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
数値解析に関する講義資料・pythonプログラム (

Update News:

- **June 11, 9:40, 2026:** Lecture materials updated: course_materials.zip
- **June 07, 8:12, 2026:** Lecture materials updated

#01 June 12, 2026: Fundamentals of c
error (誤差), Numerical differentiation

Course materials (Lecture slides and python programs):

- course_materials.zip

5-8min audio guide:

- 日本語: ▶ 0:00 / 6:35 (VOICEVOX 四国めたん&ずんだもん)
- English: ▶ 0:00 / 7:26

Slide files and Videos (monologue):

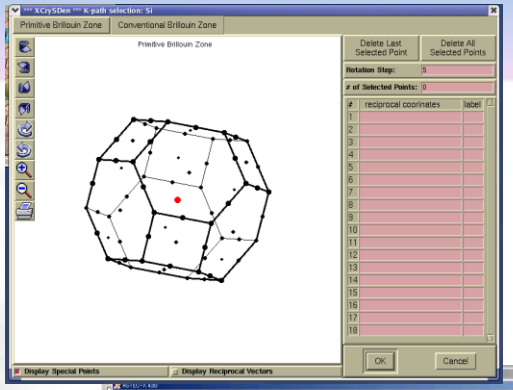
1. **Introduction:** 20260612-01-1.pptx
2. **Fundamentals:** 20260612-01-2Fundamentals.pptx
   - ▶ Fundamentals of computer (English)
   - ▶ - 原稿 (monologue, English)) (download/show)
   - ▶ コンピュータの基礎 (日本語)

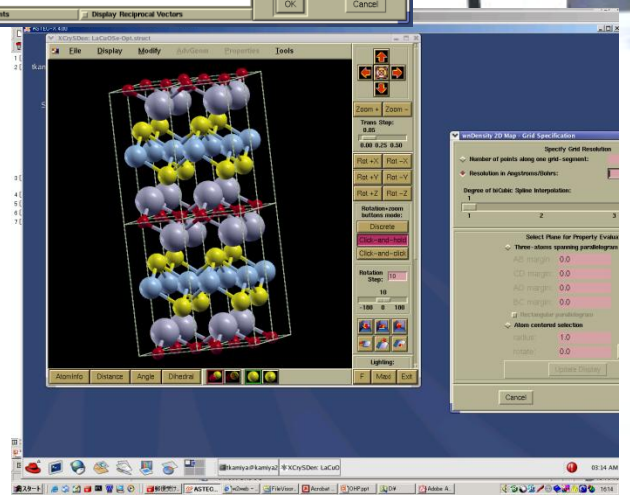
We would wait for five minuities (i.e., till 8:55).
In meantime

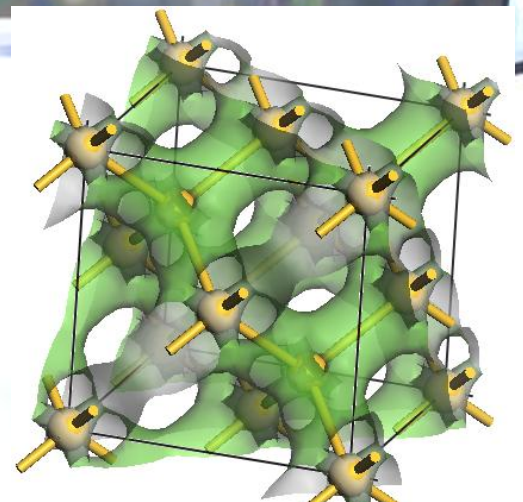
- **download the latest lecture materials**
- **hear the short audio guide.**
  English and Japanese versions available

