PROS
Centro de Investigación en Métodos de Producción de Software

UNIVERSIDAD POLITECNICA DE VALENCIA

Conceptual Modeling of Life: Beyond the "Homo Sapiens"

ER 2016 - 11/14/2016

The 35th International Conference on Conceptual Modeling

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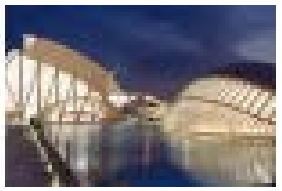


Passion for Conceptual Modeling!!!

I have had a dream…

A world plenty of Conceptual Modelers

species in our planet

Genius

qualified. M. L. Barker. 1408 Chap-
man Bldg.

MEN WANTED

for hazardous journey, small wages, bitter cold, long months of complete darkness, constant danger, safe return doubtful, honor and recognition in case of success.

Ernest Shackleton 4 Burlington st.

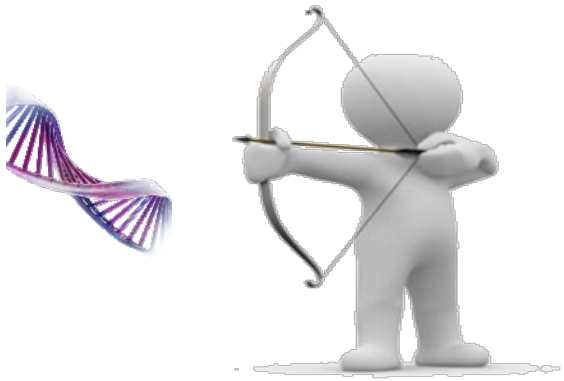
MEN—Neat-appearing young men of pleasing personality, between ages of and 40 to work

Goals of the Keynote

- to discuss the notion and the scope of CM
- to analyze how CM can help us to understand the world that comes (within what we could call a "social perspective")
- to analyze how CM can open promising and challenging scenarios in the domain of the genome understanding (a more “biological-oriented” perspective)

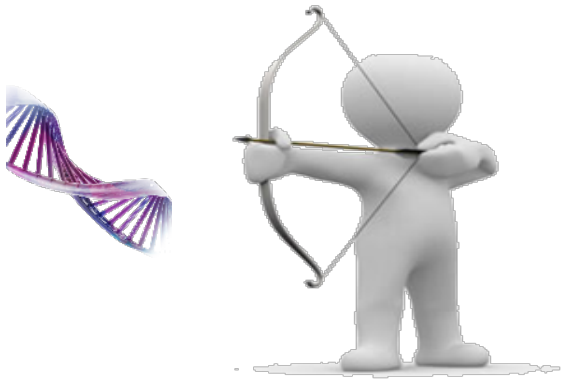
PREFACE

- What are the main inhibitors of modelling in practice?
- What could be done to improve the popularity of conceptual modelling in practice?
- What lessons did you learn from teaching conceptual modelling?



PREFACE

- What is an especially promising research direction in conceptual modelling?
- What is/should be the role of conceptual modelling in the digital transformation?
- What are especially promising areas of using models at runtime?



What are the main inhibitors of modelling in practice (I)?

- Software Engineering is not really recognized in practice as a true engineering.
- More as a handicrafts-centered activity
- Strong dependence on skilled programmers

What are the main inhibitors of modelling in practice (II)?

- Lack of a conceptual modeling perspective: product focus instead of process focus
- Conceptual Modeling on the top of Programming should be the basic topic in SE teaching
- Lack of a universal, widely-based, ontologically-supported definition

What could be done to improve the popularity of CM in practice?

- Conceptual Programming (CP)-based tools
- Assess flexibility, efficiency and effectiveness of those CP-based tools
- Emphasizing the relevance of CM in Software Engineering teaching

What lessons did you learn from teaching conceptual modelling?

- Big difference in CM abilities among students
- Or more precisely…lack of CM abilities!
- Should a Software Engineer be graduated without assessing a solid CM ability?

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What is an especially promising research direction in CM?

- Conceptual Modeling of Life
- The role of CM to guide/lead the digital transformation of our society
- From an Homo Sapiens to an "Homo Genius"

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What are especially promising areas of using models at runtime?

- Big Data is not Schemaless!
- Conceptual Modeling of the human genome and Precision Medicine implications
- Efficient and flexible Enterprise Modeling
- Full conceptual alignment between enterprise models and software application
- From Requirements to Code

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Models, Models, Models…

Sorry!

CONCEPTUAL MODELS, CONCEPTUAL MODELS, CONCEPTUAL MODELS…!!!

AGENDA

1. What is a Conceptual Model?
2. Conceptual Modeling of Life: *the Social Perspective*
3. Conceptual Modeling of Life: *the Biological Perspective*
4. Why "*beyond the Homo Sapiens*"?
5. Clinical Applications: *Precision Medicine (PM)*
6. Conclusions

What is a Conceptual Model?

A simplification of a system built with an intended goal in mind

An abstraction of a system to reason about it (either a physical system or a real or language-based system)

A description or specification of a system and its environment for some certain purpose

One main conclusion that we can reach is that the distinction between "model" and "conceptual model" is not always as precise at it should be.

What is a Conceptual Model?

While much has already been written on this topic, there is however neither precise description about what we do when we model, nor rigorous description about of the relations among modeling artifacts (Muller, 2009)

Nobody can just define what a model is, and expect that other people will accept this definition: endless discussions have proven that there is no consistent problem understanding of models (Ludewig, 2003)

What is a Conceptual Model?

- Back to the conceptualization human capability, we can see a CM as the result of making explicit a conceptualization process applied to a part of the world considered relevant for the conceptual modeler purpose

A "CS/IS" perspective

- The connection between the conceptual model and the corresponding software product that materializes it
- The CM is the code
- MDD / Conceptual Programming / CS-Centric Software Development / XNP…
- Conceptual Modeling is programming

The CM discipline (Mylopoulos, 1992)

- The activity of formally describing some aspects of the physical and social world around us for purposes of understanding and communication. Conceptual modelling supports structuring and inferential facilities that are psychologically grounded. After all, the descriptions that arise from conceptual modelling activities are intended to be used by humans, not machines... The adequacy of a conceptual modelling notation rests on its contribution to the construction of models of reality that promote a common understanding of that reality among their human users..."

CM (Thalheim, 2011)

- CM is a widely applied practice and has led to a large body of knowledge on constructs that might be used for modeling and on methods that might be useful for modeling. Modeling is ruled by its purpose, e.g., construction of a system, simulation of real-world situations, theory construction, explanation of phenomena, or documentation of an existing system. Modeling is also an engineering activity with engineering steps and engineering results.
- Conceptual models are models that incorporate concepts or conceptions

CM (Olivé 2007)

- CM refers to the activity that elicits and describes the general knowledge a particular information system needs to know. Its main objective is to obtain that description, which is called a conceptual schema.
- Conceptual schemas are written in languages called conceptual modeling languages.
- CM is an important part of RE, the first and most important phase in the development of an IS

The Ontological Perspective

- If behind a CM there is a conceptualization process, the ontological perspective becomes a first-order issue to understand what CM is.
- In IS, ontologies are the basis for creating conceptual schemas, and the languages in which they are written are called conceptual modeling languages.
- This perspective provides a solid basis to link ontologies and CM, through the use of a foundational ontology

Ontology-driven CM…

- …to characterize the different sets of meta-ontological choices that can produce different types of conceptual models
- …to understand what methaphysical choices are taken when a given foundational ontology is proposed (as these choices characterize the type of CMs that can be generated)

Dimensions to classify types of conceptualizatons

- Realism vs idealism
- Endurantism vs perdurantism
- Physical vs abstract objects
- Higher order types
- Possible worlds

- The application of meta-ontology to CM and IS development is still relatively underexplored, with a scarce literature.
- Useful to conduct comparative analysis of two or more FOs (and their subsequent CM languages).
  - to make explicit their theoretical differences,
  - to understand the different expressiveness of the resultant conceptual models
  - to investigate the implications of such differences on CM within IS development.

Required further work, already in progress...

- ...to provide a precise view on what CM is
  - Ontologically-supported
  - Conforming a widely accepted body of kwnowledge, ER/CM leaded

- Word in progress by
  - Delcambre
  - Storey, Liddle, Pastor

CM of Life: the Social Perspective

- Assuming that our capability of conceptualizing is essential as it makes us -humans- different from any other species in our planet…
- How can conceptual modeling help us to understand and to improve the world that comes?

In a world heavily influenced by "doers", just doing something without understanding with a sound conceptual basis why to do it and how to do it better, appears to be too often the selected approach

A world of conceptual modelers

- What if sound CM-based were applied to first understand, later solve through a reasoned, conceptual agreement "big problems" as?
  - A CM of the European Union
  - Is Brexit good or bad?
  - Clinton vs Trump?
  - Should Scotland / Catalonia…become independents?
  - What is behind the social distortion and alineation of a suicide terrorist?

Basic issues that create the context for the new world to come...

- Hyperconnectity
- Technological acceleration
- Raising of world-wide emerging citizens, coming potentially from any country of the world and ready to consume and compete

Conceptual Modelers should act as the knowledge architects of relevant data and information generated by this hyperconnected world, composed by last-generation technologies in continuous evolution and reached by virtually all the human population.

- A sound process of conceptualization should identify the basic issues that lead the change,
  - to understand how they affect the current social context and…
  - to develop strategies to implement an accurate transformation

- CM should provide a solid basis to discuss and materialize the opportunities demanded by this new world that is coming.

The CM role....

- Need of strong conceptual support for essential concepts as context, adaptability, decision, luck, user experience, satisfaction, sustainability…
- Educating CM skills: a challenge to form citizens whose capabilities go beyond the Homo Sapiens traditional behavior

CM for different types of knowledge

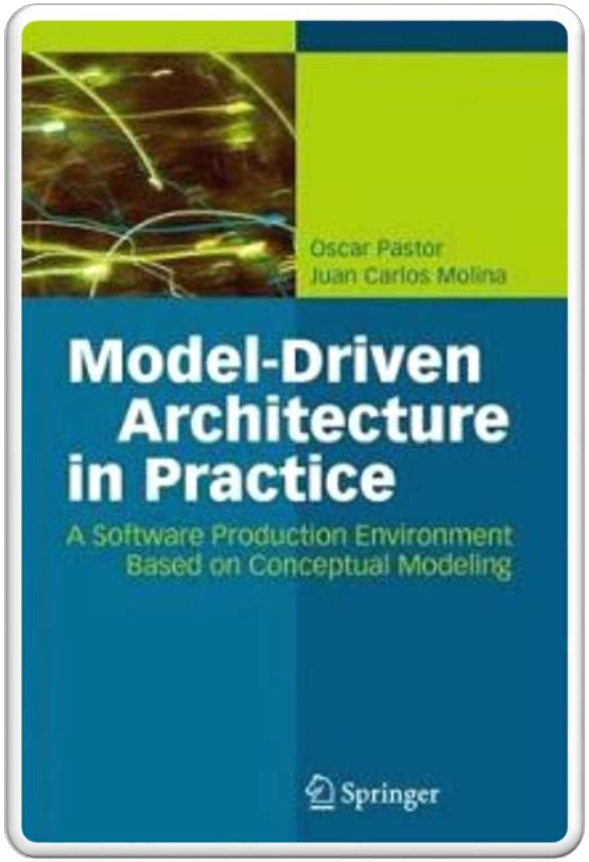
- Known knowns: expressible, articulated and relevant.
- Known unknowns: not expressible or articulated, but accessible and potentially relevant.
- Unknown knowns: potentially accessible but not articulated.
- Unknown unknowns: not expressible, articulated or accessible but still potentially relevant.

CM of Life: the Biological Perspective

- And now, let's move to the biological perspective of the conceptual modeling of life…
  1. Experience in CM: the "move" to the Genome Understanding
  2. CM of the Human Genome
  3. Bio-implications and applications to the Medicine of Precision

...Experience in Conceptual Modeling

- **We have been building**
  - Traditional Information Systems
  - Web-based Information Systems
  - SOA-based systems
  - Pervasive Systems
- **…but, what is next?**

