Interdisciplinary research collaboration

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Overview

- What is interdisciplinary working
- Why research in an interdisciplinary manner
- Pitfalls and benefits
- Examples

Multi, Inter, Intra

• Multi

Inter

• Intra

Multi, Inter, Intra

Multi – more than one; many (Latin multus 'many')

 Inter – (i) between, among; (ii) mutually, reciprocally. (Latin inter 'between, among')

• Intra – inside, within (Latin intra 'inside')

Multi, Inter, Intra

- Multi more than one; many (Latin multus 'many')
 - Multicellular, multicast, multichannel, multilingual, ...
- Inter (i) between, among; (ii) mutually, reciprocally. (Latin inter 'between, among')
 - Intercellular, intercity, internet, international, ...
- Intra inside, within (Latin intra 'inside')
 - Intercranial, intracellular, intramolecular, intranet, ...

Discipline

- A branch of knowledge
- Latin disciplina 'instruction, knowledge'

- Examples?
 - Computer science
 - Information systems

—

EPSRC Pioneering research UK Research Councils and skills



Arts and Humanities Research Council (AHRC)

Biotechnology and Biological Sciences Research Council (BBSRC)

Engineering and Physical Sciences Research Council (EPSRC)

Economic and Social Research Council (ESRC)

Medical Research Council (MRC)

Natural Environment Research Council (NERC)

Science and Technology Facilities Council (STFC)





Leading science for better health







Multidisciplinary research: UKRC

- Multidisciplinary research takes place at the edges of traditional disciplines and across traditional subject boundaries. The Research Councils believe that novel multidisciplinary research is needed to solve many, if not all, of the next decade's major research challenges, such as:
 - how does the brain work and how will this understanding lead to new forms of computing?
 - can we predict rapid climate in Europe, its impacts and sustain solutions to managing or mitigating these impacts?
 - how and why do human cultures, languages and beliefs evolve and differentiate from each other?
 - how does the UK cope with its aging population, in terms of healthcare, transport, accommodation and financial support?
 - how can manage increasing demands for energy and natural resources (fossil fuels, water, land and food)?
- Experience shows that multidisciplinary research works best when scientists from different research backgrounds are able to work together free from discipline or structural barriers. As such each Research Council seeks to foster, where appropriate, multidisciplinary research either between disciplines central to their Councils' mission or by drawing together a wide range of disciplines to address a specific problem.

Multidisciplinary research: UKRC

- Both individually and collectively, the Research Councils, stimulate multidisciplinary approaches to research, employing a broad portfolio of flexible funding mechanisms and approaches including:
 - working with researchers and users to identify important research questions, and using Research Councils funding mechanisms to publicise, promote or direct funding to multidisciplinary areas;
 - funding university research centres and Research Council Institutes to bring together researchers, setting clear goals for multidisciplinary research and providing long-term support to help develop new ways of working;
 - establishing and participating in multidisciplinary Funders Forums;
 - promoting multidisciplinarity when working with other funders in the UK and abroad.
- RCUK enables dialogue about research priorities, facilitating an open and collective approach to investing in multidisciplinary research and training. As well as providing a recognised forum in which to exchange and discuss multidisciplinary priorities

Interdisciplinary research Institute for the Study of Science, Technology and Innovation, Edinburgh www.issti.ed.ac.uk

- Interdisciplinary research -- occurring where the contributions of the various disciplines are integrated to provide holistic or systemic outcomes.
 - Research which aims to further the expertise and competence of academic disciplines themselves, e.g. through developments in methodology which enable new issues to be addressed or new disciplines or sub-disciplines to be formed
 - Research which is problem focused and addresses issues of social, technical and/or policy relevance with less emphasis on discipline-related academic outcomes
- Multidisciplinary research, where each discipline works in a self-contained manner with little cross-fertilisation among disciplines or synergy.

www.issti.ed.ac.uk

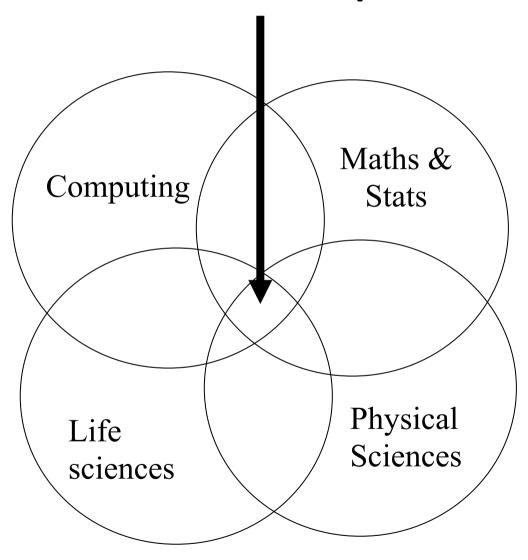
Motivations

- Setting up and funding interdisciplinary research programmes
 - the nature of the subject is interdisciplinary (e.g. transport, environment)
 - researchers are transferring information from the laboratory to the real world
 - the research is user driven (not necessarily commercial)
 - the research is particularly relevant to policy making in complex areas
 - single discipline research has encountered a bottle-neck and more than one discipline is needed to make a breakthrough
- For individuals engaging in interdisciplinary research motivations might include a desire to:
 - engage with 'real world' problems
 - tackle socially relevant issues
- contribute to the advancement of academic disciplines www.issti.ed.ac.uk

Bioinformatics (Computational Biology - USA)

- Bio Molecular Biology
- Informatics Computer Science
- Bioinformatics the study of the application of
 - molecular biology, computer science, artificial intelligence, statistics and mathematics
 - to model, organise, understand and discover interesting information associated with the large scale molecular biology databases,
 - to guide assays for biological experiments.

Bioinformatics in context - a new discipline?

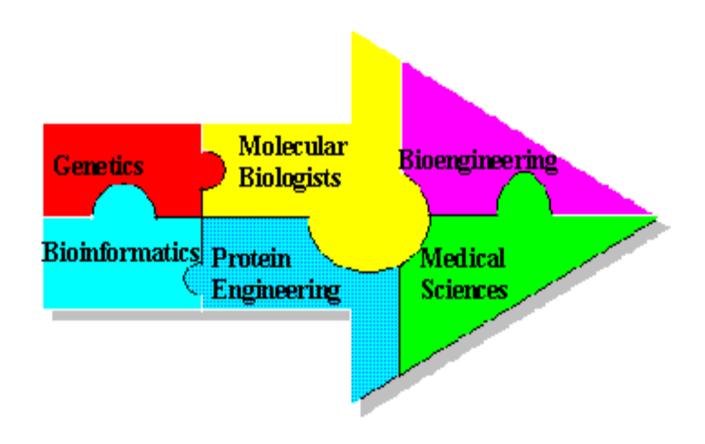


Aim of research in Bioinformatics

Understand the functioning of living things - to "improve the quality of life".

- drug design
- identification of genetic risk factors
- gene therapy
- genetic modification of food crops and animals, etc.
- application to e.g. biotechnology

Bioinformatics in context (applications)



Related but different...

Apply principles from biology to derive novel approaches in computer science:

