

Computational Materials Science (計算材料学特論)

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



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 29, 10:49, 2026: Lecture materials for June 30 has been uploaded: [course_materials.zip](#)
- June 26, 11:31, 2026: Final version: Lecture materials for June 26 has been updated: [course_materials.zip](#)
- June 23, 11:42, 2026: Final version: Lecture materials for June 23 has been updated: [course_materials.zip](#)
- June 21, 16:25, 2026: Lecture materials for June 23 has been uploaded
- June 19, 10:49, 2026: Final version: Lecture materials for June 19 has been updated: [course_materials.zip](#)

FY2026

#06 June 30, 2026: Nonlinear optimization (非線形最適化), Fourier transform (フーリエ変換) (応用)

Course materials (Lecture slides and python programs):

- [course_materials.zip](#)

5-8min audio guide:

- 日本語: ▶ 0:00 / 4:47 (VOICEVOX 四国めたん&ずんだもん)
- English: ▶ 0:00 / 6:00

#05 June 26, 2026: Solution of equations (方程式の解法), Nonlinear optimization (非線形最適化)

Course materials (Lecture slides and python programs):

- [course_materials.zip](#)
- Slide files and Videos (monologue): [tutorial web](#)

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

- **download the latest lecture materials
(uploaded yesterday)**

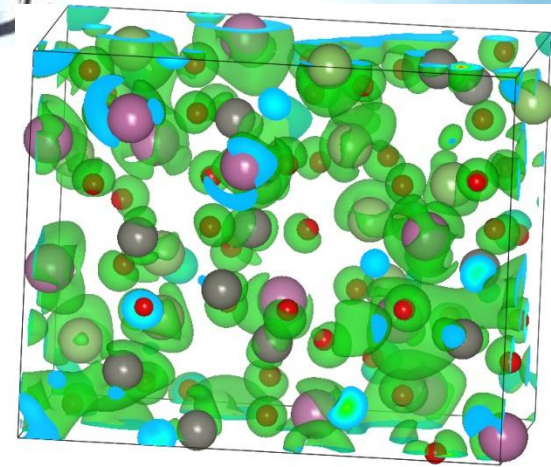
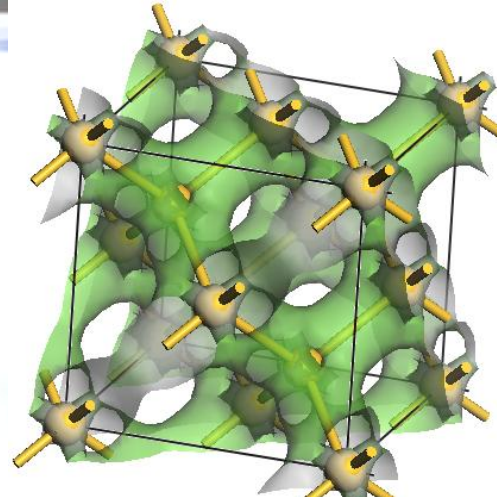
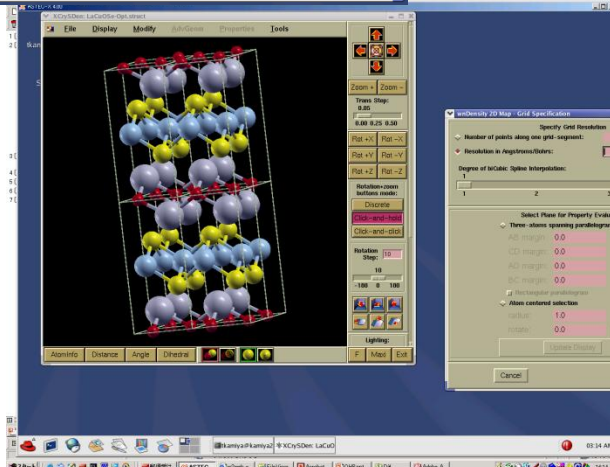
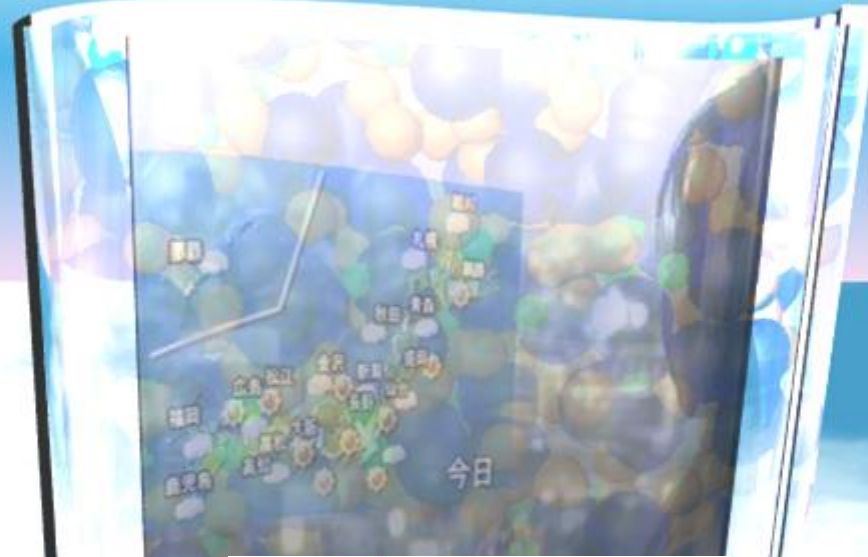
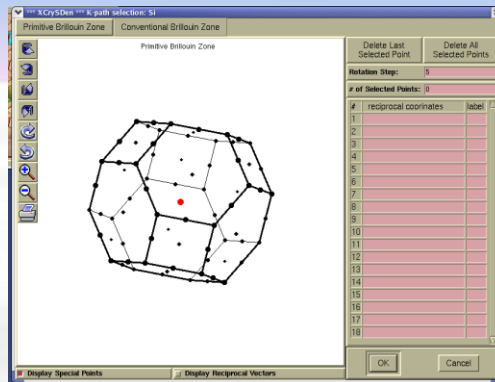
- **hear the short audio guide.**