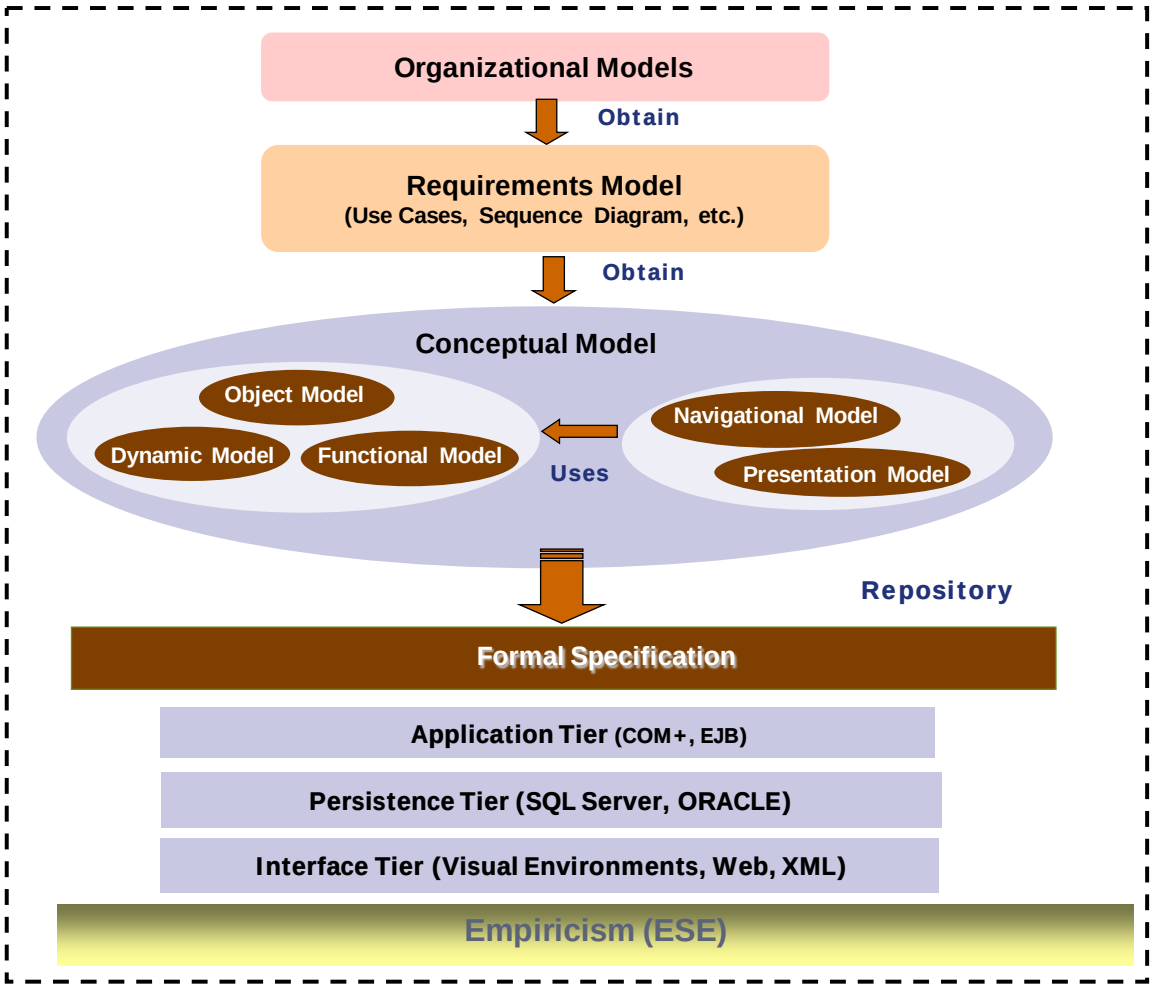


The OO-Method Approach

Problem Space Level

Automated Translation

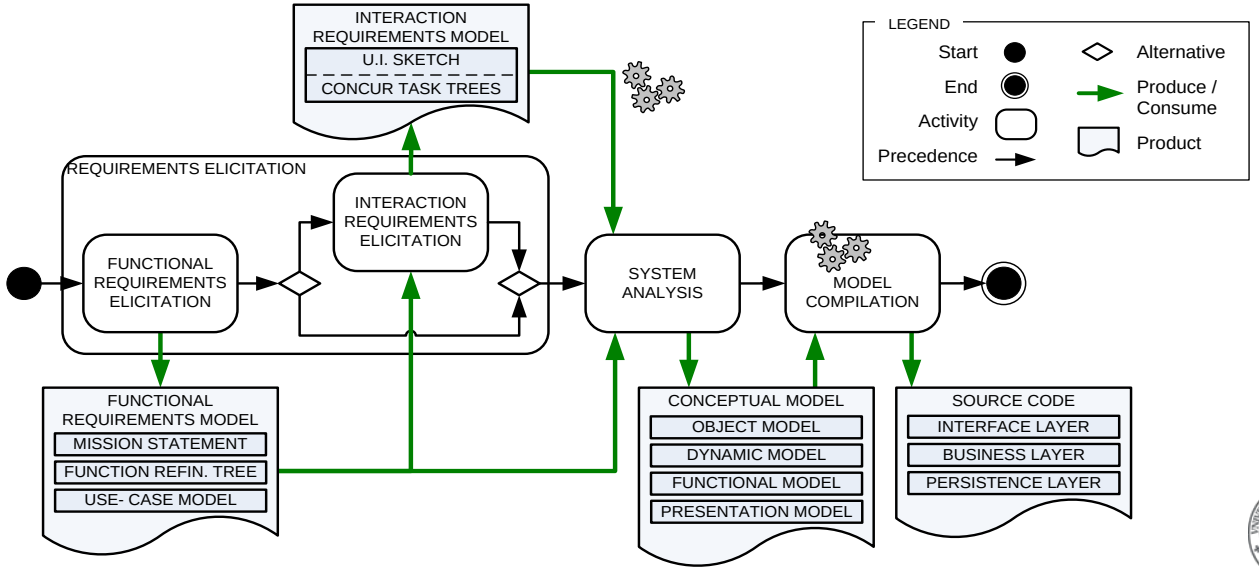
Solution Space Level



The OO-Method Approach

- We try to clarify our software development process

- Also, some gaps are being filled: an Interaction Requirements Model is being proposed, based on user-interface sketches that are supported a forest of task trees (ConcurTaskTrees notation)



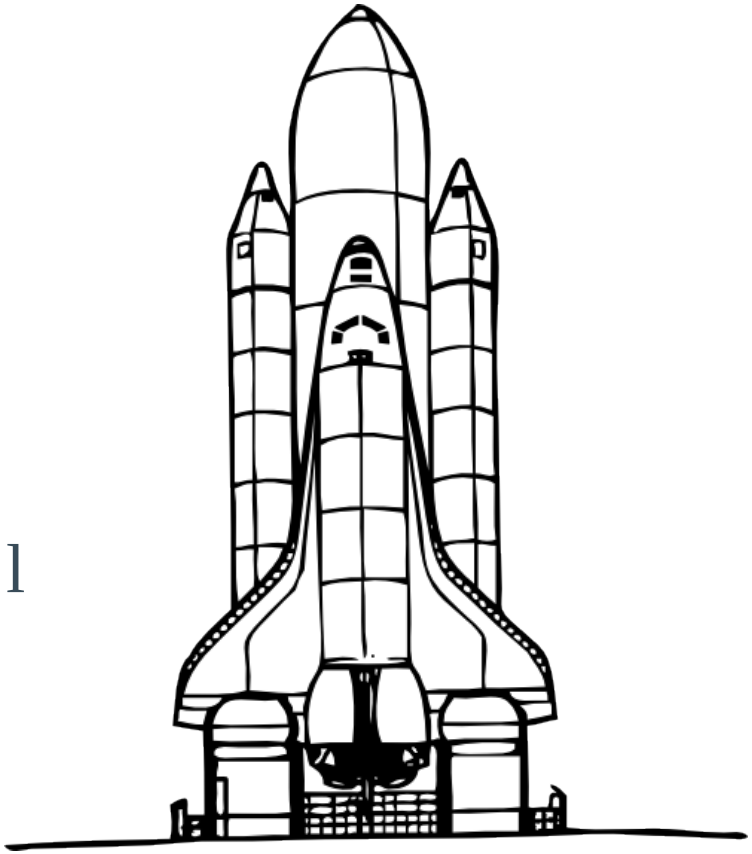
The Dream... (from Nicola Guerino, 2008)

An ontology-driven conceptual modeling system conceived as an extension of current tools such as IntegraNova, extended with

- ontological competence
- linguistic (terminological) competence
- capability to reason and criticize the designer's choice
- with reusability and understandability in mind.

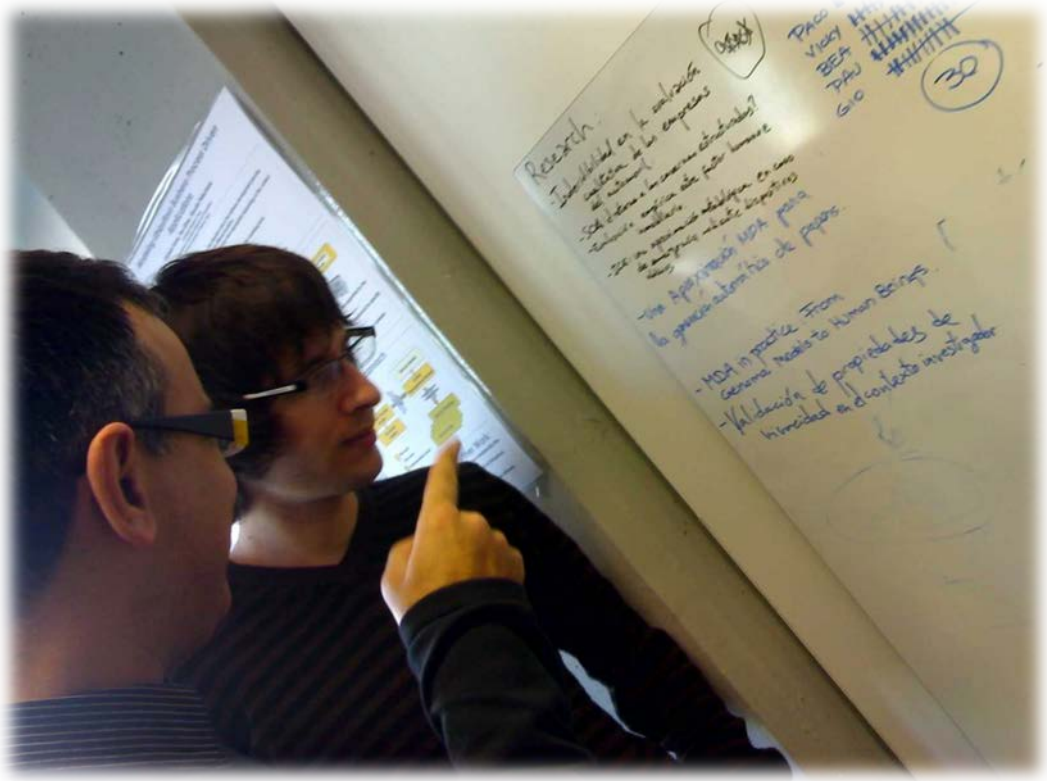
Which is the most complex system you can imagine?

- Aircraft control?
- Weather prediction?
- Digital TV?
- Videogames?
- Web n.0 socio-geographical mashups?



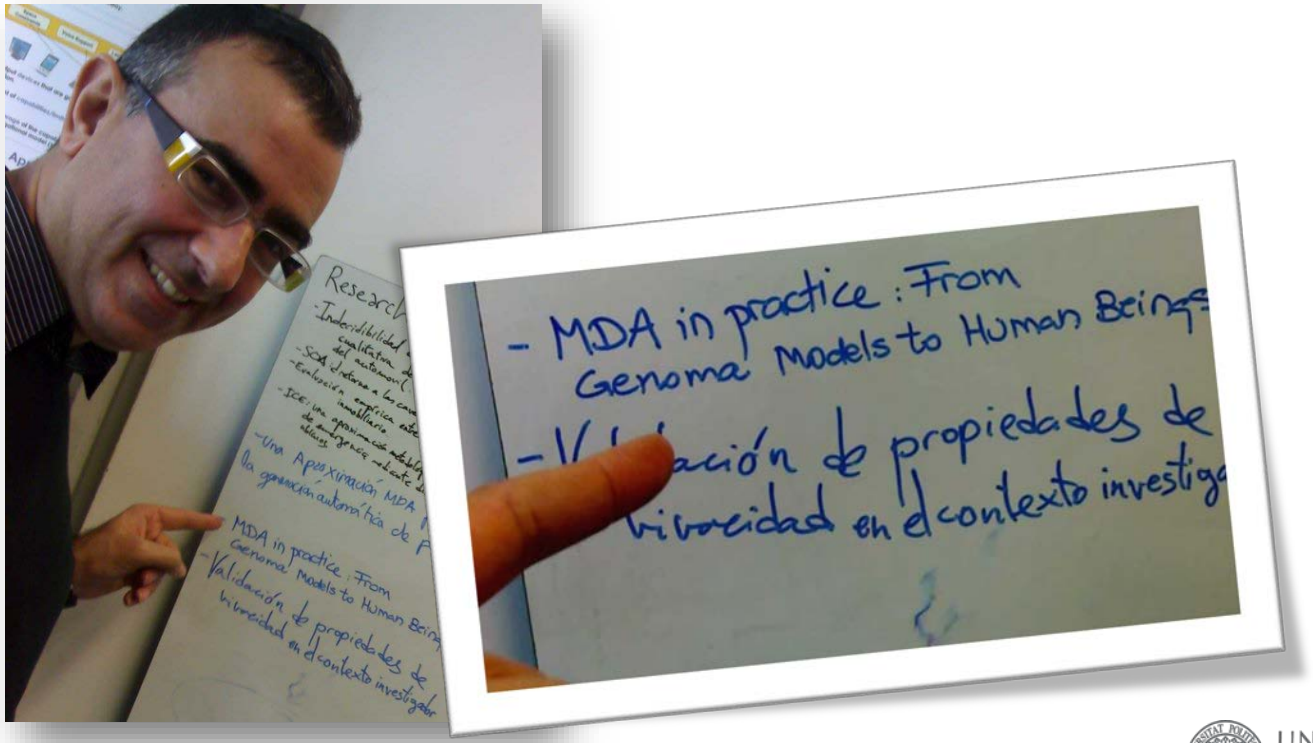
Which is the most complex system you can imagine?

- Discussion started…



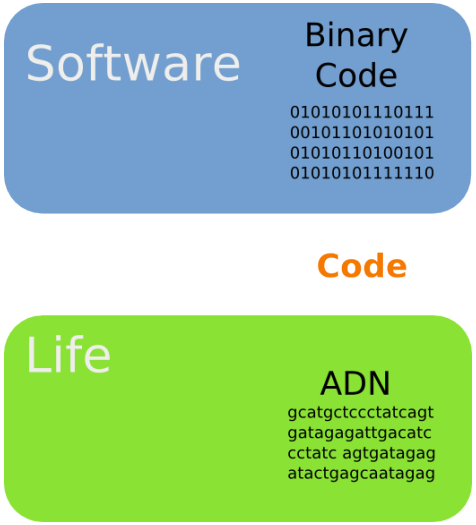
We found it

- Maybe, the **answer** is not so far from you…
- ..it is **you**!!