- biocomputing
- neural computing
- genetic algorithms
- evolutionary computing







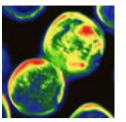
Arabidopsis thaliana



Buchnerasp. **APS**



Aquifex aeolicus



Archaeoglobus *fulgidus*



Borrelia ourgorferi



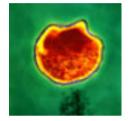
Mycobacterium tuberculosis



Caenorhabitis elegans



Campylobacter jejuni



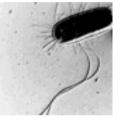
Chlamydia pneumoniae



Vibrio cholerae



Drosophila melanogaster



Escherichia Thermoplasma acidophilum coli



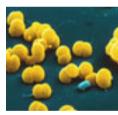
Helicobacter pylori



Mycobacterium *leprae*



mouse



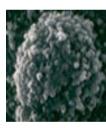
Neisseria meningitidis **Z2491**



Plasmodium falciparum



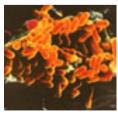
Pseudomonas aeruginosa



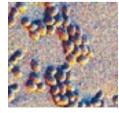
Ureaplasma urealyticum



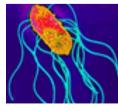
rat



Rickettsia David Gilk prowazekii



Saccharomyces cerevisiae

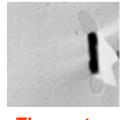


Salmonella enterica

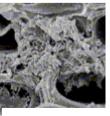


Bacillus subtilis

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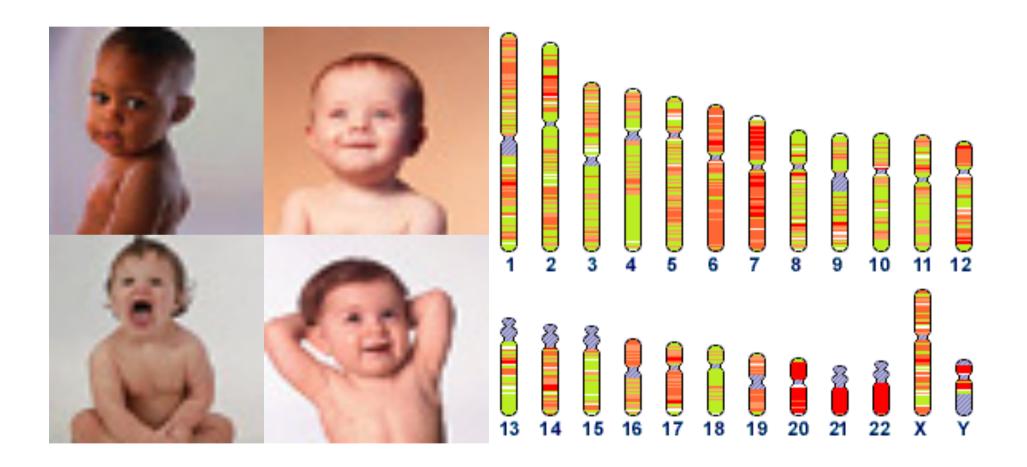


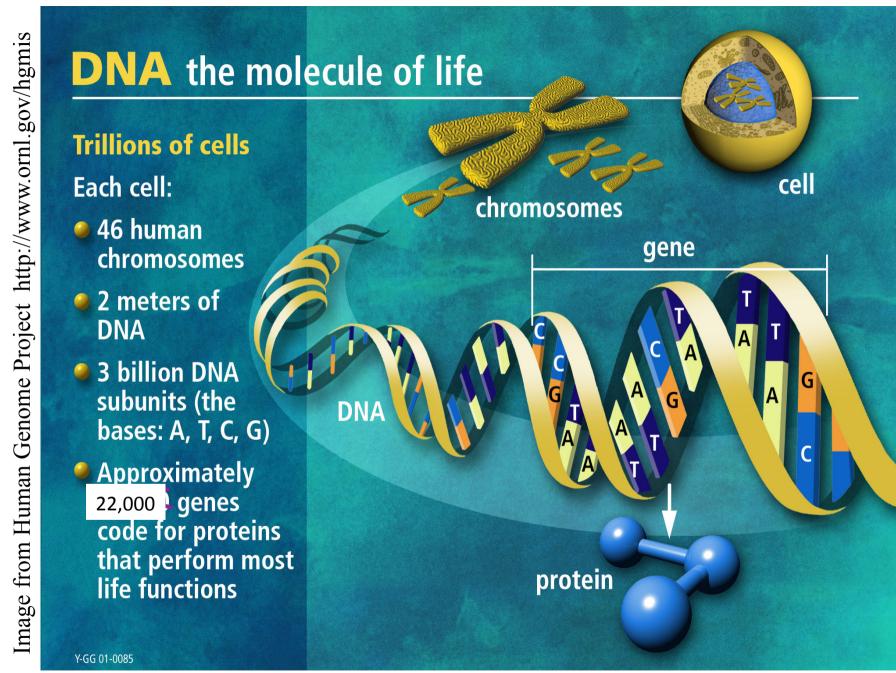
Thermotoga maritima



Xylella fastidiosa

Human Genome





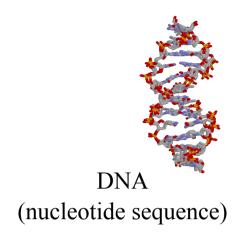
Genes to systems

DNA "gene" METABOLIC PATHWAYS **mRNA** Protein sequence **Folded** Protein

The genetic code

First Position	Second Position								Third Position
(5' end)	T		С		A		G		(3' end)
	TTT	Phe	TCT	Ser	TAT	Tyr	TGT	Cys	T
T	TTC	Phe	TCC	Ser	TAC	Tyr	TGC	Cys	C
	TTA	Leu	TCA	Ser	TAA	Stop	ΓGA	Stop	A
	TTG	Leu	TCG	Ser	TAG	Stop	ГGG	Trp	G
	CTT	Leu	CCT	Pro	CAT	His	CGT	Arg	T
C	CTC	Leu	CCC	Pro	CAC	His	CGC	Arg	C
	CTA	Leu	CCA	Pro	CAA	Gln	CGA	Arg	A
	CTG	Leu	CCG	Pro	CAG	Gln	CGG	Arg	G
	ATT	Ile	ACT	Thr	AAT	Asn	AGT	Ser	T
A	ATC	Ile	ACC	Thr	AAC	Asn	AGC	Ser	C
	ATA	Ile	ACA	Thr	AAA	Lys	AGA	Arg	A
	ATG	Met*	ACG	Thr	AAG	Lys	AGG	Arg	G
	GTT	Val	GCT	Ala	GAT	Asp	GGT	Gly	T
G	GTC	Val	GCC	Ala	GAC	Asp	GGC	Gly	C
	GTA	Val	GCA	Ala	GAA	Glu	GGA	Gly	A
	GTG	Val	GCG	Ala	GAG	Glu	GGG	Gly	G





acatttgctt ctgacacaac tgtgttcact agcaacctca aacagacacc atggtgcacc tgactcctga ggagaagtct gcggttactg ccctgtgggg caaggtgaac gtggatgaag ttggtggtga ggccctgggc aggctgctgg tggtctaccc ttggacccag aggttctttg agtcctttgg ggatctgtcc actcctgatg cagttatggg caaccctaag gtgaaggctc atggcaagaa agtgctcggt gcctttagtg atggcctggc tcacctggac aacctcaagg gcacctttgc cacactgagt gagctgcact gtgacaagct gcacgtggat cctgagaact tcaggctcct gggcaacgtg ctggtctgtg tgctggccca tcactttggc aaagaattca ccccaccagt gcaggctgcc tatcagaaag tggtggctgg tgtggctaat gccctggccc acaagtatca ctaagctcgc tttcttgctg tccaatttct attaaaggtt cctttgttcc ctaagtccaa ctactaaact gggggatatt atgaagggcc ttgagcatct ggattctgcc taataaaaaa catttattt cattgc

Amino-acid (protein sequence)

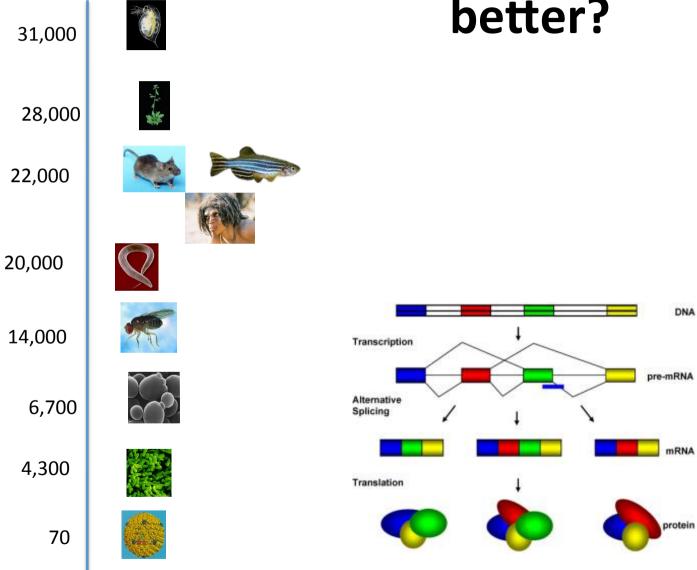
MVHLTPEEKSAVTALWGKVNVDEVGGEALGRLLVVYPWTQRFFESFGDLSTPDAVMGNPKVKAH GKKVLGAFSDGLAHLDNLKGTFATLSELHCDKLHVDPENFRLLGNVLVCVLAHHFGKEFTPPVQAAY QKVVAGVANALAHKYH



