# Computational Thinking in the Sciences and Beyond

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Microsoft Research Asia Faculty Summit – Beijing China 30 October 2014

## My Grand Vision

- Computational thinking will be a fundamental skill used by everyone in the world by the middle of the 21<sup>st</sup> Century.
  - Just like reading, writing, and arithmetic.
  - Incestuous: Computing and computers will enable the spread of computational thinking.
  - In research: scientists, engineers, ..., historians, artists
  - In education: K-12 students and teachers, undergrads, ...

J.M. Wing, "Computational Thinking," *CACM* Viewpoint, March 2006, pp. 33-35. Paper off <u>http://www.cs.cmu.edu/~wing</u>/

## What is Computational Thinking?

Computational thinking is the *thought processes* involved in formulating a problem and expressing its solution(s) in such a way that a computer—human or machine—can effectively carry out.

#### Computational Thinking, Philosophically

- Complements and combines mathematical and engineering thinking
  - C.T. draws on math as its foundations
    - But we are constrained by the physics of the underlying machine
  - C.T. draws on engineering since our systems interact with the real world
    - But we can build virtual worlds unconstrained by physical reality
- Ideas, not artifacts
  - It's not just the software and hardware that touch our daily lives, it will be the computational concepts we use to approach living.
- It's for everyone, everywhere

#### Sample Classes of Computational Concepts

- Algorithms
  - E.g., mergesort, binary search, string matching, clustering
- Data Structures
  - E.g., sequences, tables, trees, graphs, networks
- State Machines
  - E.g., finite automata, Turing machines
- Languages
  - E.g., regular expressions, ..., VDM, Z, ..., ML, Haskell, ..., Java, Python
- Logics and semantics
  - E.g., Hoare triples, temporal logic, modal logics, lambda calculus
- Heuristics
  - E.g., A\* (best-first graph search), caching
- Control Structures
  - Parallel/sequential composition, iteration, recursion
- Communication
  - E.g., synchronous/asynchronous, broadcast/P2P, RPC, shared memory/message-passing
- Architectures
  - E.g., layered, hierarchical, pipeline, blackboard, feedback loop, client-

#### NOT

- Computer literacy, i.e., how to use Word and Excel or even Google or Bing
- Computer programming, i.e., beyond Java Programming 101

# Examples of Computational Thinking in Other Disciplines

# One Discipline, Many Computational Methods

## **Computational Thinking in Biology**

- Shotgun algorithm expedites sequencing of human genome
- Abstract interpretation in systems biology
- Model checking applied to arrhythmia, diabetes, pancreatic cancer
- DNA sequences are strings in a language
- Boolean networks approximate dynamics of biological networks



- Cells as a self-regulatory system are like electronic circuits
- Process calculi model interactions among molecules
- Statecharts used in developmental genetics
- Protein kinetics can be modeled as computational processes
- Robot Adam discovers role of 12 genes in yeast
- PageRank algorithm inspires ecological food web

Insight: Models and languages for expressing computational processes are good for expressing the dynamics of biological processes.

#### **Stem Cell Prediction**

[Dunn et al., "Defining an essential transcription factor program for naïve pluripotency," *Science*,

June 2014, pp. 1156-1160]





# Embryonic Stem (ES) Cells



Transient in tissue: A culture-dependent phenomenon

Pluripotent: Generate all adult cell types, and can be re-injected back into the developing embryo

We can **reprogram** adult cells to this state

## **Extrinsic Signals Control ES Cell Behaviour**

Whether an ES cell will remain self-renewing, or differentiate towards an adult cell lineage depends on the signals that it receives.





The signals required to sustain ES cells in culture have been progressively refined. Any two of LIF, CH and PD are sufficient.

We can measure the expression of key genes under different combinations of signals to gain insight into the dynamic behavior of the system.

# A Reasoning Engine for Interaction Networks





RE:IN is a tool built on Z3 that utilizes Satisfiability Modulo Theories to synthesize only those (out of 10^43) Boolean networks that provably satisfy experimental constraints.

IF (signalA AND signalB AND NOT signalC OR ...) THEN remain a stem cell ELSE (IF NOT signalA ...) differentiate

LIF(13)

Stat3(9)

KIf4(0)

Klf2(9)

Gbx2(10)

PD(3)

MEKERK(17)

Nanog(12)

Esrrb(9)

Oct4(13)

Sox2(6)

Tbx3(6)

Sall4(8)

CH(15)

Tcf3(17)

Tfcp2l1(13)

## **Biological Computation in Stem Cells**



- The set of possible models was constrained by experimentally-observed behaviours
- This set was used to make a large number (53) of non-intuitive predictions of the response of the network to genetic perturbations. These predictions were experimentally validated with over 70% accuracy rate.
- The highlighted interactions show the minimal set required to explain stem cell behaviour: **the essential program governing naïve pluripotency**

# One Computational Method, Many Disciplines

Machine Learning has transformed the field of Statistics.