A parallelism

"A living organism is a **computer** or machine made up of genetic circuits in which DNA is the **software** that can be hacked." — *Drew Endy, MIT*



Modeling Life

- Synthetic Biology can create new forms of life from scratch
  - A microbe that would help in **fuel production**
  - Biological films as a basis of new forms of lithography for **assembling circuits**
  - Cell division inhibitors to **prevent cancer**
  - Re-designed seeds that the tree is programmed to grow into **a house**

..but, how is this *"software"* developed?

Modeling Life

"Using a laptop computer, published gene sequence information and **mail-order synthetic DNA**, just about **anyone** has the potential to construct genes or entire genomes from scratch." — *Drew Endy, MIT*

Software

Binary Code

01010101110111
00101101010101
01010110100101
01010101111110

Code

Life

ADN

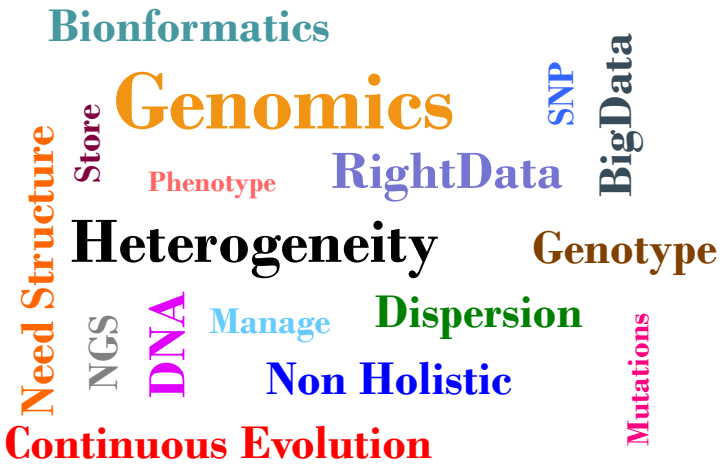
gcatgctccctatcagt
gatagagattgacatc
cctatc agtgatagag
atactgagcaatagag

Modeling Life

What would distinguish *Homo Genius* from *Homo Sapiens*?

The capability to understand and manipulate the Genome

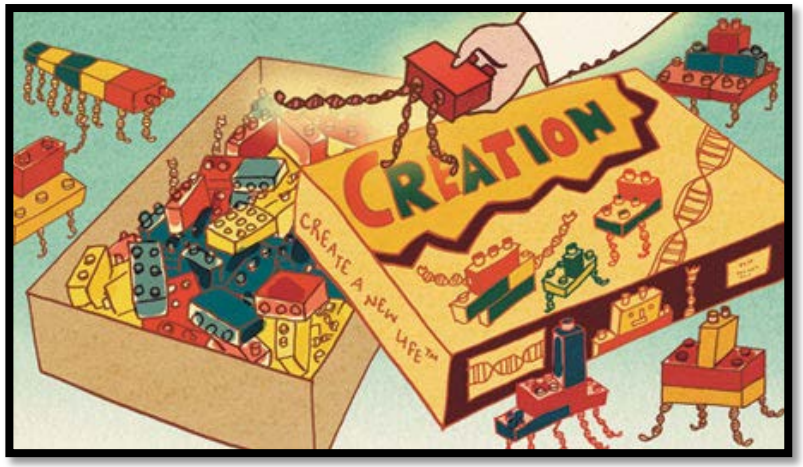
Modeling Life

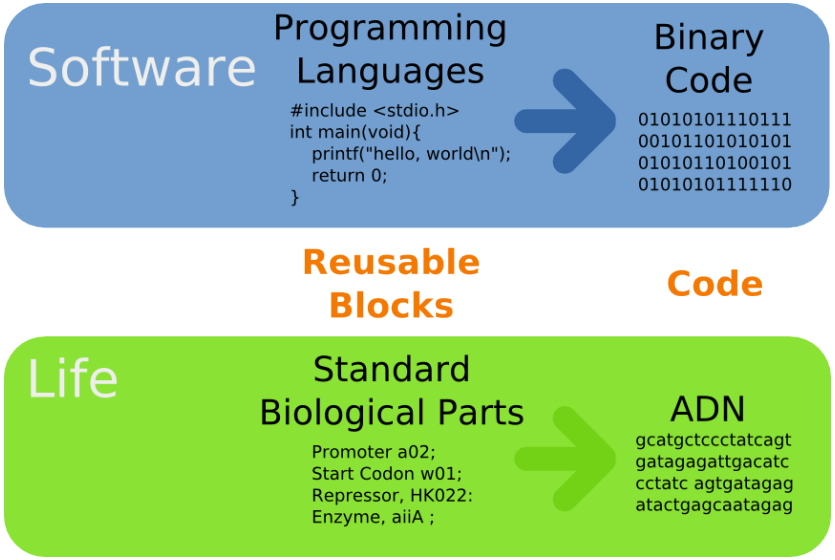


Information Systems — Conceptual Schema — Genomics

First step: Assembling

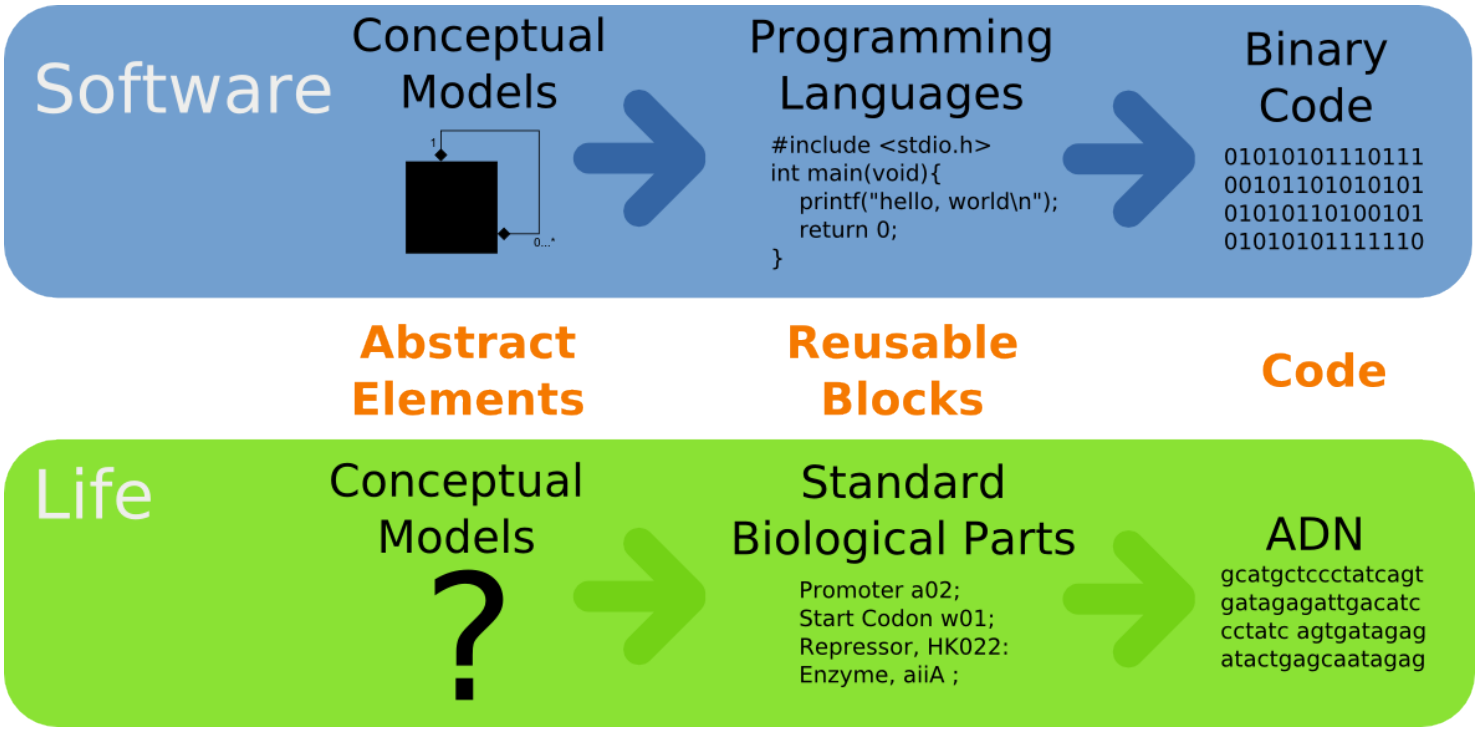
- First abstraction step
  - Standard Biological Parts





One step further: Modeling

- Conceptual models are needed for a systematic development of biological systems



From Genome To Reality

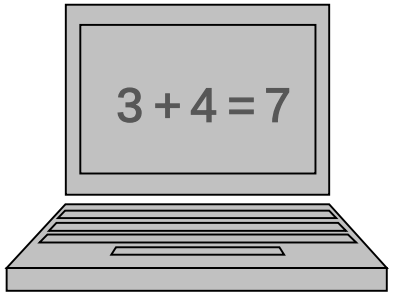
00010011	00000111	00000011	00001000

Physical Level

ADD $7 $3 $8

Instruction Level

Semantics: Add the values from the processor registers '3' and store the result in the register '8'



Representation Level

From Genome To Reality

AUG	GAA	CAC	GAC	GAG	UAA

Physical Level

START Glu His Asp Glu STOP

Instruction Level

Semantics: Process a protein with the four selected aminoacids

However, ¿Why?

Representation Level

The Genome Project

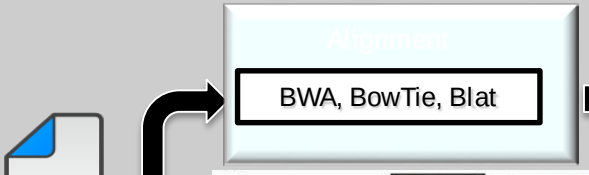
Genetic Sample

Next Generation Sequencing

TECHNOLOGIES

- SOLiD (Life Tech)
- 454 (Roche)
- Illumina

BIOINFORMATICS



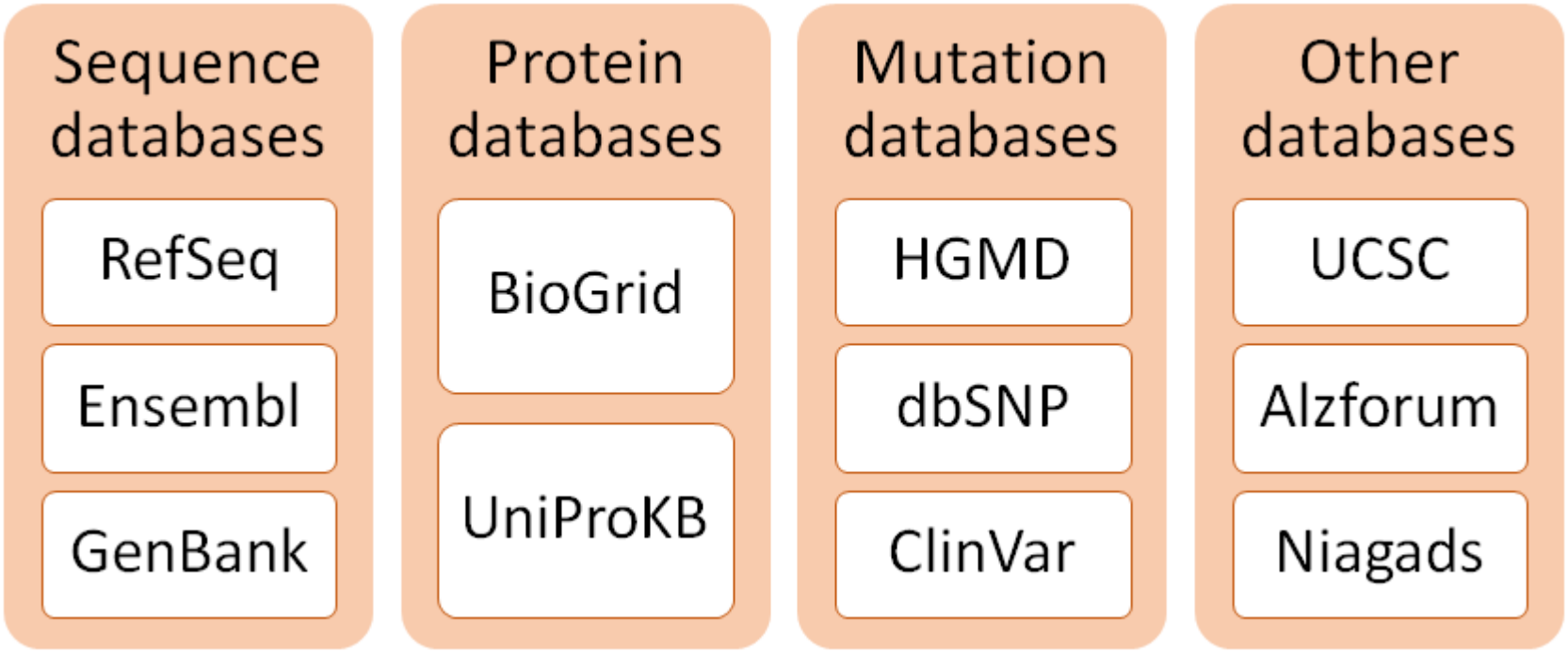
Design of Genomic Information Systems

ECGH

genes.me
www.geneslove.me

The Genomic Data Chaos

Data Quality Errors in Genomic Databases



Manual Methods of data analysis

Tedious and repetitive

No explicit methods

Human error

Navigation through hyperlinks

Data Quality Errors in Genomic Databases (Accuracy)

- Mostly found in primary databases (unreviewed data warehouses).
- SwissProt takes information from TrEMBL and when it is reviewed by experts any sequence conflict is annotated.
- Conflict annotations in the Human dataset: ~87%
  - Sequence conflicts: ~54%
  - Errors in sequence initiation: ~23%
  - Other errors: ~23%