Search using BLAST

http://www.ncbi.nlm.nih.gov/BLAST/
or
http://www.ebi.ac.uk/blastall/

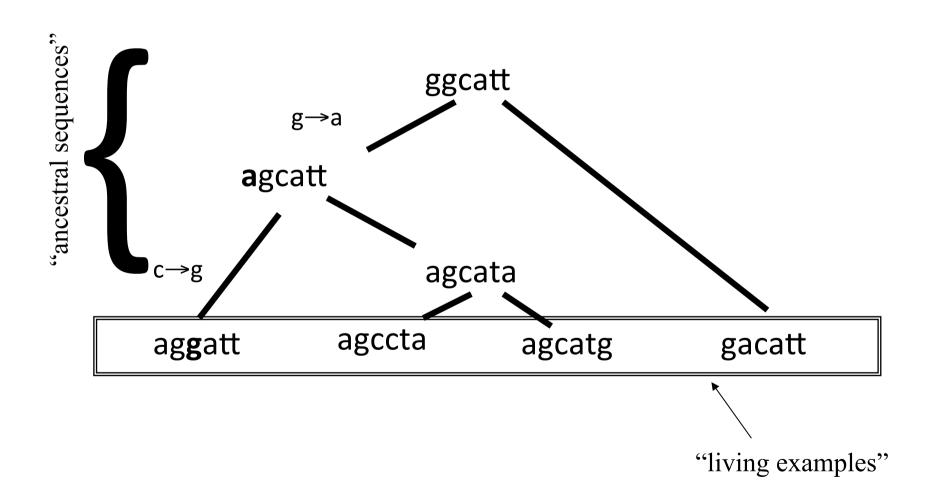
More genes – better?



RMT David Gilbert

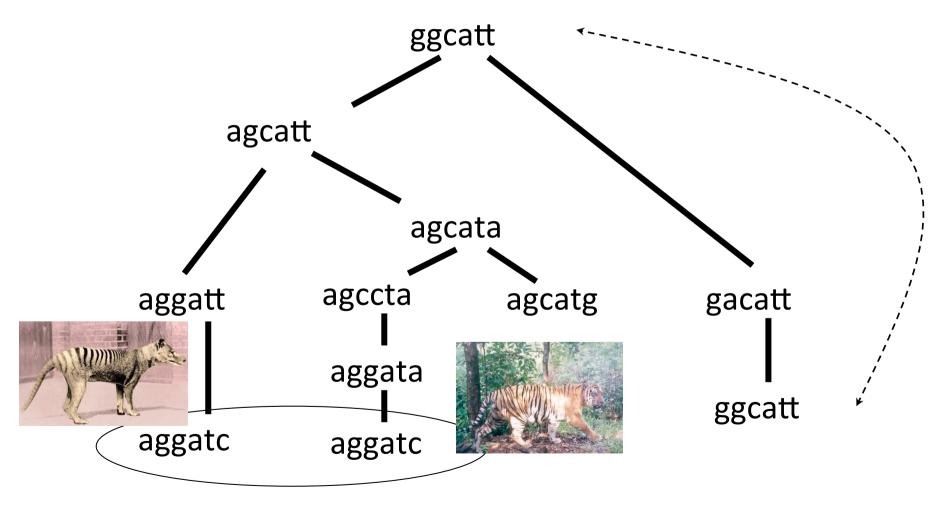
Interdisciplinary research

Evolution - related sequences



Other evolutionary issues

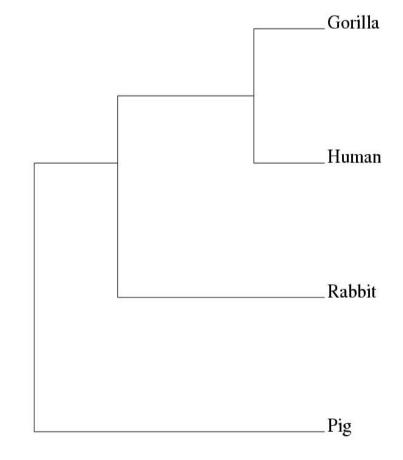
- Convergent evolution: same sequence evolved from different ancestors
- back evolution mutate to a previous sequence



How can we analyse the flood of data?

Data: don't just store it, analyse it! By comparing sequences, one can find out about things like

- How organisms are related
 & evolution
- How proteins function
- Population variability
- How diseases occur

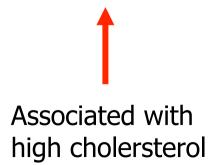


Human genetic variations (Single Nucleotide Polymorphisms)

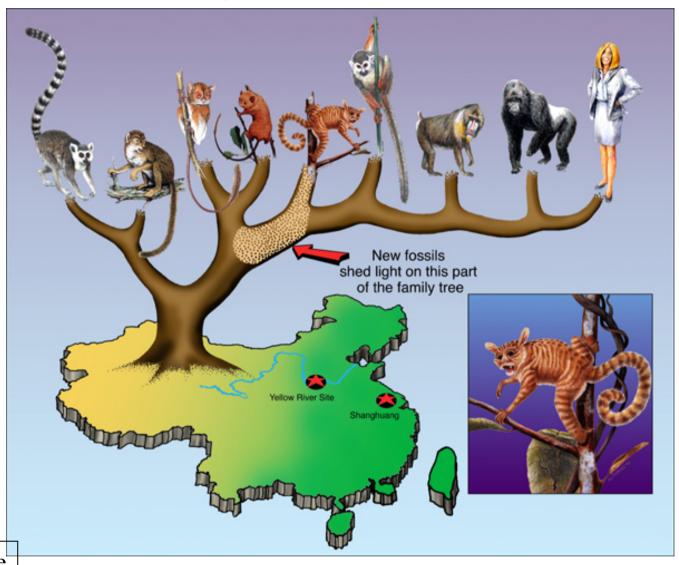
- SNP's "genetic indivuality"
- ~ 1/1000 bases variable (2 humans)
- Make us more/less susceptible to diseases
- May influence the effect of drug treatments

```
TTT TAC GGC ATC
Phe Tyr Asn Met
```

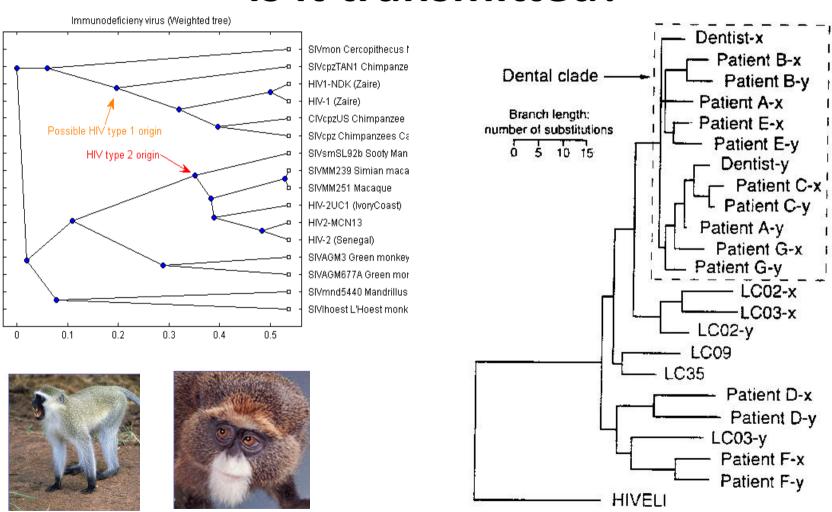
```
TTT TAC GTC ATC
Phe Tyr Ser Met
```



Our place in Nature



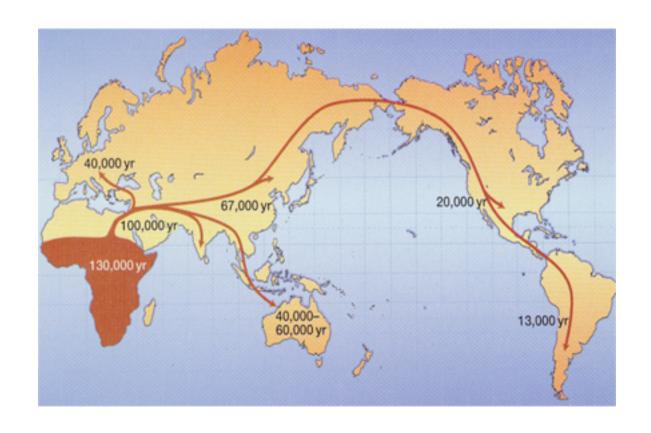
HIV: where did it come from and how is it transmitted?