# Machine Learning in the Sciences

#### Astronomy

- Brown dwarfs and fossil galaxies discovery via machine learning, data mining, data federation
- Very large multi-dimensional datasets analysis using KD-trees

#### Medicine

- Anti-inflammatory drugs
- Chronic hepatitis
- Mammograms
- Renal and respiratory failure

#### Credit: LiveScience

#### Meteorology

- Tornado formation

#### **Neurosciences**

fMRI data analysis to understand language
 via machine learning







Credit: SDSS

# Fighting Spam and Fighting HIV



Spammers mutate their messages to work around filters

Solution: Go after the weak link



HIV mutates to avoid attack by immune system

Solution: Go after the weak link

Strategy: Identify vulnerable regions on HIV and create a vaccine that directs the immune system to target those regions



		amino acid			
•	Identify a set of "controllers" who are	sequence	protein	begin	end
	infected with HIV, but don't get very	KAFSPEVIPMF	p24	30	40
	sick	RLRDLLLIVTR	gp41	259	269
•	Look for differences between where	GIPHPAGLK	pr	192	200
	immune systems of controllers vs	HTQGYFPDW	nef	116	124
	where those of normal people are	AEAMSQVTNS	p2	1	10
	attacking HIV	SAEPVPLQL	rev	67	75
•	These differences point to the	QAISPRTLNAW	p24	13	23
	vulnerable regions	RIKQIINMW	gp120	419	427

From data from hundreds of controllers and non-controllers, machine learning helped identified 8 regions of HIV proteins where controllers are much more likely to attack.

# **Finding More Vulnerable Regions**



Use in silico prediction under the assumption that vulnerable regions are where the amino acid changes protein stability (increases "structural entropy")

Estimate protein stability with simulations using the FoldX algorithm

These regions are new candidate vulnerable regions.

# Machine Learning Everywhere



# Computational Thinking in the Sciences and Beyond

#### **Computational Thinking in Other Sciences**



#### Geosciences

- Abstractions for Sky, Sea, Ice, Land, Life, People, etc.
  Hierarchical, composable, modular,
  - traceability, allowing multiple projections
  - along any dimension, data element, or query
- Cornell's NSF Expedition on Computational Sustainability

## Computational Thinking in Math and Engineering

#### **Mathematics**

- Discovering E8 Lie Group: 18 mathematicians, 4 years and 77 hours of supercomputer time (200 billion numbers). Profound implications for physics (string theory)
- Four-color theorem proof

Credit: Wikipedia



Credit: Boeing

Credit: Wikipedia

#### Engineering (electrical, civil, mechanical, aero & astro,...)

- Calculating higher order terms implies more precision, which implies reducing weight, waste, costs in fabrication
- Boeing 777 tested via computer simulation alone, not in a wind tunnel
- Hybrid automata for modeling and analyzing cyber-physical systems



# Computational Thinking for Society

#### Microsoft Digital Advertising Solutions

erstock.com®

#### **Economics**

- Automated mechanism design underlies electronic commerce,

- e.g., ad placement, on-line auctions, kidney exchange
- Internet marketplace requires revisiting Nash equilibria model
- Use intractability for voting schemes to circumvent impossibility results
  - Inventions discovered through automated search are patentable
  - Stanford CL approaches include AI, temporal logic, state machines, process algebras, Petri nets
  - POIROT Project on fraud investigation is creating a detailed ontology of European law
  - Sherlock Project on crime scene investigation

#### Healthcare

- Algorithmic medicine
- Software design principles and debugging applied to prescriptions of painkillers
- ONC SHARP Program, NSF Smart Health and Wellness Program, NITRD Senior Steering Group on Health IT

## Fast and Accurate Decision-Making

## 2012 Xbox

- Polling daily and during live debates
- 350k respondents: age, race, gender, state, edu, party id, ideology, previous votes, registration
- 750k polls in 45 days
- 30,000 respondents 5 or more polls
- Data and engagement great, but accuracy?



Cite: Forecasting elections with non-representative polls; Gelman, Goel, Rothschild, and Wang (2014)

## **Data Collection**

Two-party Obama Support



Cite: Forecasting elections with non-representative polls; Gelman, Goel, Rothschild, and Wang (2014)

#### **Data Analytics**

![](_page_26_Figure_1.jpeg)

Cite: Forecasting elections with non-representative polls; Gelman, Goel, Rothschild, and Wang (2014)

Use convex optimization to keep millions of interrelated predictions consistent

![](_page_27_Picture_0.jpeg)

# **Computational Thinking for Society**

#### Archaeology

- eHeritage Project, Microsoft Research Asia
- Digital Forma Urbis Romae Project, Stanford
- Cathedral Saint Pierre, Columbia

![](_page_28_Picture_5.jpeg)

- Algorithmic approach to validate credibility of sources
- Digital Media and Learning Initiative, MacArthur Foundation

#### Journalism

![](_page_28_Picture_9.jpeg)

#### **Humanities**

- Digging into Data Challenge: What could you do with a million books? Nat'l Endowment for the Humanities (US), JISC (UK), SSHRC (Canada)
- Music, English, Art, Design, Photography, ...