Data Quality Errors in Genomic Databases (Consistency)

- Genomic databases are very diverse, making integration a laborious process.
- Clasification of variations attending to the type:
  - Ensembl: 21 variation types.
  - dbSNP: 8 variation types.
  - UCSC: 3 variation types.
- Variation type name:
  - Ensembl: “Insertion”, “Deletion” and “Substitution”.
  - dbSNP: “DIV”
  - UCSC: “I”, “D” and “S”

ClinVar Variant Interpretation Comparison

11% (12,895/118,169) of variants have ≥ 2 submitters in ClinVar

17% (2,229/12,895) are interpreted differently

The NEW ENGLAND JOURNAL of MEDICINE

SPECIAL REPORT

ClinGen — The Clinical Genome Resource

Heidi L. Rehm, Ph.D., Jonathan S. Berg, M.D., Ph.D., Lisa D. Brooks, Ph.D., Carlos D. Bustamante, Ph.D., James P. Evans, M.D., Ph.D., Melissa J. Landrum, Ph.D., David H. Ledbetter, Ph.D., Donna R. Maglott, Ph.D., Christa Lese Martin, Ph.D., Robert L. Nussbaum, M.D., Sharon E. Plon, M.D., Ph.D., Erin M. Ramos, Ph.D., Stephen T. Sherry, Ph.D., and Michael S. Watson, Ph.D., for ClinGen

NEJM May 27th, 2015

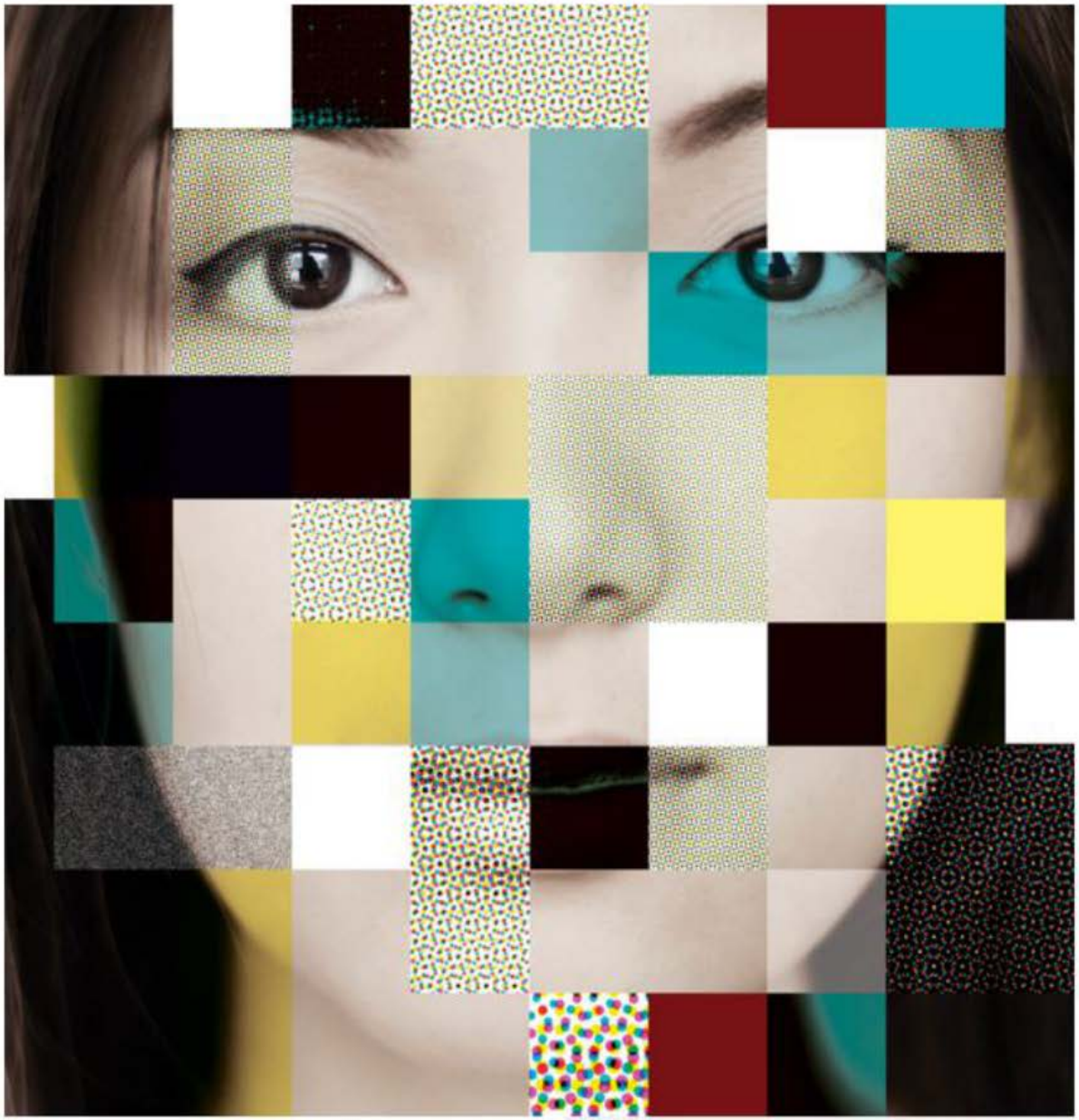
RESEARCH 6 min read

Open to Interpretation

Increasingly, genetic tests provide ambiguous results, leaving doctors and scientists searching to make sense of these 'variants of unknown significance.'

BY ERIC CELESTE

November 24, 2014 | Print | 0 Comments



The Atlantic
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Clinical Genetics Has a Big Problem That's Affecting People's Lives

nreliable research can lead families to make health decisions they ight regret.

For Heidi Rehm, it looked like a straightforward case. Her lab at Partners Healthcare offers tests for genetic diseases. They had received a blood sample from a fetus after a doctor conducting an ultrasound spotted signs of Noonan syndrome—an inherited disorder involving heart problems and stunted growth. The fetus turned out to have a mutation in PTPN11, a gene that affects the risk of Noonan syndrome.

Rehm found that another team of scientists had published on that very same mutation before. (Not every mutation of PTPN11 increases the rick of Noonan syndrome.) They found that it was more common among Noonan patients than in healthy people, and had billed it as "pathogenic"—that is, likely to cause disease. Rehm reported it as such to the doctor who sent her the sample.

Sometime later, she was listening to a talk by a colleague who had found the same mutation in a patient with Noonan syndrome and, based on the same published study, had also classified it as pathogenic. But this time, the patient—an adult—had contacted the researchers behind the paper. And they had admitted that their conclusions were wrong. In later work, they had found that the mutation is so common in certain ethnic groups that it couldn't possibly be responsible for a rare disease like Noonan syndrome. It wasn't pathogenic after all.

"I immediately contacted the physician to find out the story with that baby," Rehm says. "And that's when I found out that the parents had terminated it."

Mother's Negligence Suit Against Quest's Athena Could Broadly Impact Genetic Testing Labs

Mar 14, 2016 | Turna Ray

NEW YORK (GenomeWeb) – Christian Millare had a severe seizure on Jan. 5, 2008, and died. He was two years old.

His mother Amy Williams is convinced, based on his medical records, the opinions of experts, and the published liter[illegible] Quest Dia tes

In the complaint, Williams accuses Athena of misclassifying her son's SCN1A mutation as a variant of unknown significance (VUS), meaning that the lab determined there wasn't sufficient evidence in 2007 to link the mutation to epilepsy or determine it was benign. Williams asserts there was enough evidence at the time that her son's mutation was disease-causing. The complaint cites two papers, one published in June 2006 and one published in March 2007, which mention Christian's specific mutation had been studied and seen in another patient who had epileptic encephalopathy.

Motivation

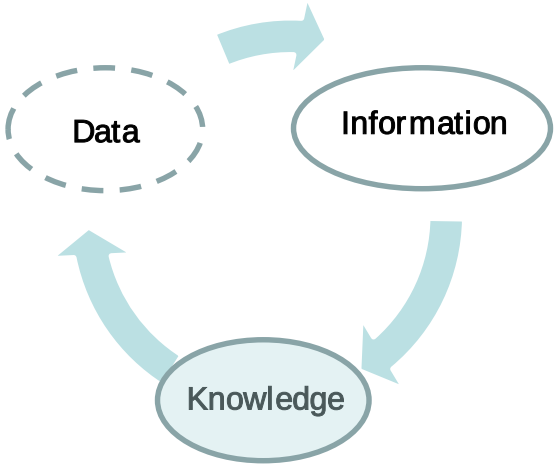
Motivation

2003

2010

2015

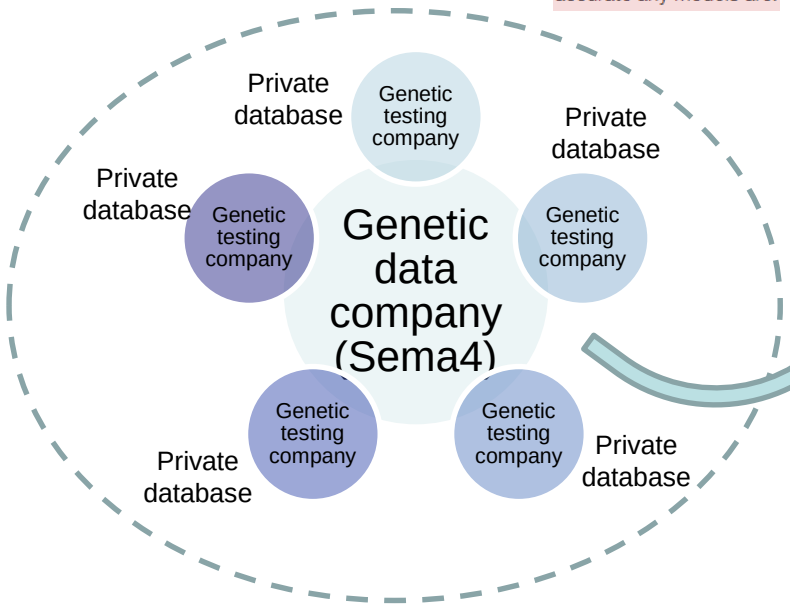
Data, information or knowledge?

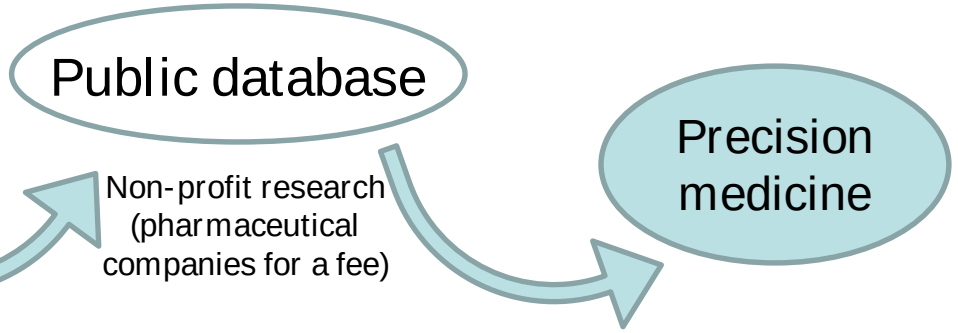


More Data, Please

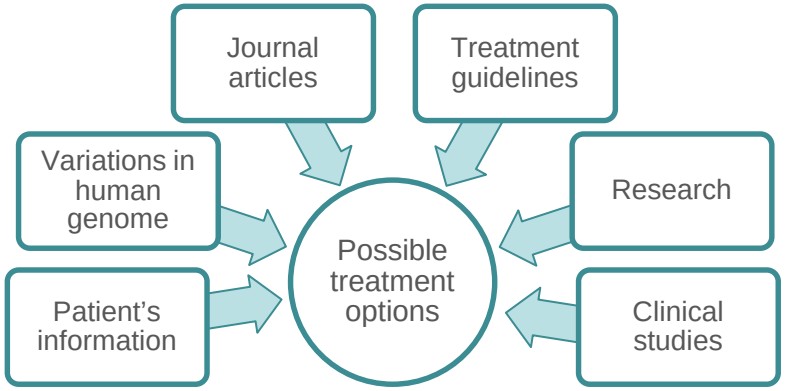
Oct 19, 2016

To tease out disease patterns, particularly for cancers, Mount Sinai's Eric Schadt tells *Wired* that data from many individuals is required — the more data, the more accurate any models are.





Dealing with genomic's Big Data



Medical data is expected to double every 73 days by 2020:

- How to clean, normalize, and manage large datasets?
- How to look for algorithmically interesting patterns?
- How to structure data that is unstructured?

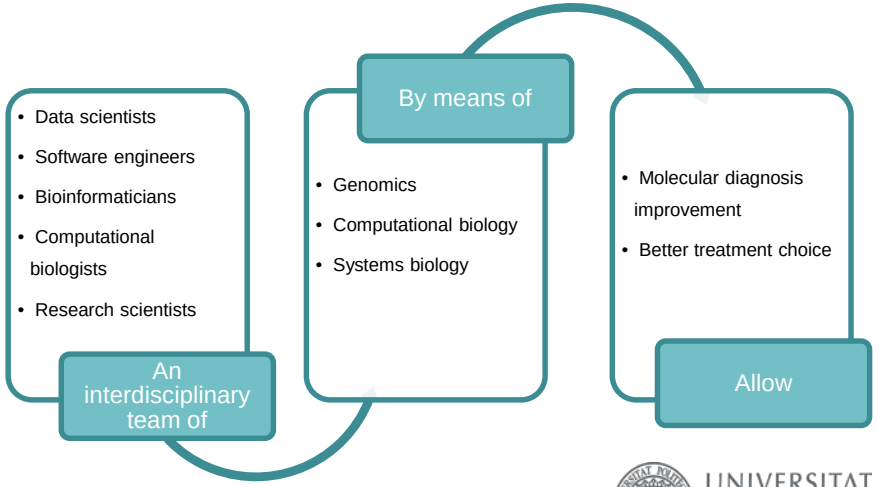
IBM's Watson (from unstructured data)

Able to read scientific literature and interpret scans.

