THE CHINESE UNIVERSITY OF HONG KONG
Print Course Catalog Details

Academic Org: Div of Computer Science & Engg – Subject: AI: Systems & Tech

Course: AIST5040 **Course ID:** 015376 **Eff Date:** 2026-07-01 **Crse Status: Active** **Apprv. Status:** Approved **[**New Course**]**
PhysAI and GenAI for Natural Science 面向自然科學的物理啟發和生成式的人工智能

This course introduces PhysAI and GenAI as complementary approaches to natural scientific discovery. PhysAI refers to physics-inspired AI models that embed domain knowledge, physical laws, and invariances into learning frameworks, enabling models to achieve greater robustness, accuracy, and interpretability. In contrast, GenAI leverages generative modeling to create hypotheses, design candidates, and explore novel scientific paradigms beyond the limits of existing data. Together, PhysAI and GenAI form a powerful synergy: PhysAI accelerates and strengthens established paradigms, while GenAI opens pathways to entirely new directions of research. Through this integration, PhysAI and GenAI hold the potential to transform discovery in chemistry, materials science, and biology.

Advisory: Students are expected to have taken AIST1000 or AIST 3120 or AIST 4010 or CSCI3230 or CSCI3320.

本科介紹 PhysAI 和 GenAI 作為自然科學的互補方法。 PhysAI 是指受物理啟發的人工智能模型，將領域知識、物理定律和不變性嵌入學習框架，使模型能夠實現更高的穩健性、準確性和可解釋性。相較之下，GenAI 利用生成模型來創建假設、設計候選模型，並探索超越現有資料限制的全新科學模式。 PhysAI 和 GenAI 形成強大的協同效應：PhysAI 加速並強化了既有模式，而 GenAI 則開闢了通往全新研究方向的道路。透過這種整合，PhysAI 和 GenAI 有望徹底改變化學、材料科學和生物學領域的發現。

建議：學生應曾修讀 AIST1000、AIST 3120、AIST 4010、CSCI3230 或 CSCI3320 科目。

Grade Descriptor:

A

EXCELLENT – exceptionally good performance and far exceeding expectation in all or most of the course learning outcomes; demonstration of superior understanding of the subject matter, the ability to analyze problems and apply extensive knowledge, and skillful use of concepts and materials to derive proper solutions.

有關等級說明的資料，請參閱英文版本。

B

GOOD – good performance in all course learning outcomes and exceeding expectation in some of them; demonstration of good understanding of the subject matter and the ability to use proper concepts and materials to solve most of the problems encountered.

有關等級說明的資料，請參閱英文版本。

C

FAIR – adequate performance and meeting expectation in all course learning outcomes; demonstration of adequate understanding of the subject matter and the ability to solve simple problems.

有關等級說明的資料，請參閱英文版本。

D

MARGINAL – performance barely meets the expectation in the essential course learning outcomes; demonstration of partial understanding of the subject matter and the ability to solve simple problems.

有關等級說明的資料，請參閱英文版本。

F

FAILURE – performance does not meet the expectation in the essential course learning outcomes; demonstration of serious deficiencies and the need to retake the course.

有關等級說明的資料，請參閱英文版本。

Equivalent Offering:
Units: 3 (Min) / 3 (Max) / 3 (Acad Progress)
Grading Basis: Graded
Repeat for Credit: N
Multiple Enroll: N
Course Attributes: MSc Computer Science
MPhil-PhD Computer Sci & Erg

Topics:

COURSE OUTCOMES

Learning Outcomes:

At the end of the course of studies, students will be able to:

1. Critically evaluate the strengths and limitations of PhysAI and GenAI approaches in scientific applications.
2. Implement and experiment with AI models that incorporate physics priors or generative capabilities using modern machine learning frameworks (e.g., PyTorch, PyTorch-Geometric, Transformers).
3. Design and prototype workflows that combine physics-based constraints with generative modeling for real-world scientific problems.
4. Communicate complex ideas and findings effectively through coding projects, written reports, and oral presentations.

Course Syllabus:

Week 1: Overview on AI for Science
Week 2: Generative AI
Week 3: Physics-inspired AI
Week 4: Pretraining, Foundation Model, and Large Language Model
Week 5: The Multi-modal Learning and Alignment
Week 6: PhysAI for Chemistry: Energy and Force, AI MD
Week 7: GenAI for Chemistry: Molecule Generation, Molecule Optimization, Reaction Mechanism
Week 8: PhysAI for Material Science: Crystallization, Phase Detection
Week 9: GenAI for Material Science: Material Generation, Structure Generation
Week 10: PhysAI for Biology: Folding, Binding, Structure-based Drug Design
Week 11: GenAI for Biology: Protein Design and Engineering, Structure Generation, Metabolism Pathway
Week 12: Group Presentation (1)
Week 13: Group Presentation (2)

Assessment Type:

Homework or assignment	: 40%
Presentation	: 20%
Project	: 40%

Feedback for Evaluation:

1. Course evaluation and questionnaire
2. Question-and-answer sessions during class
3. Student consultation during office hours or online

Required Readings:

To be provided by course teacher.

Recommended Readings:

1. Yang Song, Diederik Kingma, (2021), How to Train Your Energy-Based Models. ArXiv.
2. Shengchao Liu, (2025), Tutorial on Physics-Inspired Geometric Pretraining for Molecule Representation. AAAI.
3. Shengchao Liu, (2025), Tutorial on Multi-modal Foundation Model for Scientific Discovery: With Applications in Chemistry, Material, and Biology. AAAI

OFFERINGS

1. AIST5040 — Acad Organization=CSEGV; Acad Career=RPG

COMPONENTS

LEC : Size=30; Final Exam=N; Contact=3

ENROLMENT REQUIREMENTS

1. AIST5040

Enrollment Requirement Group:
For students in MSc Computer Science; or
For students in MPhil-PhD Computer Science & Engineering; or
For students in UG AISTN or CDASN or CENGN or CSCIN

New Enrollment Requirement(s):
Other Requirement = For students in MSc Computer Science; or
For students in MPhil-PhD Computer Science & Engineering; or
For students in UG AISTN or CDASN or CENGN or CSCIN

Additional Information

VTL-Onsite face-to-face hrs 0
VTL-Online synch. hrs 0
VTL-Online asynch. hrs 0

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