# Computational Social Science: Learning about Crowdworkers

 <u>Computational</u>: digital studies produce the nodes (people) and edges (relationships) in a network

![](_page_29_Picture_2.jpeg)

• <u>Anthropology</u>: qualitative studies produce the variety of nodes (individuals, institutions) and meaning of edges (motivations, hierarchies, power dynamics)

# Mapping the Crowd

![](_page_30_Figure_1.jpeg)

Self-reported locations for ~10,000 participants in a map task on Amazon Mechanical Turk. Coloration of counties/districts is by *population density*.

# Computational Thinking in Education

#### Pre-K to Grey

- K-6, 7-9, 10-12
- Undergraduate courses
  - Freshmen year
    - "Ways to Think Like a Computer Scientist" aka Principles of Computing
  - Upper-level courses
- Graduate-level courses
  - Computational arts and sciences
    - E.g., entertainment technology, computational linguistics, ..., computational finance, ..., computational biology, computational astrophysics
- Post-graduate
  - Executive and continuing education, senior citizens
  - Teachers, not just students

#### **Education Implications for K-12**

Question and Challenge for the Computing Community:

What is an effective way of learning (teaching) computational thinking by (to) K-12?

- What concepts can students (educators) best learn (teach) when? What is our analogy to numbers in K, algebra in 7, and calculus in 12?
- We uniquely also should ask how best to integrate The Computer with teaching the concepts.

Computer scientists are now working with educators and cognitive learning scientists to address these questions.

## **Computational Thinking in Daily Life**

## Getting Morning Coffee at the Cafeteria

![](_page_35_Figure_1.jpeg)

## Getting Morning Coffee at the Cafeteria

![](_page_36_Figure_1.jpeg)

## Getting Morning Coffee at the Cafeteria

![](_page_37_Figure_1.jpeg)

#### Better: Think Computationally—Pipelining!

![](_page_38_Figure_1.jpeg)

![](_page_39_Picture_0.jpeg)

## **United Kingdom Efforts**

#### British Royal Society (2012): Shut down or restart? report

...

Shut down or restart?

The way forward for computing in UK schools

THE ROYAL SOCIETY

January 2012

`` "Computational thinking" offers insightful ways to view how information operates in many natural and engineered systems.

- 3. *Every child should have the opportunity to learn Computing at school.* We believe that:
- Every child should be expected to be 'digitally literate' by the end of compulsory education, in the same way that every child is expected to be able to read and write. "

# Computing At School (K-12)

Establish computer science as a foundational subject discipline, like math or physics, that ever child should learn, from primary school onwards.

## **COMPUTING AT SCHOOL**

EDUCATE · ENGAGE · ENCOURAGE In collaboration with BCS, The Chartered Institute for IT

![](_page_41_Picture_4.jpeg)

An entirely new K-12 subject, Computer Science, started in England, Sept 2014.

## **International Efforts**

![](_page_42_Figure_1.jpeg)

تحو نتس فكرة التقكير الحوسبي في مصر والعالم العربي . Towards spreading computational thinking in Egypt and the Arab world

Asia

# **Computational Thinking in China**

Prof. Guoliang Chen (陈国梁 院士) is one of the key influencers who put Computational Thinking as the core ability for CS Fundamental Courses in all China universities.

Prof. Guoliang Chen also started the first CS Fundamental Course of Computational Thinking.

![](_page_43_Picture_3.jpeg)

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服务大厅	行政审批	1	办事公开	1	项目指南	I.	招生考试	1	就业指导	1	名单查阅	T	学历查询	Ĕ	学历认证	1	学位查询	学位认证		
互动平台	部长信箱	1	政策咨询	Ĩ	专家答疑	1	政策解读	1	征求意见	1	在线访谈	1	热线电话	Г	滇西开发	1	移动客户端	新闻办微博	微信	
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- In 2012, The Chinese Ministry of Education (MOE) announced a program to reform Computing Fundamental Courses focusing on Computational Thinking.
- In 2014, MOE and Microsoft jointly put forward a new program to sponsor 16 full Computational Thinking Courses and 100 case studies.
- Empower 7 Million students with Computational Thinking ability through CS Fundamental Courses.

#### Computational Thinking, International

![](_page_45_Picture_1.jpeg)

<sup>建型使我们敢于去处</sup> In Bulletin of Specif, December 2008

#### La pensée informatique

par Jeannette M. Wing

Cet article fait suite aux divers interviews que nous avons faits et qui nous invitaient à une réflexion sur les fondements de notre discipline et ses aspects philosophiques et épistémologiques. Aujourd'hui l'article de Jeannette Wing nous conduit à réfléchir sur l'utilité et l'ubiquité de la pensée informatique et ses implications, mais aussi sur l'essence même de cette pensée.

#### Spread the Word

• Help make computational thinking commonplace!

To fellow faculty, students, researchers, administrators, teachers, parents, principals, guidance counselors, school boards, teachers' unions, congressmen, policy makers, ... Thank you!

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