Neanderthal sequenced... Humans interbred with Neanderthal

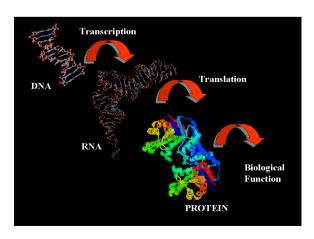


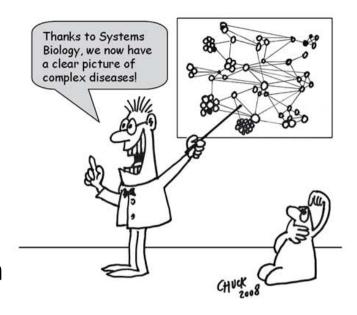
Out of Africa

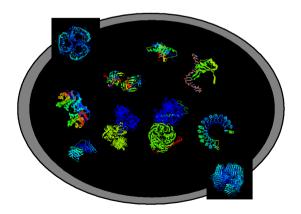


Systems Biology

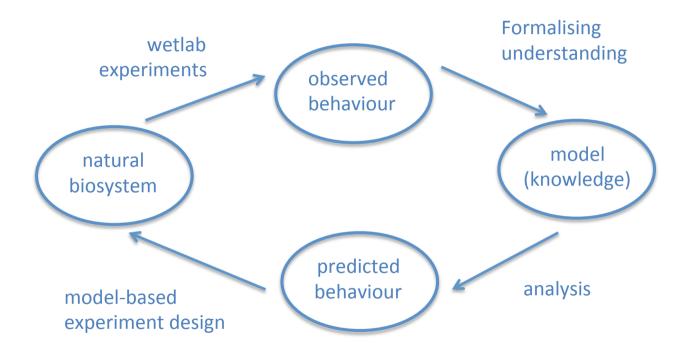
- Putting it all together
- Systems Biology studies the relationships and interactions between various parts of a biological system in order to understand how the whole system functions.

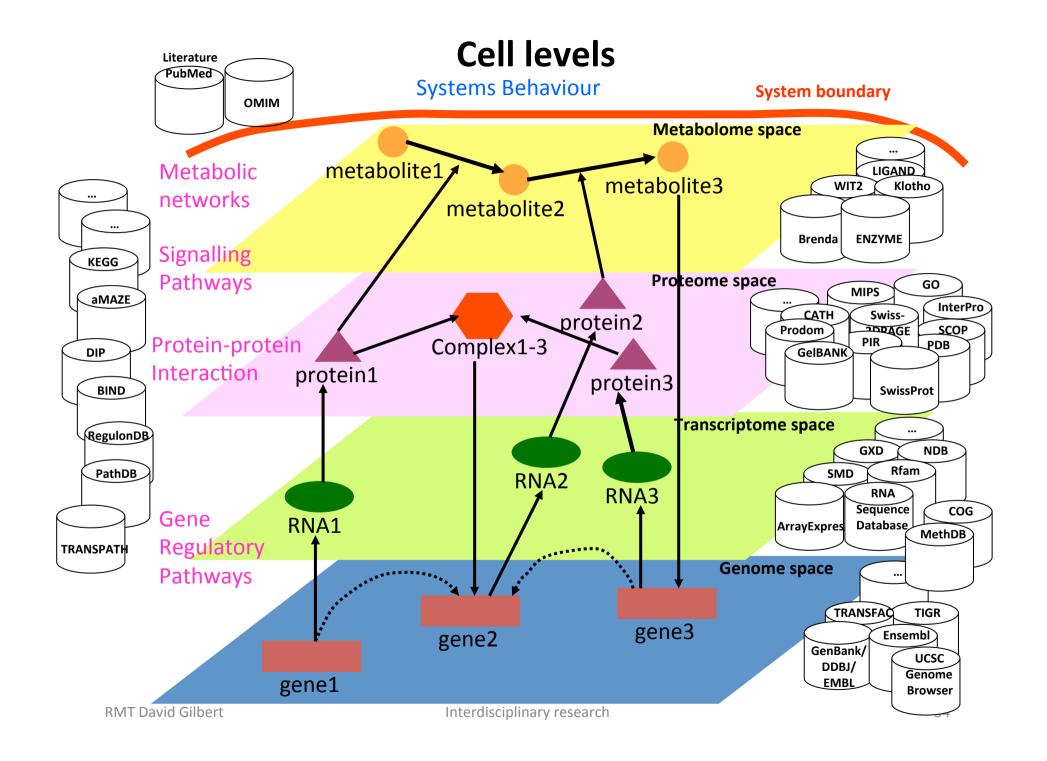






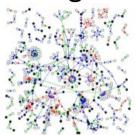
Systems biology





Networks

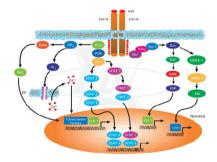
Gene regulation



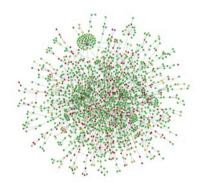
Metabolic



Signalling

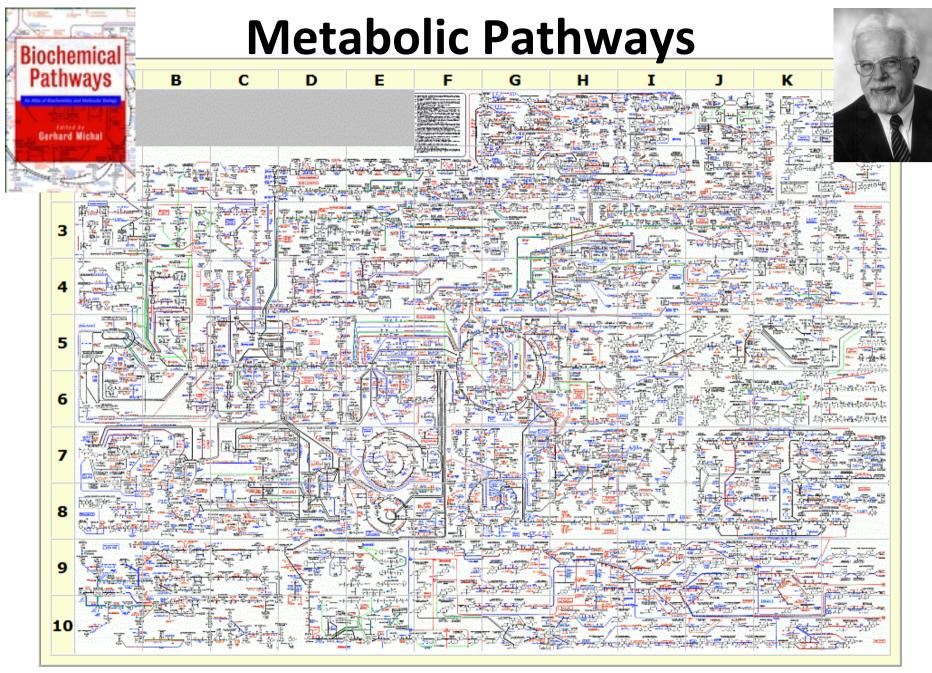


• Protein-protein interaction

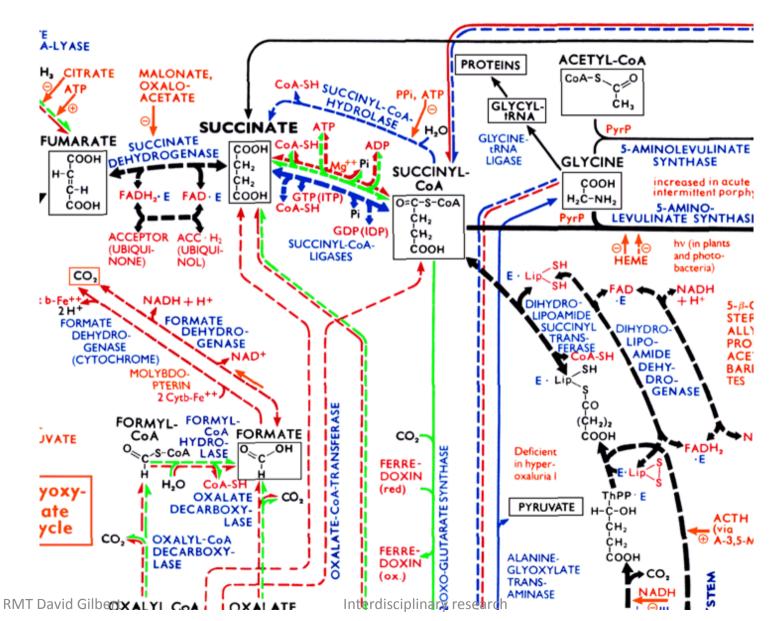


Developmental





Patterns: → general biochemical pathways, → animals, → higher plants, → unicellular organisms