English and Japanese versions available

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 (Smoothing (平滑化), Linear least-squares method (線形最小二乗法),
Numerical solutions of equations (方程式の数値解法))
- #05 June 26 (Fri) Kamiya (Numerical solutions of equations (方程式の数値解法), Nonlinear optimization (非線形最適化))
- #06 June 30 (Tue) Kamiya (Fourier transformation (フーリエ変換), Matrix (行列), Applications (応用))
- #07 July 3 (Fri) Kamiya (Montecarlo methods, Bayesian regressions, etc.)
- #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 26

- Answer in English or Japanese
- Submit electronic file(s) via LMS by midnight on June 28
(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)
- Common formats (.pdf, .txt., .docx, .xlsx, .pptx) are acceptable, but NO APPLE-ONLY files

PROBLEM:

Solve $5\cos(x) - x = 0$.

- Plot the functions $y = 5\cos(x)$ and $y = x$ in the range $x = 0 - 3$, find an initial x for Newton-Raphson method.
- Solve $5\cos(x) - x = 0$ by Newton-Raphson method at least with four significant digits.

Additional mandatory item: Choose one of the following

- Write any question, comment, opinion, or impression about the lectures
- Propose if you have any numerical analysis method / simple python program that you would like to learn

PROBLEM, June 27

See [equation_answer.xlsx](#)

Request about textbooks

NOTE: Numerical analysis covers a huge area with many algorithms and implementations. No single textbook can cover everything you may want to know.

Search the literature and check the contents first.

E.g., search by “numerical analysis”, “numerical simulation”, “数值解析”, etc.

1. Richard W. Hamming, *Introduction to Applied Numerical Analysis*
Dover publications, inc., New York (1989)
2. Anthony Ralston and Philip Rabinowitz, *A First Course in Numerical Analysis*
Dover publications, inc., New York (1978)

A practical way now: Use generative AI as a starting point.

- (i) Ask: How can I solve problem XXX in Python?**
- (ii) Ask it to generate Python code and simple test cases.**
- (iii) Ask for textbooks, papers, and accessible references.**
- (iv) Check the algorithm, implementation, and references yourself.**

Requests for additional methods

- Bayesian inversion, Markov Chain Monte Carlo (MCMC) methods, Metropolis-Hastings algorithm.
- How to implement the Lagrange multiplier method for constrained optimization in Python.
- For each type of problem, should we consider the methods introduced in this lecture to be sufficiently comprehensive for practical use, or should we regard them as only a small selection from the many methods available?
- Exact diagonalization / exact solution for Hubbard / Heisenberg model
- How to choose smoothing algorithms
- How do the numerical methods we study adapt to guarantee the conservation of physical invariants, like energy or angular momentum, over long timescales?
- Short Python comparisons of bisection, secant, Newton-Raphson, and Brent methods applied to the same equation
- **Characterize ICP-MS spectrum: Send a digital data by e-mail**

PROBLEM, June 30

- Answer in English or Japanese
- Submit electronic file(s) via LMS by midnight on July 1st
(If LMS doesn't work, send the files to kamiya.t.aa@m.titech.ac.jp.
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PROBLEM: Answer can be in Japanese or English

- (i) Find (x, y) to minimize $\exp(-x^2) * \sin(x+y)$ by your-chosen algorithms
hint: use SD method with fixed alpha
if you will approximate df/dx and df/dy , use central differences

Optional:

- (i) Propose if you have any other numerical analysis you want to learn in Computational Materials Science
- (ii) Propose if you have any python program (should be simple) you want to learn