COMP 7/8290
Molecular Computing
Fall, 2005

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1pm		1pm		1pm
Also by Appointment				

Course Description

COMP 7290 Basics of cell biology and genetics (DNA structure and enzymes, replication, transcription and translation); Feasible DNA solutions of hard computational problems; issues in the design of molecular computers; foundations of nanotechnology. PREREQUISITE: COMP 6030, or permission of instructor.

Why this course?

Computational devices at the molecular level have been envisioned since the mid 1940s, but it is only in the last decade that major strides have been taken towards actual construction of computers at nanoscales for computational and engineering purposes. This course provides a state-of-the-art survey of some of the most promising and intriguing recent developments and techniques to have molecular computers self-assemble *in silico*, *in vitro*, and *in vivo*, particularly those based on DNA molecules. Of the potential impact in real-world applications, three stand out, namely, molecular self-assembly of complex nanostructures, synthetic biology for bioinformatics, and data mining from DNA-based associative memories at terascales for business applications.

Resources

Articles selected by the instructor on cutting-edge research concerning the subject matter of the class. A variety of other tools and sources are constantly updated at http://www.cs.memphis.edu/classes/7290/.

Required Text

None. Articles in a reading selection are provided by instructor and posted on the class web site by the first days of classes.

Recommended Texts

As of yet, there is no textbook in the market that will cover a significant portion of the syllabus.
The following sources and the supplementary references provides a good coverage of most of the topics.

- **Bibliographies on Molecular Computing**
  Adleman's Lab for Molecular Science
  Seeman's lab page--DNA nanotechnology
  Molecular Computing Group in Memphis
  Winfree's Group on BMC
  Duke's Group on BMC
  Landweber's Lab for Molecular Science
  UW-Madison DNAC Lab
  DNA Microarrays (Genome chips)
  Erik Winfree's old page--Molecular Computation
  Molecular Electronics
  Survival Dictionary for BMC.

- **Class presentations**
  SampleTemplate.ppt | BMCInVivo.ppt | BMCInVitro.ppt | BMCInSilico.ppt at CEC-2003 - Special Issue
  BMC Tutorial at CEC-04
  Encoding problem in BMC

Other Resources: (Journal / Conference papers, websites, etc)

A variety of other tools and sources are constantly updated at
http://www.cs.memphis.edu/classes/7290/.

- [CP] C. Calude, Gh. Paun. *Computing with Cells and Atoms: An Introduction to Quantum, DNA and Membrane Computing*, Taylor and Francis, London, 2000. ISBN 0-7484-0899-1
- [**S**] M. Sipper, Computing in a test tube. Computer 1999. [A leisure overview of Molecular Computing.]
- [**MR**] Hard Tiling Problems with Simple Tiles. C. Moore, J.M. Robson [2001]. *J. Discrete and Computational Geometry* **26**:4, 573-390
- [**S**] J.D. Watson, The Double Helix. A Mentor Book (Penguin Putnam Inc.), 1968. [A Personal Account of the Discovery of DNA.]
- [BY] Making Things Work: Solving Complex Problems in a Complex World Yaneer Bar-Yam, Knowledge Magazine Press, 2004, ISBN 0-9656328-1-4. [CSSEdu] Complex Systems and International Security, February 1, 2005, Washington, DC.

- [GD2] Max H. Garzon and Russ J. Deaton. Codeword design and information encoding in DNA ensembles. *J. of Natural Computing* 3:4 (2004), 253-292. [An overview of the potential, challenges, and progress in Molecular Computing up to 12/2004.]

- [GD1] Max H. Garzon, R.J. Deaton. Biomolecular Computing and Programming. IEEE Trans. Evolutionary Computation 3:3 (1999), 36-50. [An overview of the potential, challenges, and progress in Molecular Computing up to 6/1999.]

- S. Ji: **The Cell as a DNA-based Molecular Computer**. BioSystems **44**(1997), 17-39.

- Tom Head: **Formal Language Theory and DNA: an analysis of the generative capacity of specific recombinant behaviors**. *Bull. Math. Biology* 49(1987), 737-759.
[Pioneering work into the power of DNA as a generating device.]

- [A94] L. Adleman: **Molecular Computation of Solutions to Combinatorial Problems**. *Science* 226 (1994), 1021-1024.

- D. Deutsch: **Quantum Theory, the Church-Turing principle, and the Universal Quantum Computer**. Proc. Royal Society (London) A400 (1985), 95-117. [A discussion of the CTT in light of Quantum Computing.]

- Max Garzon, Kiran Bobba, Andrew Neel. Efficiency and Reliability of Semantic Retrieval in DNA-based Memories, *9th Int Workshop on DNA-based Computers*, Madison, WI, 2003. [Semantic retrieval based on DNA computers.]

- Max Garzon, Andrew Neel, Hui Chen: Efficiency and Reliability of DNA-based Memories. *Genetic And Evoluctionary Computation Conference-GECCO-03*. (Best paper award) [Semantic retrieval based on DNA computers.]

- Andrew Neel, Max Garzon: Efficiency and Reliability of Genomic Information Storage and Retrieval in DNA-based Memories with Compaction. *IEEE Congress on Evolutionary Computation-CEC2003*, Canberra.