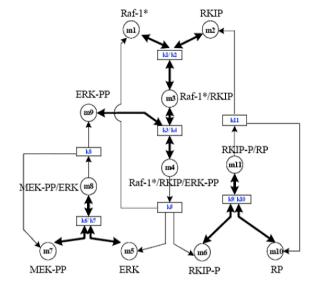
BioModel Engineering

- Takes place at the interface of computing science, mathematics, engineering and biology.
- A systematic approach for designing, constructing and analyzing computational models of biological systems.
- Some inspiration from efficient software engineering strategies.
- Not engineering biological systems per se, but
 - describes their structure and behavior,
 - in particular at the level of intracellular molecular processes,
 - using computational tools and techniques in a principled way
 - Use of patterns to guide model construction?

Rainer Breitling, David Gilbert, Monika Heiner, Richard Orton (2008). A structured approach for the engineering of biochemical network models, illustrated for signalling pathways. Briefings in Bioinformatics

Rainer Breitling, Robin Donaldson, David Gilbert, Monika Heiner (2010): Biomodel Engineering - From Structure to Behavior; : Trans. Comp Systems Biology XII, Springer LNBI 5945, pp. 1-12

Biochemical network model construction



graph **QUALITATIVE**

1. Structure

"Topology"

2. Kinetics (if you can)

$$d[Raf1*]/dt = k1*m1*m2 + k2*m3 + k5*m4$$

 $k1 = 0.53$; $k2 = 0.0072$; $k5 = 0.0315$

reaction rates

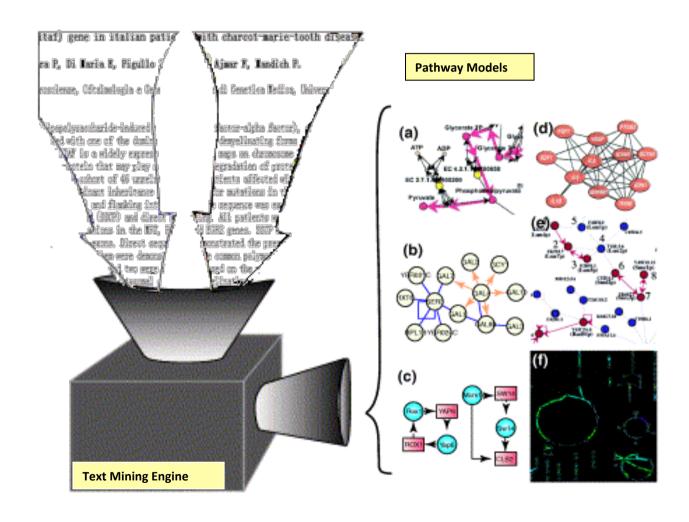
QUANTITATIVE

3. Initial conditions

$$[Raf1^*]_{t=0}$$
= 2 μ Molar

marking , concentrations **QUANTITATIVE**

Biomedical network data mined from scientific texts



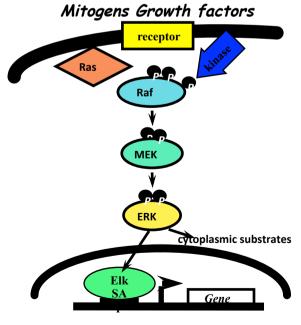
Diseases, Drugs and Systems Biology

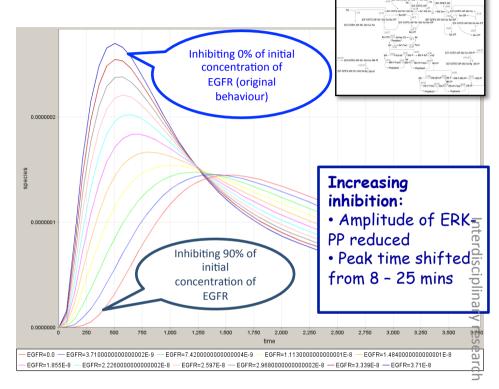
- Intra-cellular Signalling Pathway
- Key in many key cellular processes
- Deregulated in various diseases: cancer; immunological, inflammatory and degenerative syndromes





Represents an important drug target



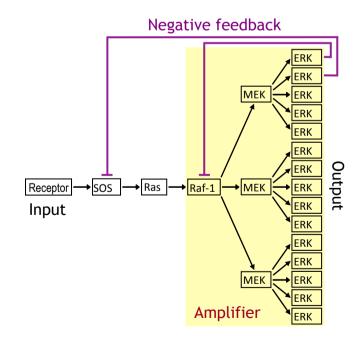


Applications

- •Understanding of human diseases
- Drug discovery (efficient & lower-cost)
- Personalized Medicine (individual therapy)
- Predictive Medicine (predict future disease)

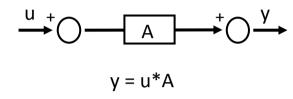
ERK cascade well known biological amplifier

- Amplifies the original signal to create effective cellular responses.
- 1:3:5 are the approximate ratios of Raf-1, MEK and ERK in fibroblasts.
- Well known negative feedback loop: phosphorylation of SOS by ERK-PP (via MAPKAP1) resulting in the dissociation of the Grb2/SOS complex.
- New negative feedback loop: ERK-PP phosphorylates Raf-1 resulting in a hyper-phosphorylated inactive form of Raf (Dougherty et al. 2005)

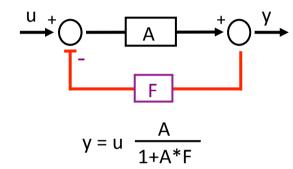


Negative Feedback Amplifier

Standard Amplifier

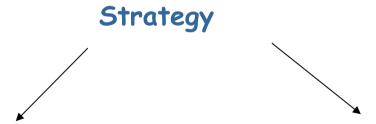


Negative Feedback Amplifier



- Negative feedback amplifier from electronics
- Amplifier with a negative feedback loop from the output of the amplifier to its input.
- NF loop \rightarrow a system much more robust to disturbances in the amplifier.
- NFA was invented in 1927 by Harold Black of Western Electric.
- Originally used for reducing distortion in long distance telephone lines.
- NFA a key electrical component used in a wide variety of applications

How to test if the ERK pathway is a NFA?

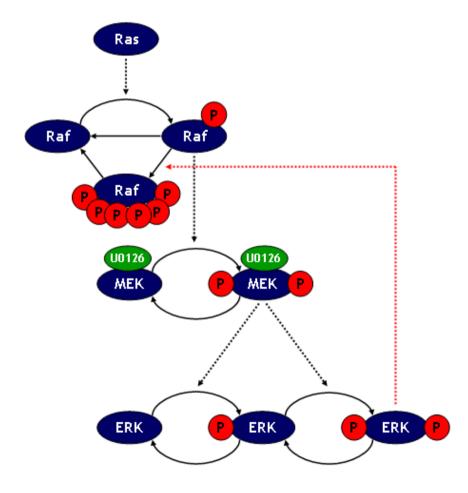


In vivo system that allows us to compare feedback broken to feedback intact model. Computational Model of ERK pathway with/without feedback

Computational Modeling 1: Build the model



- Non-linear ordinary differential equations (ODE's).
- ODE's were solved using Math Lab and Gepasi.
- Models are based on the Schoeberl et al. (2002) model
- Mass Action Kinetics instead of Michaelis Menten
- Kinetic parameters are from literature, previous models and "guesstimates"