Tested at North Carolina Cancer Hospital:

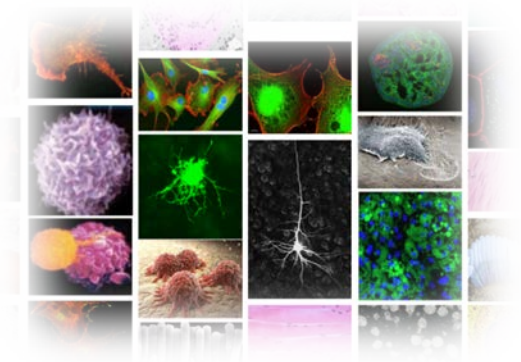
- 99% cases prescribed treatment within Watson's options
- 30% cases new treatment options not considered
- Timeline reduced from weeks to minutes!

Tempus (from structured data)

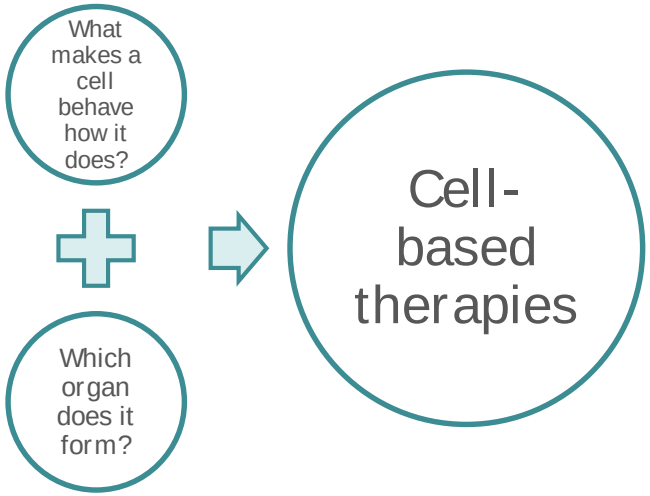


Dealing with genomic's Big Data

Human Cell Atlas project



35 billion cells, 300 major types, many more subtypes
ALMOST THE SAME GENOME!

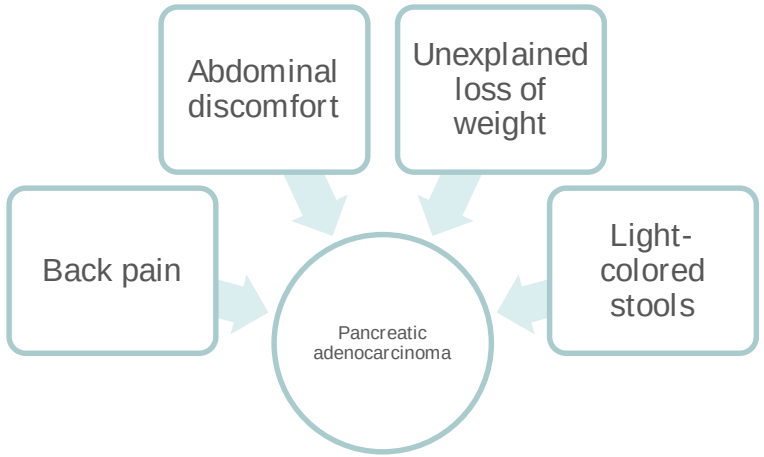


What if no biological data was needed at all?

Screening for Pancreatic Adenocarcinoma Using Signals From Web Search Logs: Feasibility Study and Results

John Paparrizos, MSc, Ryen W. White, PhD, and Eric Horvitz, MD, PhD

Search logs as sensor!



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Sharing variants

Human Genome Variation Society (HGVS) variant nomenclature format:

<sequence file identifier>:<type of reference sequence>.<position><change>

Different representations are sometimes possible ⇨ Automatically matching variations against a database may not be trivial

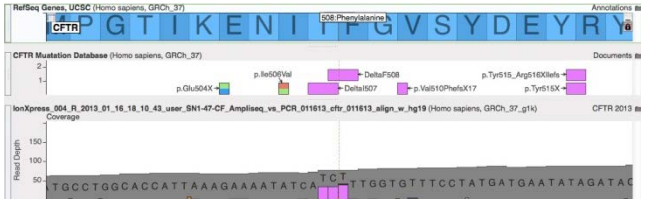
Examples of ambiguities and problems:

- Many notations for the same variant

```
Ref: GAAC    Alt: GTTC
```

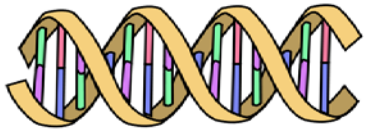
g.2_3delinsTT/ g.2_3inv

- Software ignoring the guidelines



- Discrepancies turn into bugs

GRCh37 (3,137,144,693bp)



GRCh38 (3,238,442,024bp)

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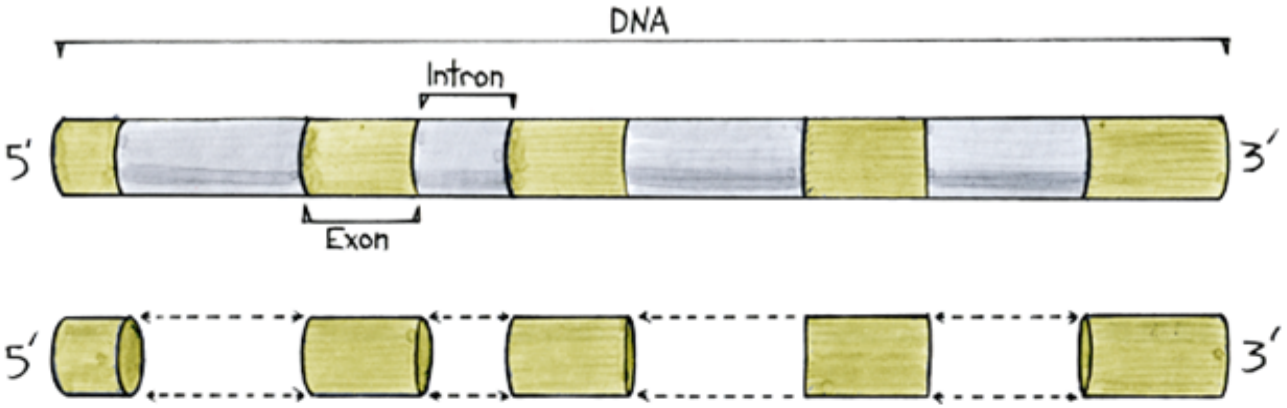
The short-time future

- The problem is getting worse!!!!!
- The DNA Sequencing hardware is evolving dramatically
- In next years, we will be able to sequence a complete human genome faster and cheaper

	2003	2006	2016
Technology	Sanger	Next generation	Next generation
Cost	$3 billion	$100000	$1000 / $6500
Duration	13 years	3 months	3 days / 26h



3,2 Gb (~20000 genes)
3GB (899MB compressed)

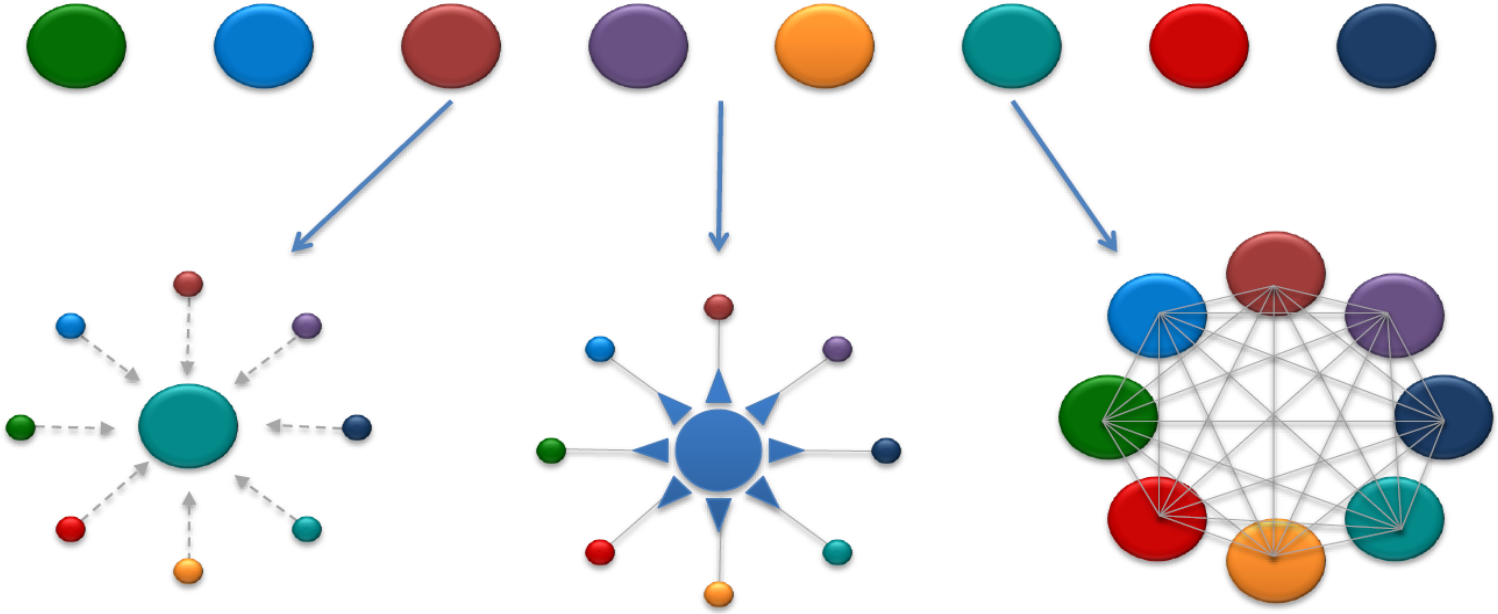
32 Mb (85% known variants)

4,8 Mb (3000 genes associated with Mendelian diseases)

To improve our DNA variation **knowledge** and variant classification **consistency**, a massive effort in **data sharing** will be required.

The genomic community needs to come together and develop its own standards to ensure safe and effective use of genetic and genomic medicine.

Connecting Data in the Big Data World



Centralized Database
Everyone submits data to a single central database

Examples:
ClinVar,
dbGaP, EGA

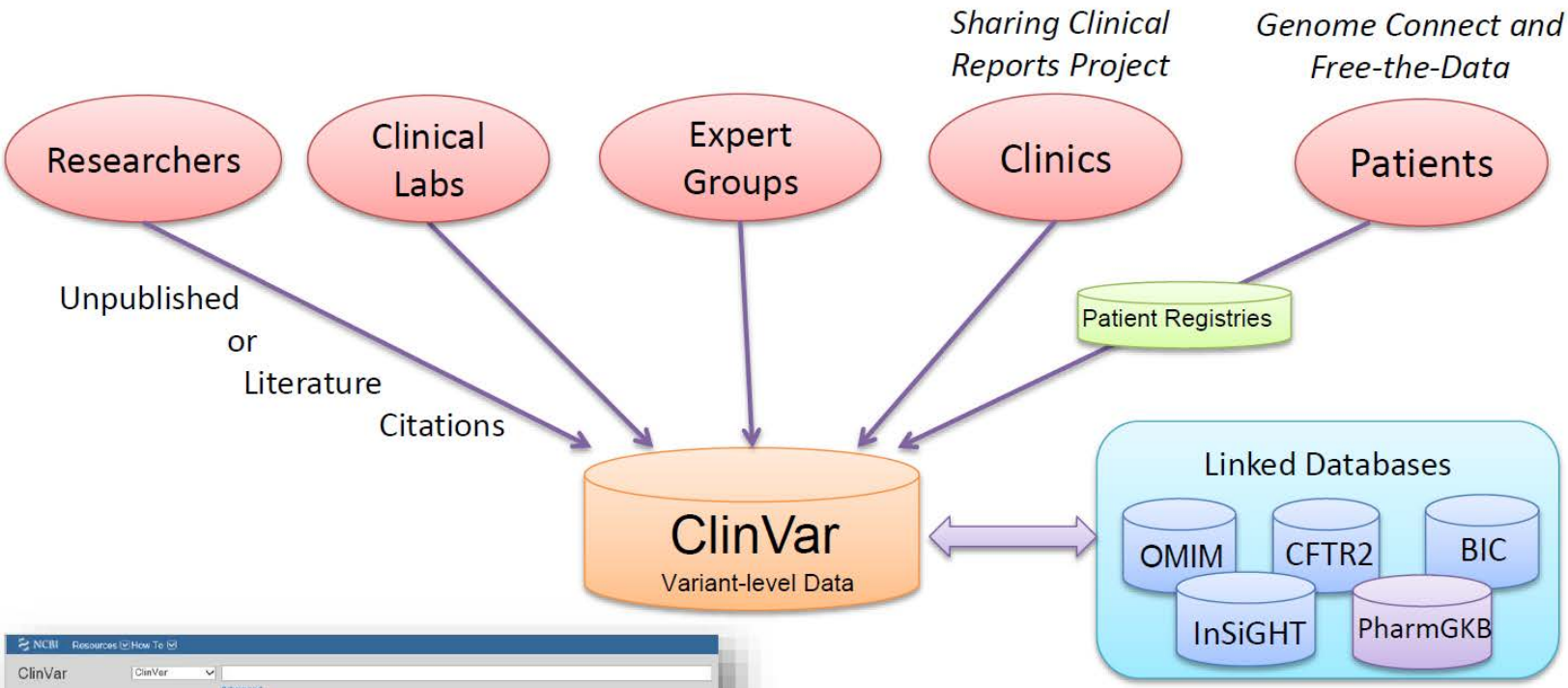
Centralized Hub
APIs connect each database to a central hub