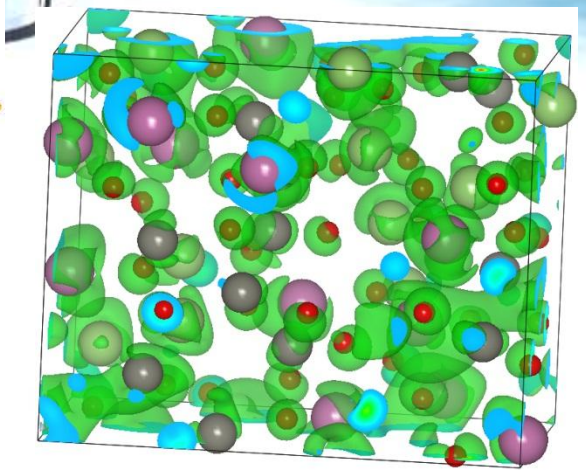
MAT.C505

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 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)

English textbooks

Search by ‘numerical analysis’, ‘numerical simulation’, ‘数値解析’ etc.

1. ***Introduction to Applied Numerical Analysis***
   Richard W. Hamming
   Dover publications, inc., New York (1989)
   ~340 pages

2. ***A First Course in Numerical Analysis***
   Anthony Ralston and Philip Rabinowitz
   Dover publications, inc., New York (1978)
   ~600 pages

For practical programming: Numerical Recipes series

1. **Numerical Recipes in C**
2. **Numerical Recipes Example Book (FORTRAN)**
3. **Numerical Recipes Source Code**
   Second Edition: C, Fortran77, Fortran 90
   Third Edition: C++

Policy

Evaluation:

1. Assignment is given in each class
2. Term-end assignment

   You can use AI like ChatGPT,

   but your answers must include your own thought and improvements.

Absence of class

1. If you can’t join a class, let me know prior to the class.

Zoom recording

1. Classes will be recorded, used only for students who request watching it.

Python: A Light Weight Language (LWL)

- **Interpreter language** (インタプリタ言語 – 逐次解釈)
  ⇔ Compiled language (コンパイル言語 – 機械語翻訳)
  Slower execution, but faster development
- Only **interpreter** and **editor** are required
- Free or public domain versions available
- Grammar similar to C, C++, perl, php, …
- Native **Object-Oriented** (オブジェクト指向) language
- Efficient functions and libraries
  Text processing: Regular expression (正規表現),
  csv, html, xml, json etc
  Science: numpy, scipy, scikit-learn etc
  Network: …
  Graph plotting: matplotlib etc
  GUI: tkinter, pygtk etc

Text editor vs Word processor

	Text editor	Word processor
Startup time (起動時間)	Shorter	Longer
Processing speed (実行速度)	Faster	Slower
Memory	Light	Heavy
Text style / format	Usually none	Required
File format	**Basically text-based**	**Application specific**
Others	**Specialized for specific program languages.** Macro (small program languages)	Print (WYSIWYG): What You See is What You Get
Examples	Linux : vi, emax Windows: TeraPad, Sakura Edtior Multi : Visual Studio Code, Sublime text, Atom	MS-Word

Recommendation:

Microsoft Visual Studio Code: https://code.visualstudio.com/

- Multiplatform (Windows, MacOS, Linux)
- Multilanguage
- Integrated Development Editor (IDE)

For those interested in Python and AI-based programming

http://d2mate.mdxes.iir.isct.ac.jp/D2MatE/?page=tutorial&id=programming

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- 学会等講演
- プレゼンテーション
- 生成AI
- プログラミング
- 物理・科学
- 半導体デバイス
- データ科学

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プログラミング

Audio guides were generated by Google NotebookLM

- ▶ pythonチュートリアル: 環境構築: Pythonとライブラリ
- ▶ pythonチュートリアル: 環境構築: Visual Studio Code
- ▶ pythonチュートリアル: Jupyter notebookを使ってpythonプログラムを動かす
- ▶ pythonチュートリアル: Fortran/Cとの比較で学ぶpython文法
- ▶ pythonチュートリアル: Debug: 全体の流れ
- ▶ pythonチュートリアル: Debug ー Tracebackメッセージの読み方

Most tutorials are currently available only in Japanese.
English versions can be prepared and uploaded upon request.

- ▶ pythonチュートリアル: Debug ー デバッガ
- ▶ Vibeコーディング (難易度★): van der Pauw法の形状補正因子を例に
- ▶ Vibeコーディング (難易度★): 非線形最小二乗法

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