- R.C. Paton: . **Glue, Verb and Text Metaphors in Biology** BioTheoretica **45**(1997), 1-15.

Evaluation

Final Grades

Your final grade will be composed as described below in FINAL GRADES. Plus/minus grading will be used. Students taking the class at the 8290 level will be expected to turn in assignments and perform at a higher level of quality and thoroughness than that of the corresponding students at the 7290 level for a comparable grade.

Grading Scale

Final letter grades will be assigned based on performance relative to the rest of the class, so no fixed total scores are preset to obtain a given grade. The best performances will be given As. Students with scores below a 65% will be given Fs. In between, comparable scores for students at the same level will be given identical and proportionate intermediate grades. The grades will reflect class participation (includes

attendance), consistency in term project work (progress reports), benefiting of readings selections, and a written and oral presentation about the results of the term project.

20% Class Participation (2)

30% Project Reports (3/4)

50% Term Project

Course Policies:

Attendance
Attendance is compulsory and is integral part of **class participation**. Students are also expected to read relevant chapters in the selected readings, and the supplementary references *before the corresponding topics are discussed* in class. Reading assignments from other sources than the selected readings will be announced as it becomes necessary at least two lectures in advance

Late Policy
No makeup is given for missed readings, project reports, or tests. They need to be uploaded ahead of presentation on the umdrive directories for the class.

Testing Policy
This is an advanced course and no tests are given. The final exam is oral and given on research completed for a term project in the course of the semester on a topic negotiated and agreed upon with the student by the third week of classes.

Plagiarism/Cheating Policy (These paragraphs are mandatory.)

Plagiarism or cheating behavior in any form is unethical and detrimental to proper education and ***will not be tolerated.*** All work submitted by a student (projects, programming assignments, lab assignments, quizzes, tests, etc.) is expected to be a student's own work. The plagiarism is incurred when any part of anybody else's work is passed as your own (no proper credit is listed to the sources in your own work) so the reader is led to believe it is therefore your own effort. Students are allowed and encouraged to discuss with each other and look up resources in the literature (including the internet) on their assignments, but ***appropriate references must be included for the materials consulted***, and appropriate citations made when the material is taken verbatim.

If plagiarism or cheating occurs, the student will receive a failing grade on the assignment and (at the instructor's discretion) a failing grade in the course. The course instructor may also decide to forward the incident to the University Judicial Affairs Office for further disciplinary action. For further information on U of M code of student conduct and academic discipline procedures, please refer to:
http://www.people.memphis.edu/~jaffairs/

Course Syllabus

Week	Date	Lecture Topics
1	***Aug 30***	**The Big picture**: What is molecular computing? [BMC Tutorial; GD99; GD00]
2	***Sep 8***	**Big challenges**: Errors; error prevention; scaling; manufacture; fault-tolerance [BMCInVivo.ppt; GD04;]
3	***Sep 20***	**Biomolecular solutions**: Biotechnology; Adleman's Solution; Head's solution [BMCInVitro.ppt; Adl94]
4	***Sep 27***	**Encodings and Word Design**: Gibbs energy models; encoding problem; word selection; PCR selection protocols [GarzonDeaton04NC.pdf; GEtAlCodes.pdf; RosSuy04.pdf; FeldkampEtAl03GPEM.pdf; NusDea03.pdf; GD96; PCRSelection]
5	***Oct 4***	**Self-Assembly**: Tilings; 3-Colorability; nanocircuits [WinEtAl98; REtAl; JonEtAl03GPEM.pdf; WestEtAl04.ppt; PEtAl; SelfAssemble1; SelfAssemble2.ppt; 3-Coloring]
6	***Oct 11***	**Characterizations of Self-Assembly**: Three regimes; robust self-assembly [WinEtAl98.pdf; Win98Thesis.pdf; PCRSChar.ppt; WestEtAl04.ppt] * Progress Report One
7	***Oct 18***	**Progress Reports and Fall Break**
8	***Oct 25***	**BMC in Silico**: Simulations; implementation in silico [Garzon03.pdf; GarEtAl05VTTs.pdf; BlainEtAl05.pdf; BMCInSilico.ppt; EdnaCo]
9	***Nov 1***	**Representation**: Information Encoding in DNA; learning wDNFs [PhanGar04DNA10.pdf; InfoRep.htm; FidelityAnalysis.ppt]
10	***Nov 8***	**DNA Microarrays**: Concepts and related biotechnology [DNA Chips; DNAChips.ppt]
11	***Nov 15***	**Applications I**: Bioinformatics, DNA Chip Design [InfoRepDNAChips.pdf; DNAChips.ppt; DNAMems.ppt] * Progress Report Two
12	***Nov 22***	**Applications II**: Semantic Retrieval [NeelEtAlCEC04.pdf; DNAMems.ppt] * Progress Report Three
13	***Dec 1***	**Applications II**: Semantic Retrieval [NeelEtAlCEC04.pdf; DNAMems.ppt] * Progress Report Three
14	***Dec 6***	**Project's Final Presentations** I: [**G1-G8**]
15	***Dec 13***	**Project's Final Presentations** II: [**G1-G8**]