kamiya’s part): **http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/?page=cms**

授業 6月10日(水)～7月28日(火), 7月30日(木) 月曜の授業 7月23日(木) 期末試験･補講 7月29日(水), 7月31日(金)～8月6日(木)

#01 June 12 (Fri) Kamiya (Fundamentals of computer, Sources of error (コンピュータの基礎、誤差), Numerical differentiation (数値微分))

#02 June 16 (Tue) Kamiya (Numerical differentiation (数値微分), Numerical integration (数値積分), Differential equation (微分方程式))

#03 June 19 (Fri) Kamiya (Differential equation (微分方程式), Molecular dynamics (分子動力学法), Interpolation (補間), Smoothing (平滑化))

#04 June 23 (Tue) Kamiya (Linear least-squares method (線形最小二乗法), Optimization (最適化), Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化))

#05 June 26 (Fri) Kamiya (Nonlinear optimization (非線形最適化), Fourier transformation (フーリエ変換)

#06 June 30 (Tue) Kamiya, Matrix (行列)

#07 July 3 (Fri) Kamiya, Review (復習)

#08 July 7 (Tue) Sasagawa (Review of quantum theory 1: 量子論おさらい1)

#09 July 10 (Fri) Sasagawa (Review of quantum theory 2: 量子論おさらい2)

#10 July 14 (Tue) Sasagawa (First principles calculations: basics 1 第一原理計算：基礎1)

#11 July 17 (Fri) Sasagawa (First principles calculations: basics 2 第一原理計算：基礎2)

#12 July 2 (Fri) Sasagawa (First principles calc.: applications 1 第一原理計算：応用1)

#13 July 24 (Fri) Sasagawa (First principles calc.: applications 2 第一原理計算：応用2)

#14 July 28 (Fri) Sasagawa (Classical and Quantum Computers 古典および量子コンピュータ)

Explanation of the answers

課題解答の解説

PROBLEM, June 12

- **Submit electronic file(s) via LMS until the midnight of June 14**
  (If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
  In this case, file name must include your STUDENT ID and FULL NAME)

Choose one of the following PROBLEM 1 or PROBLEM 2

PROBLEM 1:

(i) Convert 100101_2 to base 10

(ii) Convert 6432_{10} to base 16

PROBLEM 2:

Choose one of the python programs given today (sum_error.py, sum.py, base.py).

・Explain what each block of the source code does,

or

・list up the source code parts that you cannot understand what they do or why they are needed.

今日配布したプログラム (sum_error-plt.py, sum.py, base.py) から1つを選び、
以下のいずれかを答えよ

・ソースコードのそれぞれの部分が何をしているかを説明する

・ソースコードの中で理解できない部分、あるいは なぜそれが必要かわからない部分を述べよ

PROBLEM, June 12

(i) Convert 100101_2 to base 10

> python base.py 100101 2 10

Convert 100101 in base 2 to base 10
0 -th digit = 1_2: + 1*2^0 => + 1 _10 => 1 _10
1 -th digit = 0_2: + 0*2^1 => + 0 _10 => 1 _10
2 -th digit = 1_2: + 1*2^2 => + 4 _10 => 5 _10
3 -th digit = 0_2: + 0*2^3 => + 0 _10 => 5 _10
4 -th digit = 0_2: + 0*2^4 => + 0 _10 => 5 _10
5 -th digit = 1_2: + 1*2^5 => + 32 _10 => 37 _10

Convert 37 in base 10 to base 10
37 = 3 * 10 + 7 : base_10 => 7
3 = 0 * 10 + 3 : base_10 => 37_{10}

PROBLEM, June 12

(ii) Convert 6432_{10} to base 16

> python base.py 6432 10 16

Convert 6432 in base 10 to base 10
0 -th digit = 2_10: + 2*10^0 => + 2 _10 => 2 _10
1 -th digit = 3_10: + 3*10^1 => + 30 _10 => 32 _10
2 -th digit = 4_10: + 4*10^2 => + 400 _10 => 432 _10
3 -th digit = 6_10: + 6*10^3 => + 6000 _10 => 6432 _10

Convert 6432 in base 10 to base 16
6432 = 402 * 16 + 0 : base_16 => 0
402 = 25 * 16 + 2 : base_16 => 20
25 = 1 * 16 + 9 : base_16 => 920
1 = 0 * 16 + 1 : base_16 => 1920_{16}

WARNING: Consider the Purpose of the Assignment

- Why did I tell you not to use base.py before solving the problem by yourself?
- Does writing a Python program using built-in base-conversion features, such as an f-string, bin(), oct(), hex() etc, fulfill the purpose of the assignment?
- Should an answer that gives only the resulting values, without showing the required method or reasoning, receive credit?