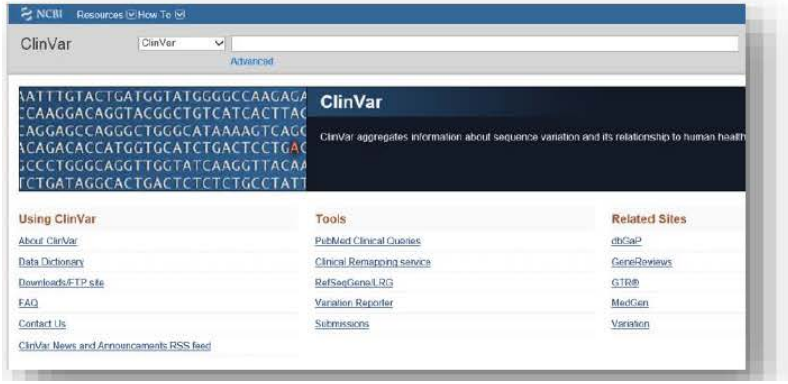
Example:
Many commercial platforms

Federated Network
All databases connected through multiple APIs

Example:
Matchmaker Exchange

Aggregating Variant Interpretations in ClinVar

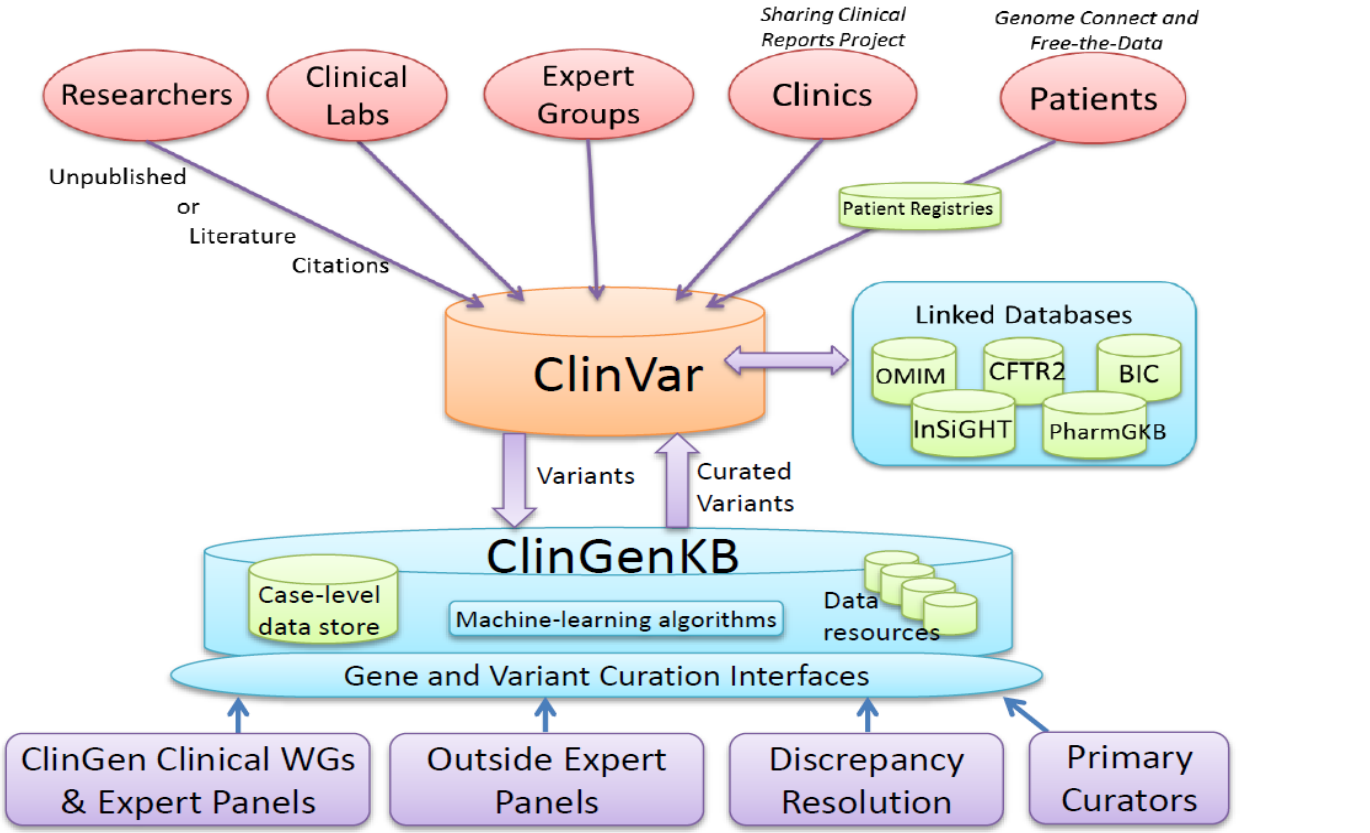


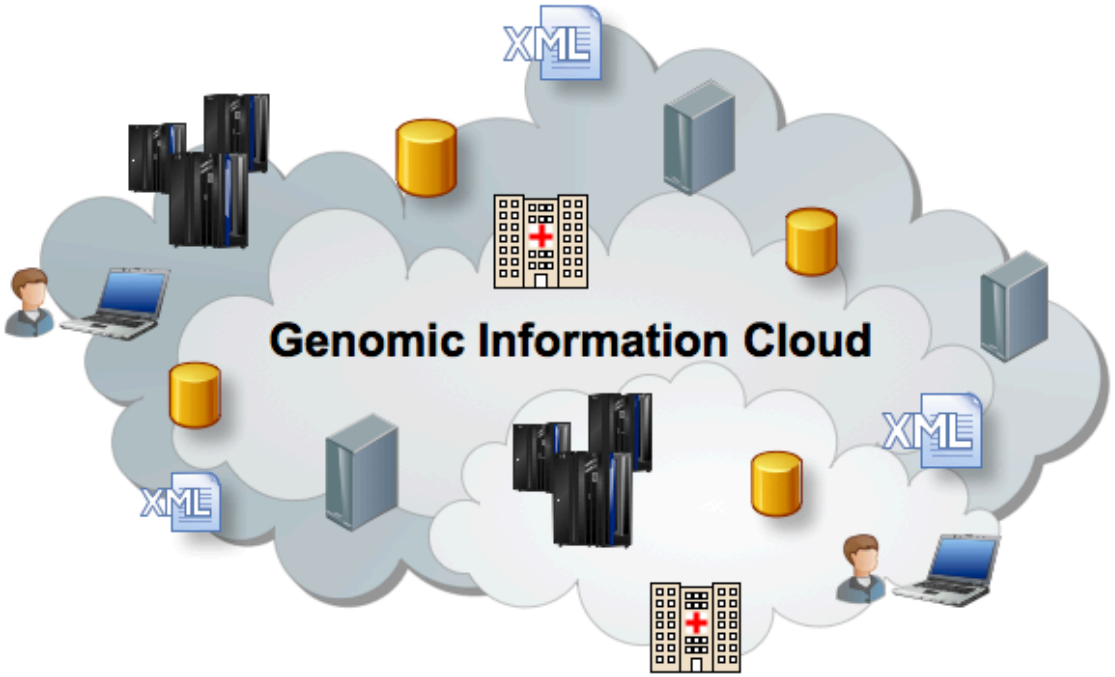


482 ClinVar submitters
179,845 variants submitted
126,247 unique interpreted variants

ClinVar as of March 21, 2016

Supporting a Curation Environment for both Crowd-Sourcing and Expert Consensus



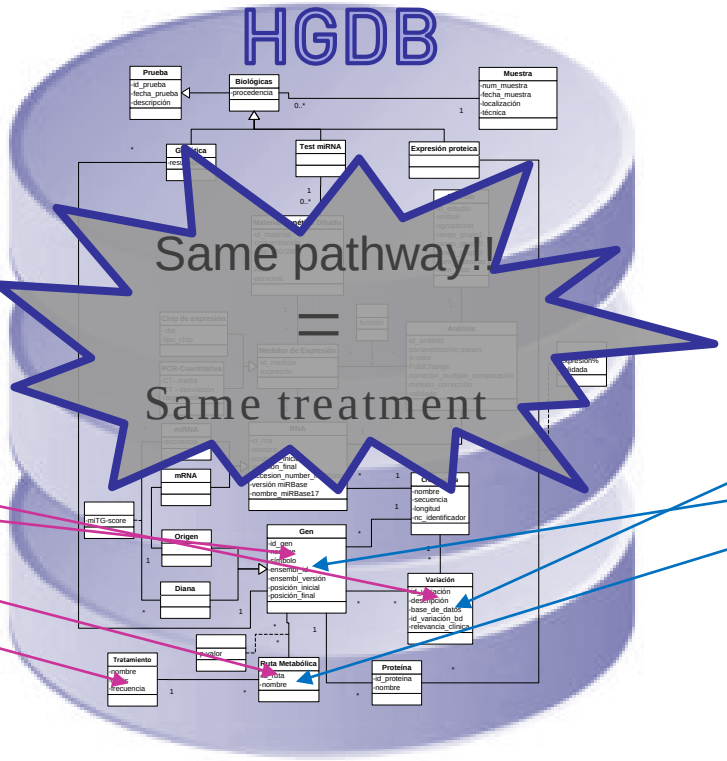


Modeling

Breast Cancer Studies

- Variation
- Gene
- Pathway
- Treatment

HGDB



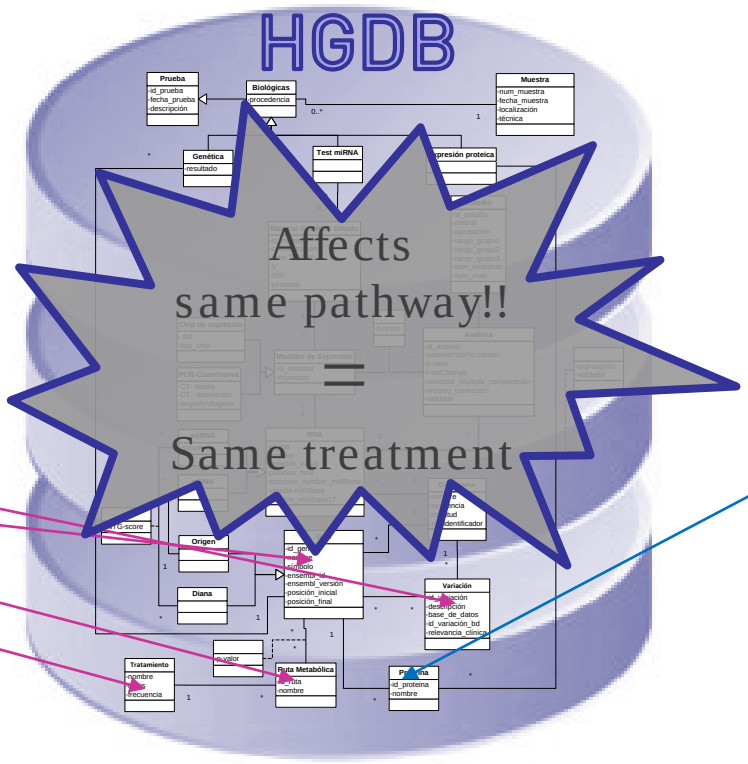
Neuroblastoma Studies

- Variation
- Gene
- Pathway

Breast Cancer Studies

- c.256A> G
- SNAP23
- Exocytosis
- Herceptin

HGDB

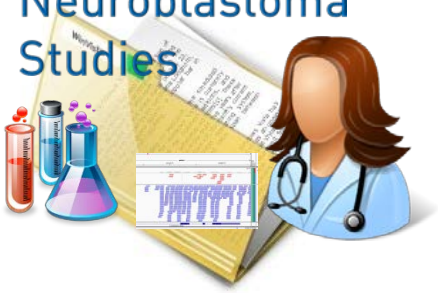


Affects same pathway!!

=

Same treatment

Neuroblastoma Studies



- p.Glu1038Ala

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Neuroblastoma gene rearrangements

Fusion partners	References (PMID)
NF1:NF1	11748857 15103551 7485153 9169039
KMT2A:FRYL	16061630 17854671 18195096
PAFAH1B2:FOXR1	21860421
NBPF1:ASIC2	18493581
TERT:ALK	25485619
KMT2A:FOXR1	21860421

Adenocarcinoma gene rearrangements

Fusion partners	References (PMID)	Treatment
TMPRSS2:ERG	16820092 16951141 17043636	-
MAP4K4:RRBP1	25204415	-
TPM3:NTRK1	10074915 10646882	-
EML4:ALK	22707299 22919003 22954507 22975805 23060067 23264847	**Crizotinib**
CAMKK2:KDM2B	25204415	-

What if crizotinib were also useful in neuroblastoma?