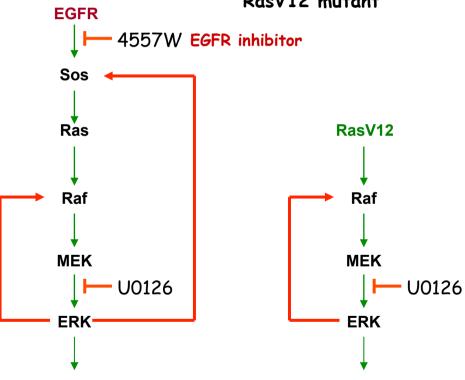


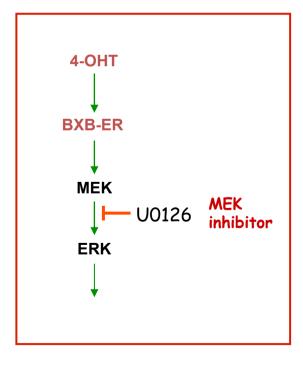
Schoeberl *et al.* (2002), Computational modeling of the dynamics of the MAP kinase cascade activated by surface and internalized EGF receptors, Nature Biotechnology 20, 370-375

The experimental systems

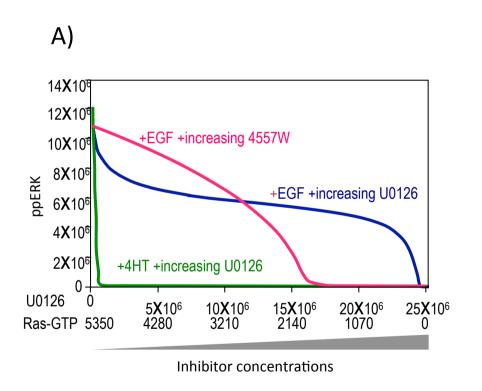
Negative feedback loops intact

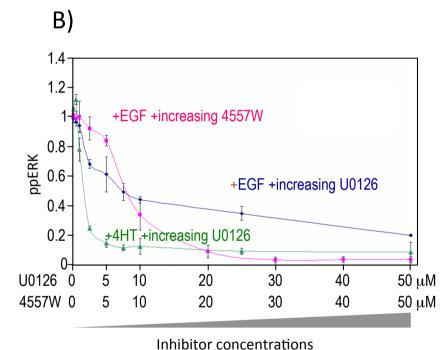
One feedback loop eliminated by constitutively active RasV12 mutant Both feedback loops eliminated by BXB-ER (4-OHT regulatable Raf-1 mutant)





(A) Model prediction (B) Biochemical validation





The Mammalian MAPK/ERK Pathway Exhibits Properties of a Negative Feedback Amplifier

- Three-tiered kinase module, signal amplifier.
- Negative feedback loops system like negative feedback amplifier
- Smoothens the output to changes in input system robust to change.
- No feedback loops: cells sensitive to inhibition of MEK
- Feedback intact: cells are resistant to inhibition there.
- Drug development: inhibitors targetting components outside NFA are more effective at inhibiting the pathway.

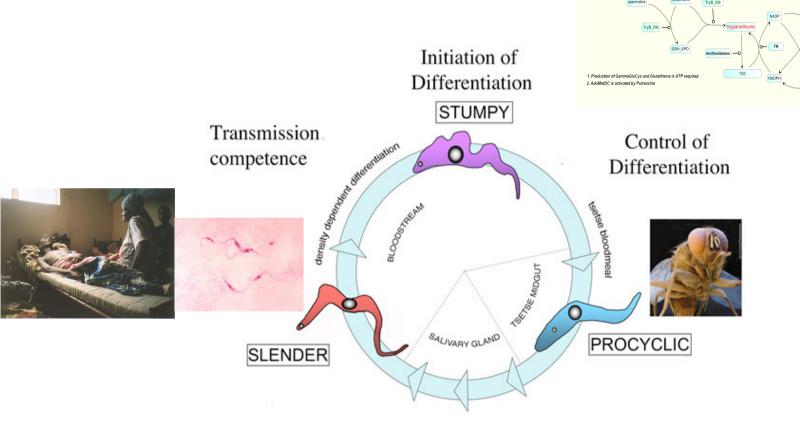
Sturm, Orton, Vyshemirsky, Grindlay, Birtwistle, Gilbert, Calder, Pitt, Kholodenko and Kolch., Science Signalling Dec 21;3

SysTryp: System Biology of Trypanosoma

metabolism













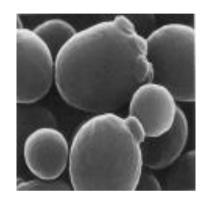




Trypanothione Metabolism in Trypanosoma brucei

What about scaling up?











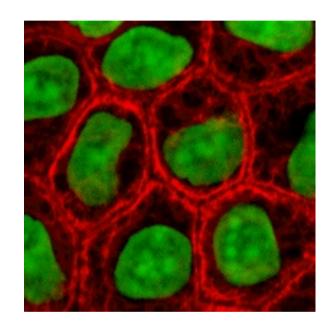






Multiscale modelling challenges

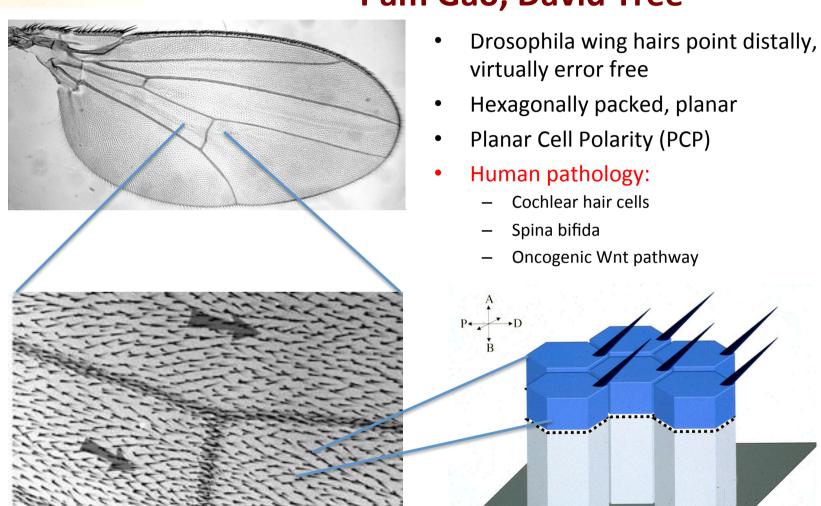
- **Repetition** multiple cells with a similar definitions
- Variation mutants.
- *Organisation* regular or irregular patterns over spatial networks in one, two or three dimensions.
- Communication between neighbours constrained by neighbour relation, and the position in spatial network.



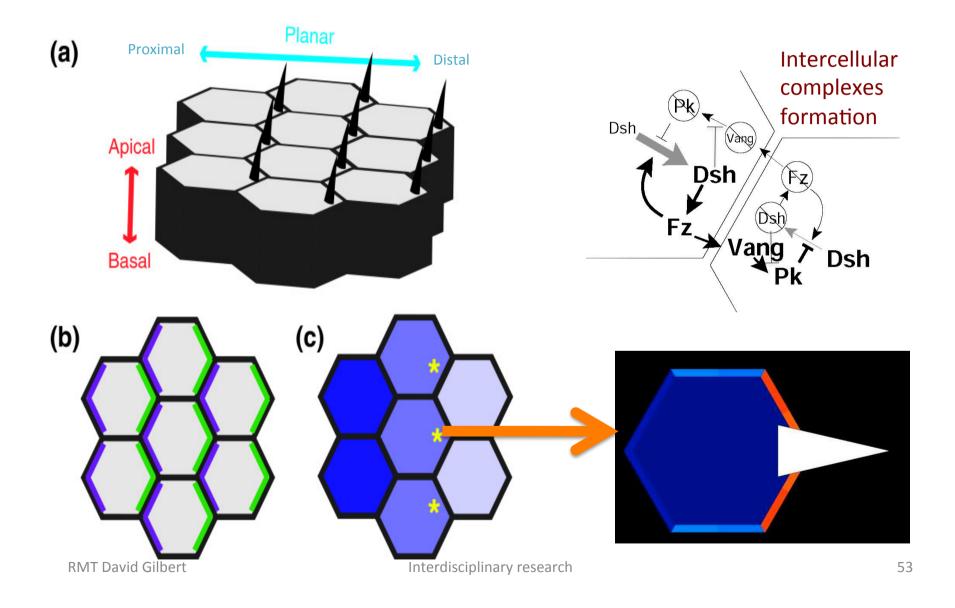
Hierarchical organisation — cells containing compartments.
 Enables abstraction over level of detail of components.