Such answers before thinking by yourself defeats the purpose of the assignment.

PROBLEM, June 16

- **Answer in English or Japanese**
- **Submit electronic file(s) via LMS until June 17**

(If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
In this case, file name must include your STUDENT ID and FULL NAME)

PROBLEM:

(i) Calculate dE(k)/dk, d^2E(k)/dk^2, and effective mass m_e^*/m_0 from E(k) in band.xlsx, and plot m_e^*/m_0 vs k.
Assume the lattice parameter is a = 4.0 Å.

(ii) Compare the results obtained by different h.

Optional: Any questions and impressions of the lecture style are welcome

Effective mass

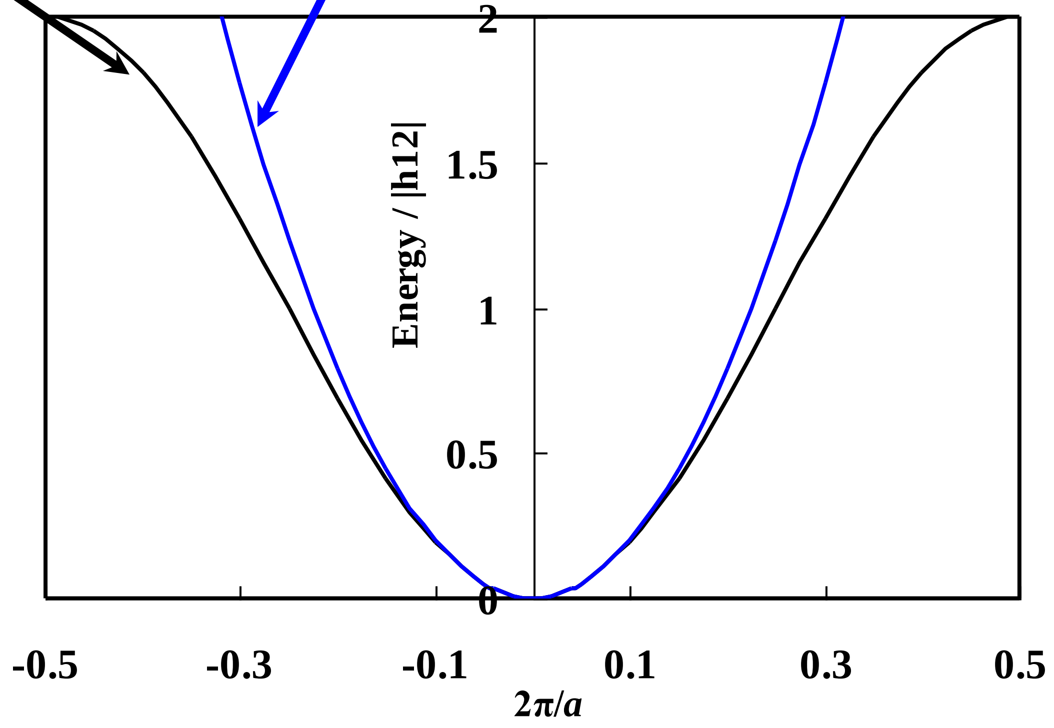
LCAO band

$$E(k) = \varepsilon_1 - 2|h_{12}|\cos(ka) \sim \varepsilon_1 - 2|h_{12}| + |h_{12}|a^2k^2 + O((ka)^4)$$

Free electron model

$$E(k) = E_0 + \frac{|\mathbf{P}|^2}{2m} = E_0 + \frac{\hbar^2}{2m}|\mathbf{k}|^2$$

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k^2}$$



Effective mass

k represents fractional coordinate in reciprocal unit cell:

generally expressed in the range **[-½ ½]**

Unit conversion $\boldsymbol{k_{real} = (2\pi/a)k}$

Note ***E*(*k*) is in eV**

$$m^* = \hbar^2 \left(\frac{\partial^2 E_J(\mathbf{k})}{\partial {k_{real}}^2} \right)^{-1} = \hbar^2 \left(\frac{2\pi}{a} \right)^2 \left(\frac{\partial^2 E_{eV}(\mathbf{k})}{\partial k^2} e \right)^{-1}$$

Very often effective mass is given by a ratio to the electron rest mass m_e^0 .

$$m^*/{m_e}^0 = \hbar^2 \left(\frac{\partial^2 E_J(k)}{\partial {k_{real}}^2} \right)^{-1} /{m_e}^0 = \hbar^2 \left(\frac{2\pi}{a} \right)^2 \left(\frac{\partial^2 E_{eV}(k)}{\partial k^2} e \right)^{-1} /{m_e}^0$$