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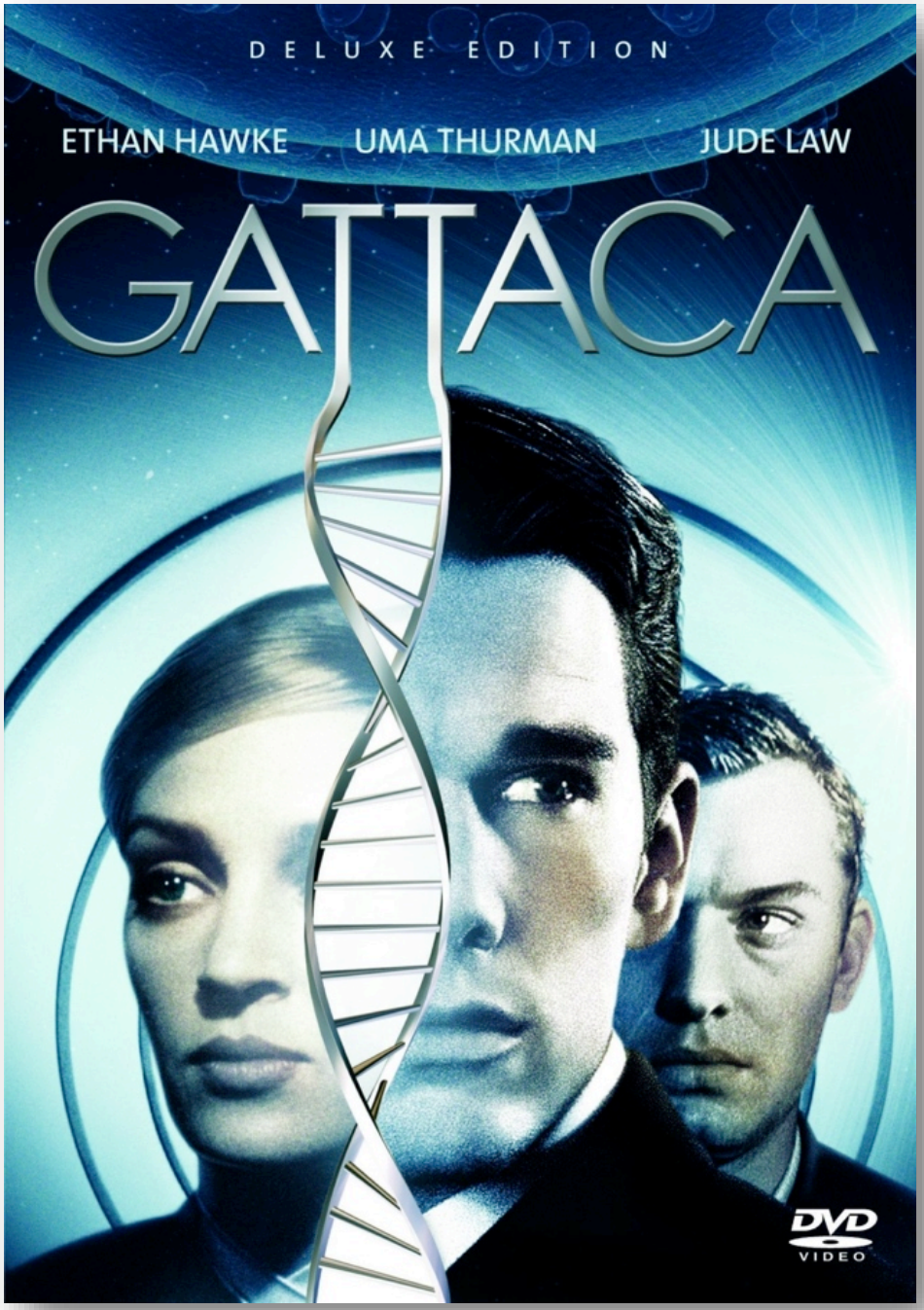
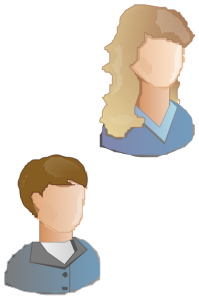

DELUXE EDITION
ETHAN HAWKE
UMA THURMAN
JUDE LAW
GATTACA
DVD
VIDEO

PROS

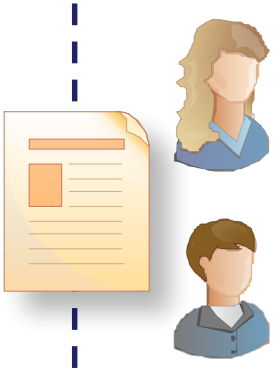
Genoma Project



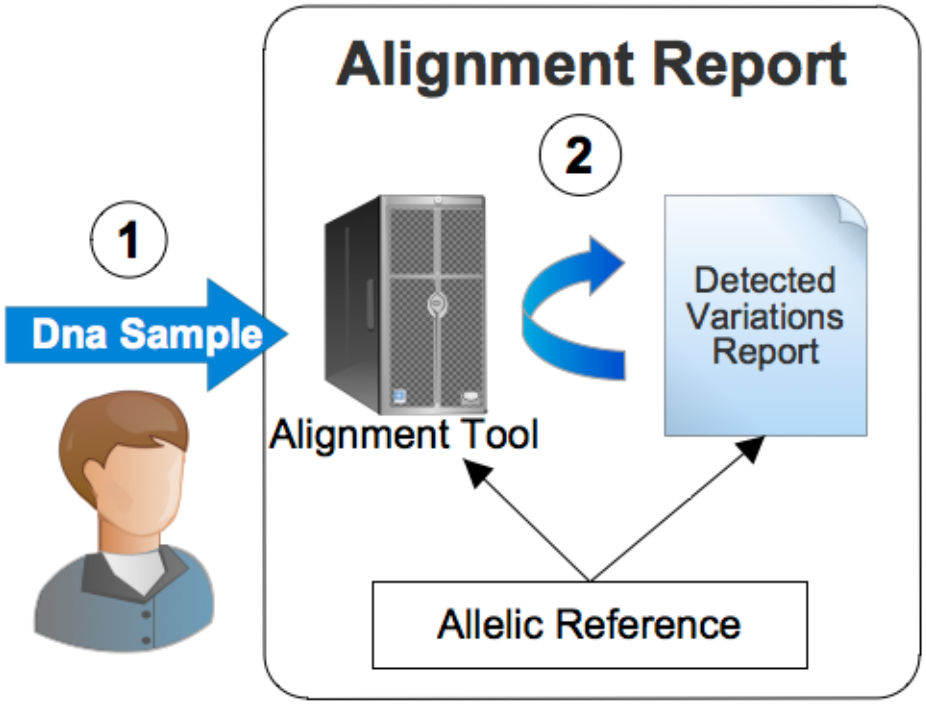
SEQUENCING PIPELINE

RIGHT DATA

RIGHT KNOWLEDGE



Variation Analysis Process

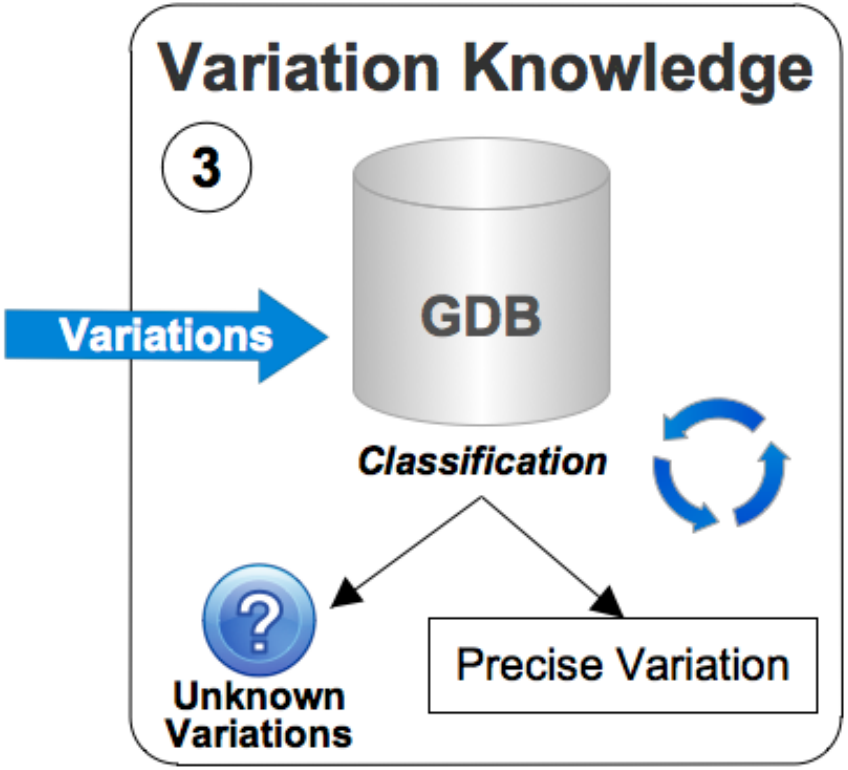


The Input of the process is a DNA sample from a sequencing machine and an allelic reference sequence.

An alignment is performed using the BLAST tool.

Each discovered difference is formalized as an instance of the variation entity. Then, a summarized report is generated.

Variation Analysis Process

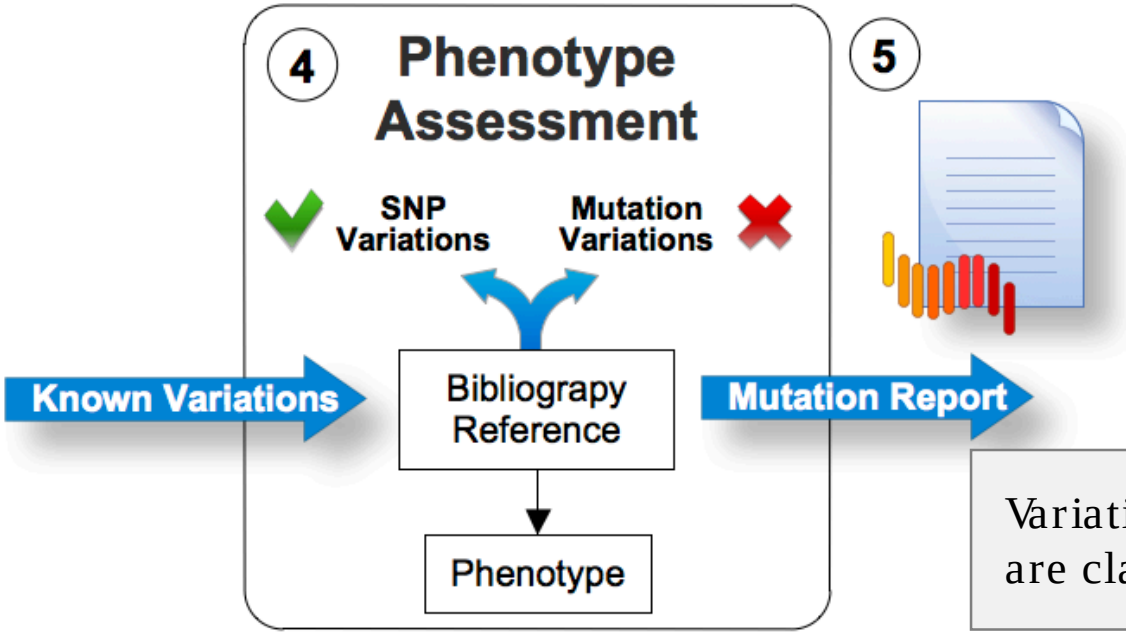


Found Variations are searched in a database conforming to the genome conceptual model.

Known variations are classified into a specific type of sequence change (Insertion, Deletion, SNP, Indel).

Unknown variations are classified as non-silent if the variation produces an effect in the expected gene product .

Variation Analysis Process



In order to assess the phenotype of an specific variation, a research publication is required.

The conceptual model describes the bibliographical reference that supports the phenotype of a variation.

Variations with a pathogenic phenotype are classified as mutations

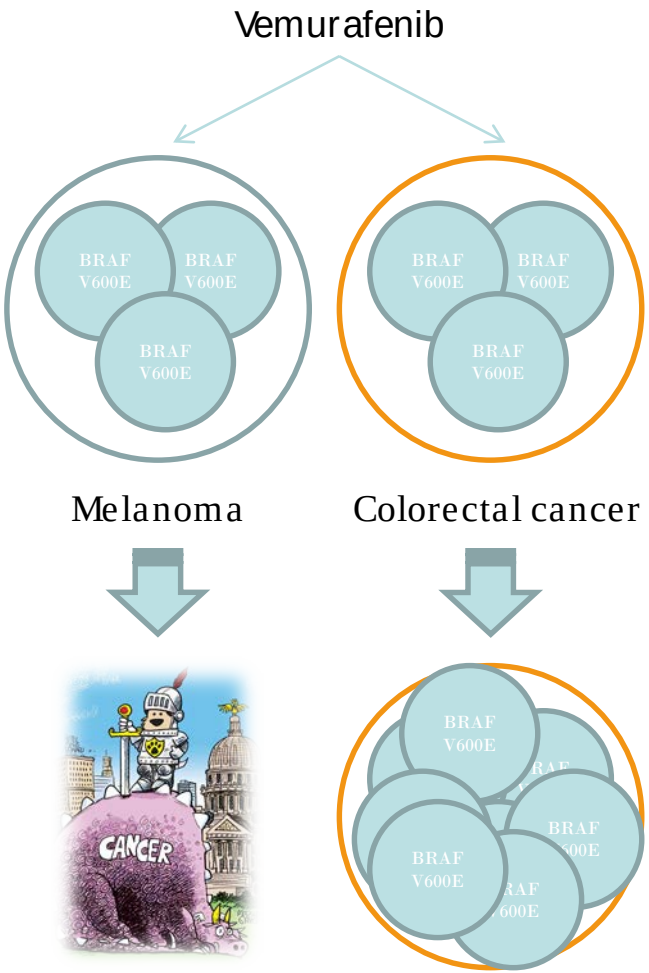
Finally, the information is gathered in a report to support the clinical diagnosis

nature biotechnology

Analysis of 589,306 genomes identifies individuals resilient to severe Mendelian childhood diseases

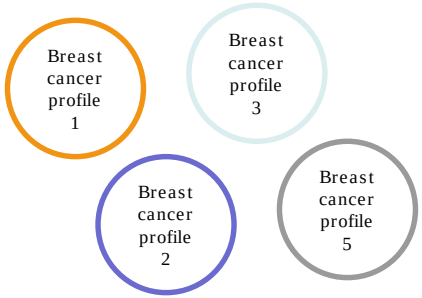
Rong Chen[1,2,12], Lisong Shi[1,2,12], Jörg Hakenberg[1,2], Brian Naughton[3,11], Pamela Sklar[1,2,4], Jianguo Zhang[5], Hanlin Zhou[5], Lifeng Tian[6], Om Prakash[7], Mathieu Lemire[8], Patrick Sleiman[6], Wei-yi Cheng[1,2], Wanting Chen[5], Hardik Shah[1,2], Yulan Shen[5], Menachem Fromer[1,2,4], Larsson Omberg[9], Matthew A Deardorff[6], Elaine Zackai[6], Jason R Bobe[1,2], Elissa Levin[1,2], Thomas J Hudson[8], Leif Groop[7], Jun Wang[10], Hakon Hakonarson[6], Anne Wojcicki[3], George A Diaz[1,2], Lisa Edelmann[1,2], Eric E Schadt[1,2] & Stephen H Friend[1,2,9]

Usually works though...