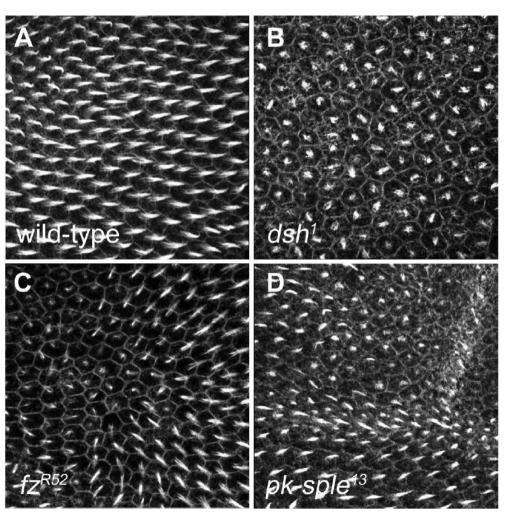
Multiscale - morphology, images, patterns Planar Cell Polarity in Drosophila wings Pam Gao, David Tree



Planar Cell Polarity



PCP: Mutants

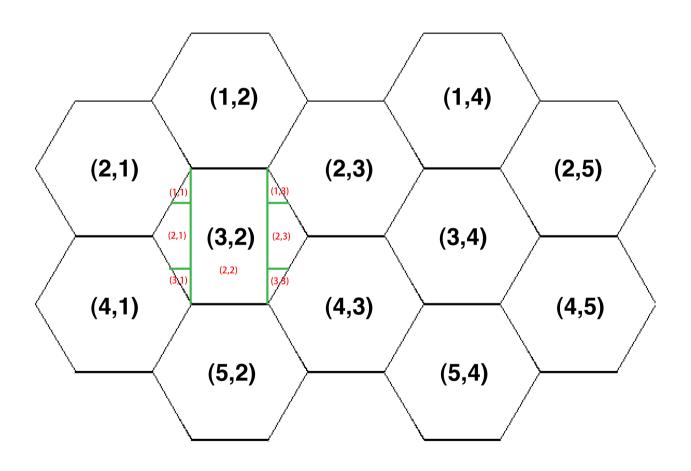


Disruption of the signal produces stereotypical swirls and patterns of misoriented hairs and in some cases produces significant numbers of cells with multiple hairs

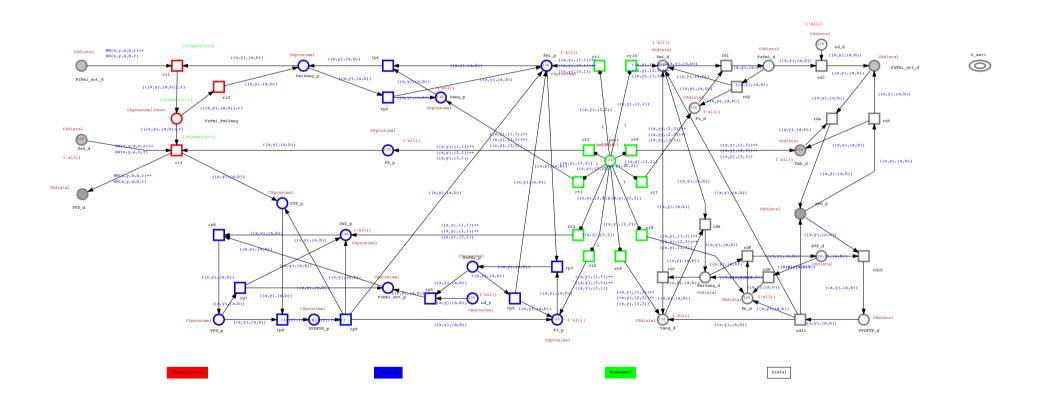
Mutant Fz clones



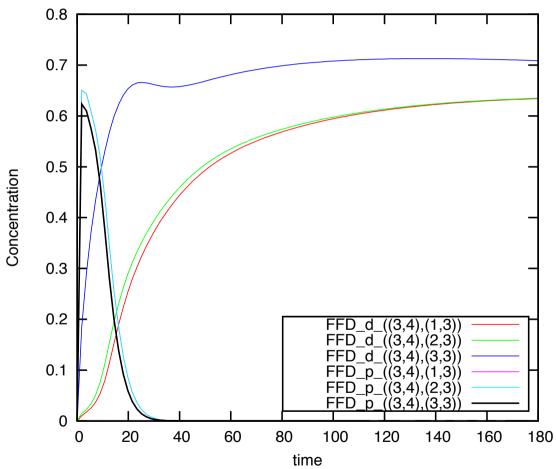
Wing tissue tissue: Cells with logical compartments



CPN model of PCP signalling

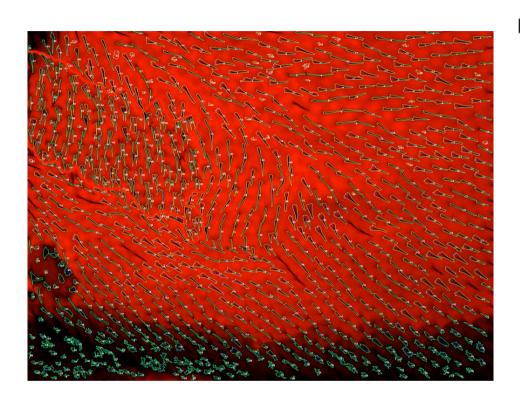


FFD in one cell (3,4) Continuous simulation

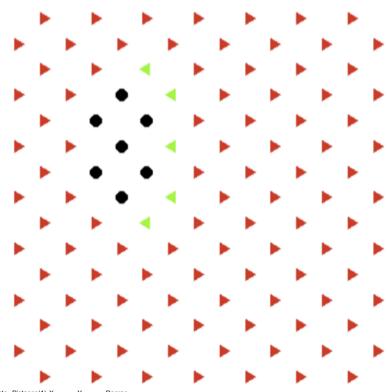


FFD accumulates at the distal edge of the cell rather than the proximal edge at the end of signalling.

Fz clone in WT background



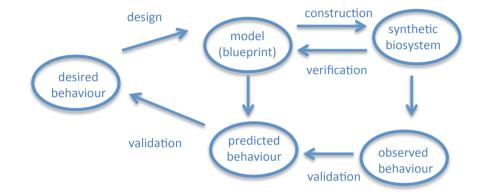
FFD at distal vs FFD at proximal over Tissue



Object	Area	Perimeter I	Roundness E	Eccentricity I	_y l	Lx .	Alpha :	Sk width	Sk width std	Skeleton length	Branch points	End points	Maximum length	Length estimate	Distance(1) X	Y	De	egree
1	72	42.73	0.70	0.97	2.68	10.33	1.36	2.15	1.05	17	7 0	2	18.68	17.82	38.95	5.04	48.69	78
2	150	84.04	0.52	0.99	2.68	21.69	-1.35	2.19	0.97	35	5 0	2	38.08	38.96	23.65	8.91	306.77	-77
3	69	79.50	0.37	0.84	5.79	10.66	1.56	0.50	0.88	32	2 3		21.21	38.63	22.96	8.80	955.96	89
4	82	48.28	0.66	0.68	4.85	6.63	-1.08	2.01	1.60	27	7 3		13.60	20.67	35.18	10.65	382.76	-62
5	77	84.38	0.37	1.00	1.40	23.23	-1.42	0.15	0.53	40) 0	2	39.62	41.02	20.75	8.06	636.34	-82
6	87	72.18	0.46	0.92	4.10	10.76	-0.96	1.18	1.11	31	1 3		19.85	34.21	30.36	13.09	902.91	-55
7	439	132.08	0.56	0.90	9.59	21.83	1.54	4.89	3.21	57	' 1	4	44.55	59.96	34.06	17.26	273.65	88
8	68	52.87	0.55	0.74	4.87	7.25	0.39	1.42	1.14	22	2 2	. 4	13.42	24.11	22.96	12.18	933.25	23
9	470	152.37	0.50	0.79	12.60	20.61	-0.43	5.24	3.57	63	3 1	3	43.42	70.98	35.21	23.53	729.00	-24
10	246	129.11	0.43	0.99	3.50	30.34	-1.51	2.32	2.16	57	' 0	2	58.22	61.74	38.95	14.10	86.58	-87
11	113	81.90	0.46	1.00	1.91	22.09	1.56	1.38	1.00	39	0	2	39.01	38.79	31.52	10.92	210.87	89
12	199	95.05	0.53	0.99	2.91	24.73	-0.98	3.25	0.86	33	3 0	2	42.72	43.88	28.67	21.01	570.89	-56
13	104	59.11	0.61	0.93	3.70	10.35	1.51	2.05	1.38	24	. 2	. 4	18.68	26.14	19.94	15.83	782.50	87
14	81	43.11	0.74	0.83	4.05	7.22	-0.60	2.22	1.93	24	. 2	. 4	15.26	17.51	19.95	18.58	978.42	-35