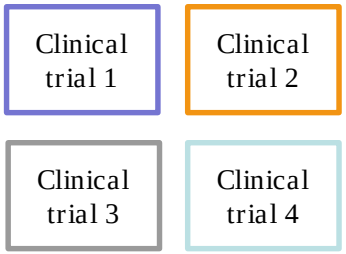


Signaling pathways may be important in cancer

Genetic testing company (integrating sequencing, expression and proteomic data)



Breast cancer screening program



Let's hope we are never in that situation but…do you like wine?

Genetic profile 1

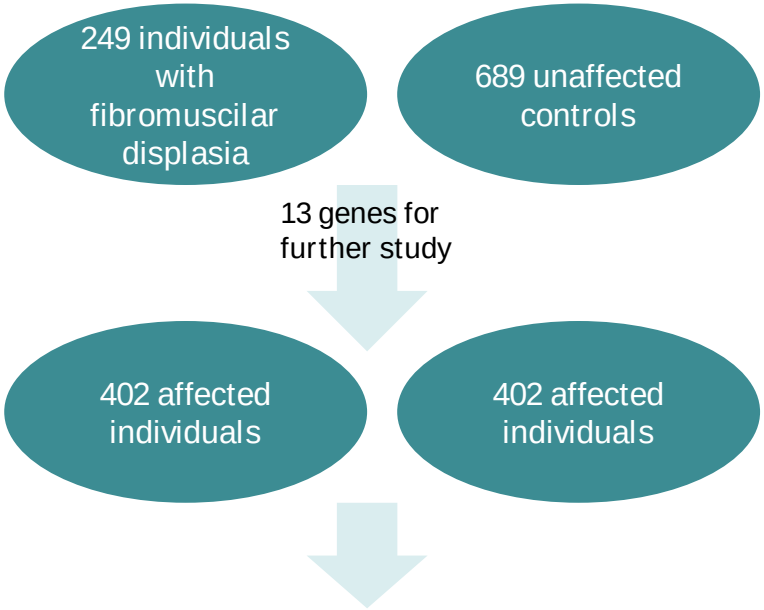
Genetic profile 2

Usually works though...

PHACTR1 Is a Genetic Susceptibility Locus for Fibromuscular Dysplasia Supporting Its Complex Genetic Pattern of Inheritance

Soto Romuald Kiando, Nathan R. Tucker, Luis-Jaime Castro-Vega, Alexander Katz, Valentina D'Escamard, Cyrielle Tréard, Daniel Fraher, Juliette Albuisson, Daniella Kadian-Dodov, Zi Ye, Erin Austin, Min-Lee Yang, Kristina Hunker, […], Nabila Bouatia-Naji [view all]

Published: October 28, 2016 • http://dx.doi.org/10.1371/journal.pgen.1006367

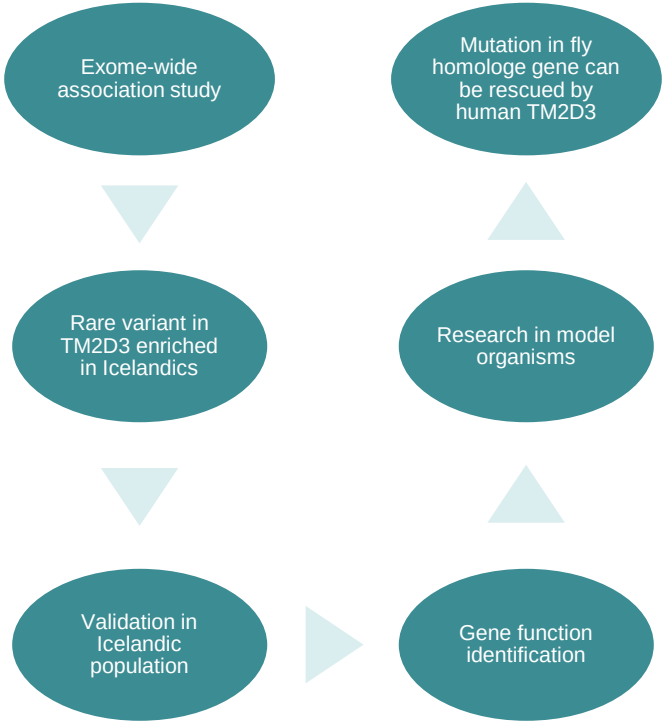


Intron variant associated with fibromuscular dysplasia which can alter the gene's expression

Rare Functional Variant in *TM2D3* is Associated with Late-Onset Alzheimer's Disease

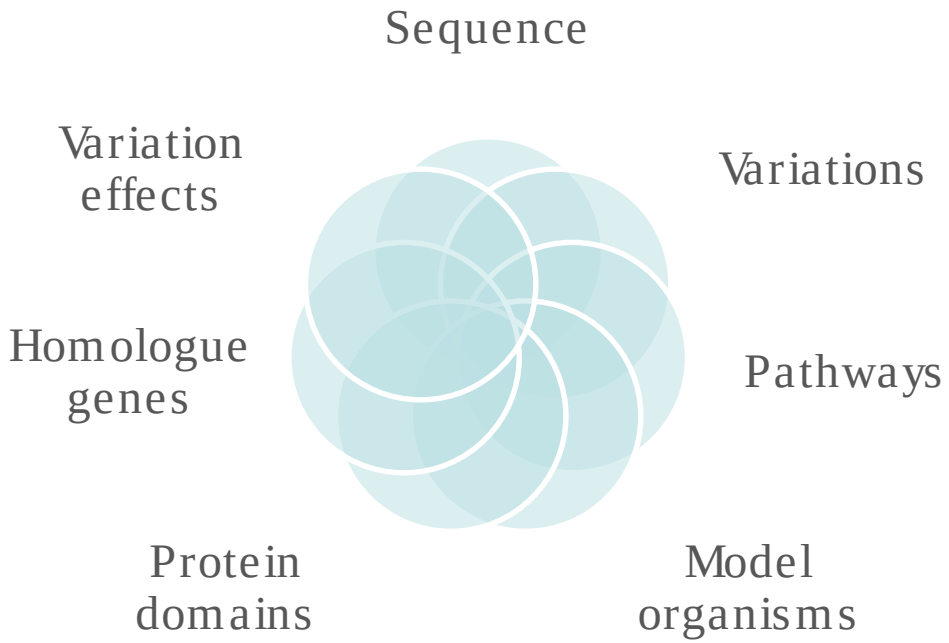
Johanna Jakobsdottir, Sven J. van der Lee, Joshua C. Bis, Vincent Chouraki, David Li-Kroeger, Shinya Yamamoto, Megan L. Grove, Adam Naj, Maria Vronskaya, Jose L. Salazar, Anita L. DeStefano, Jennifer A. Brody, Albert V. Smith, […], Cornelia M. van Duijn [view all]

Published: October 20, 2016 • http://dx.doi.org/10.1371/journal.pgen.1006327



Conclusions

- With **Conceptual Models** targeted at digital elements, we can improve Information Systems Development
- With Conceptual Models targeted at **life** we can directly improve **our living**



Conclusions

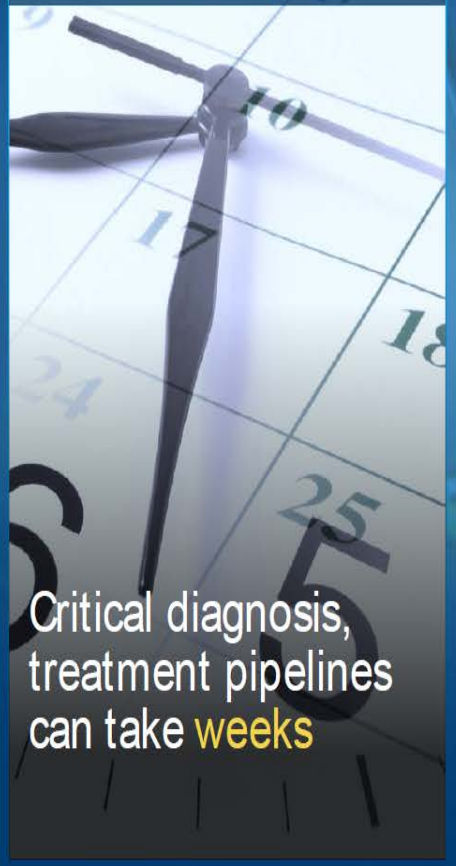
- A world plenty of conceptual modelers making true a "from Homo Sapiens to Homo Genius" evolution in two main directions:
  - Understanding and leading the human adaptation to "the world to come" (social perspective)
  - Understanding life through genome understanding and management (the "biological perspective"

MAIN COMPUTING CHALLENGES TO ACHIEVE 'ALL IN ONE DAY'

Size
Data management

Raw sequencing data sets are large, impractical to share

Speed
Workflow efficiency



Critical diagnosis, treatment pipelines can take weeks

Secure sharing
Privacy protection

Difficult to protect patient privacy while sharing diagnosis, treatment data

Scalability
Increasing requirements

Genomic sequencing outpacing capabilities of current architectures

DESIGN CHALLENGES WE'VE BEEN FOCUSING ON

Get new insights in a secure, shared way without giving up control of your data

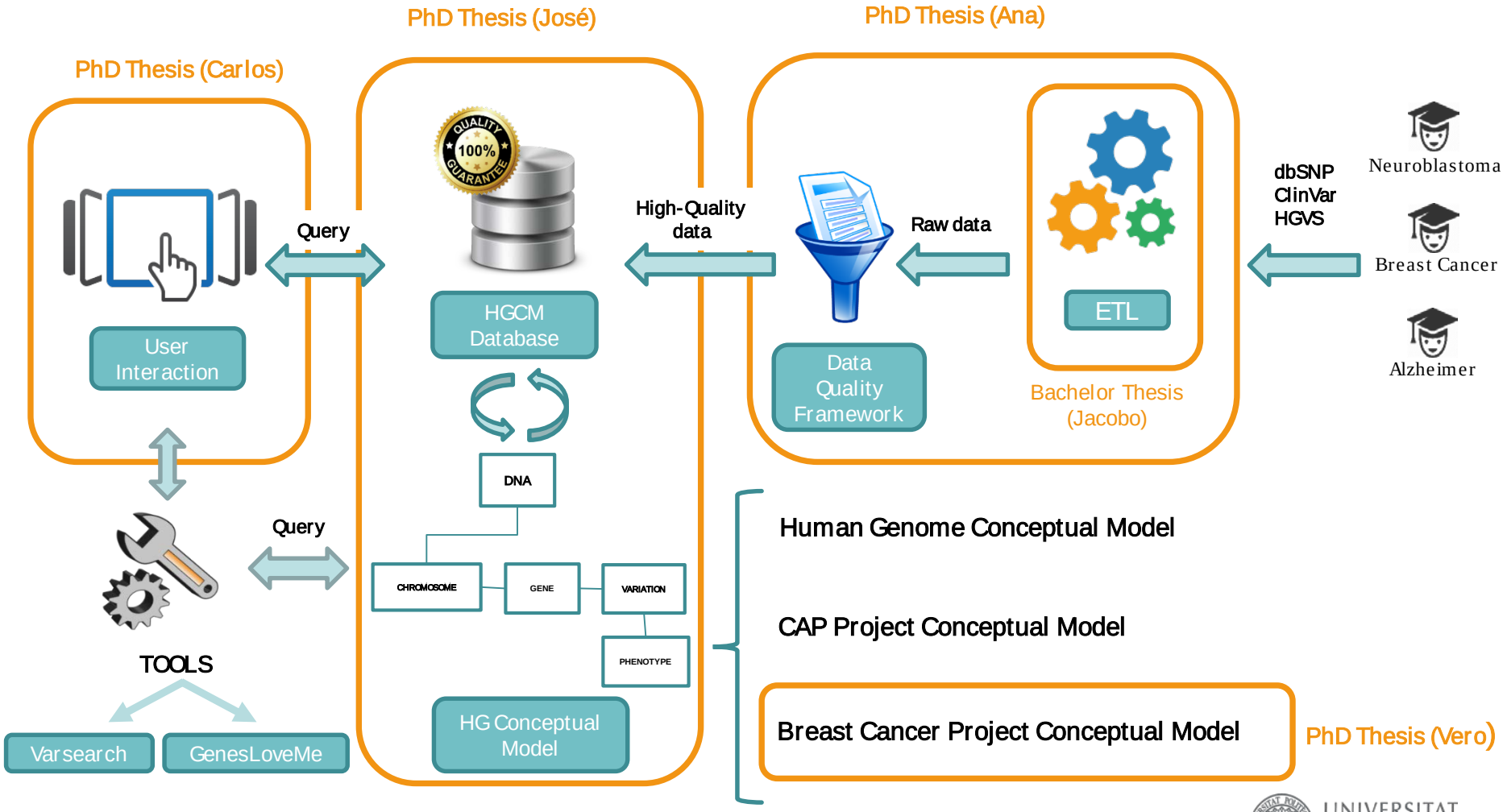
Move the **analytics**, not the data

Do it in an **open, secure** trust model

Do it at **scale**, for any researcher

Bring your own **tools** and **infrastructure**

Conclusions



I love to model!

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