Synthetic Biology

- Make a new one:
 - System, or
 - product



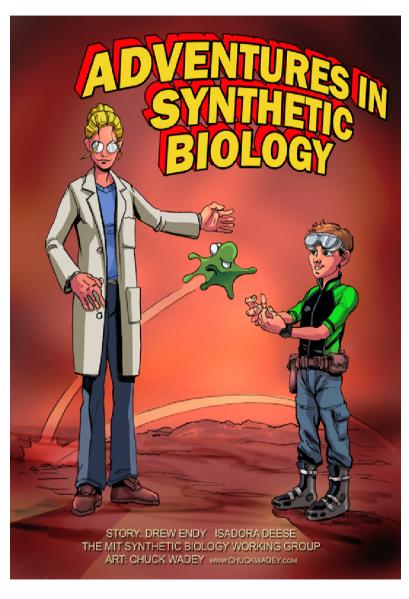
 Synthetic Biology - the structured engineering of biological systems for useful purposes.



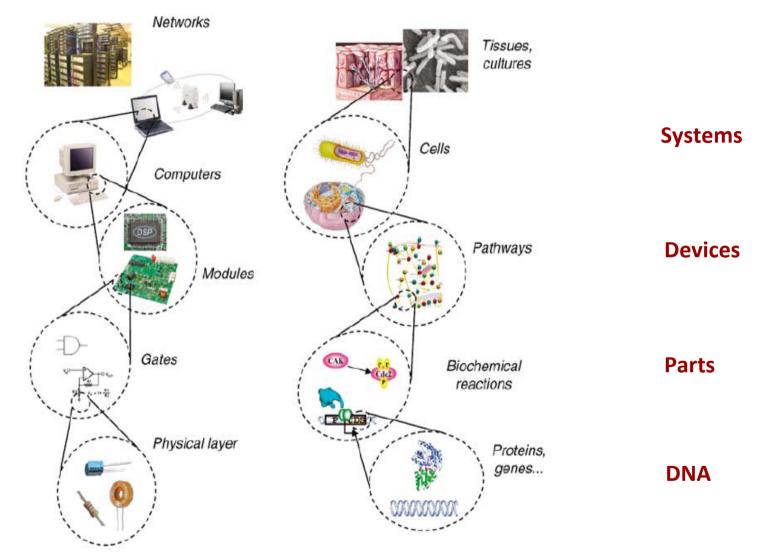




What is synthetic biology?

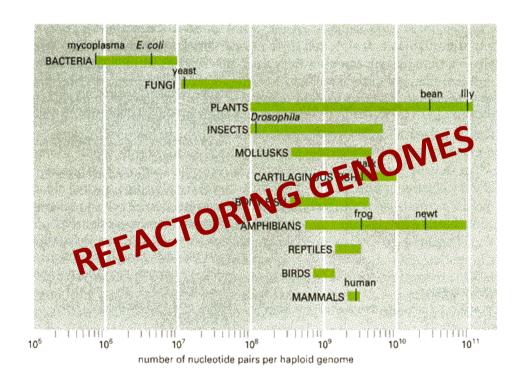


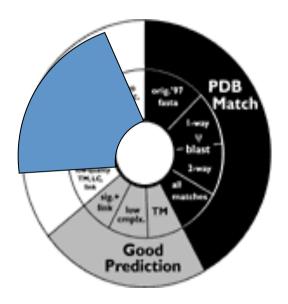
- Design & construction of new biological parts, devices, and systems
- Re-design of existing, natural biological systems for useful purposes
- Involves
 - Standardisation
 - Decoupling
 - Abstraction



Adrianantoandro et al. Mol Sys Bio 2006

Top-Dowr - The "North American" model

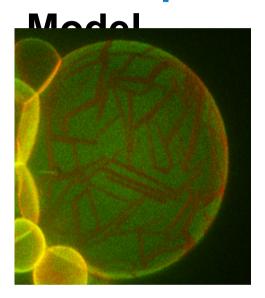




Mycoplamsa genitalium Genome 580kbp

PNAS 103, 425-430, 2006

Bottom-Up – The "Far-Eastern"



Introduce to the vesicle only what is needed for your uses

- Synthetic DNA
- Refactored organelles
- Membrane pores

Creation of artificial life!

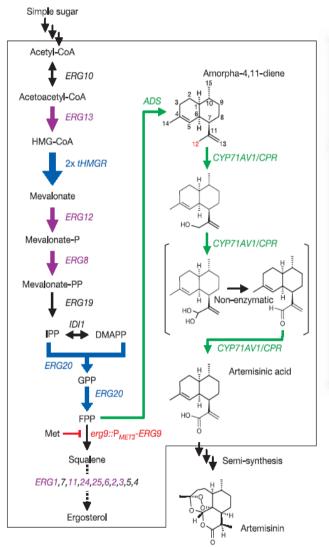
A drug manufacturing plant

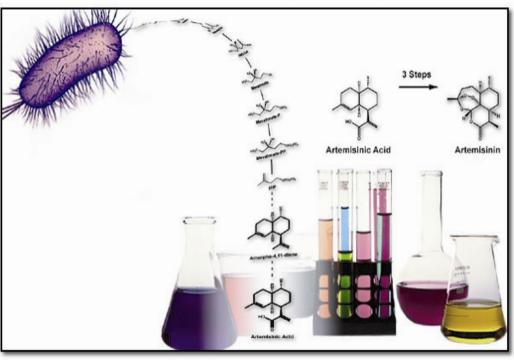
- "Audacious plan" New Scientist, May 2006
- Engineer e.coli / yeast to synthesise the anti-malarial artemisinin
- \$42.6 million, Bill & Melinda Gates Foundation



Artemisia annua

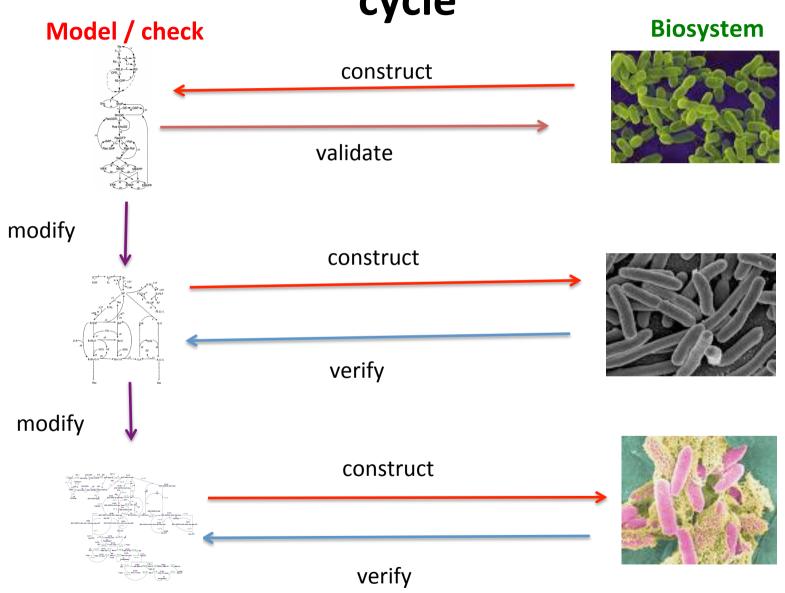
- Plant difficult to grow and only yield minute quantities of drug per kilo
- Artemisinin is expensive
 - Engineer cheaper alternative and save the world!



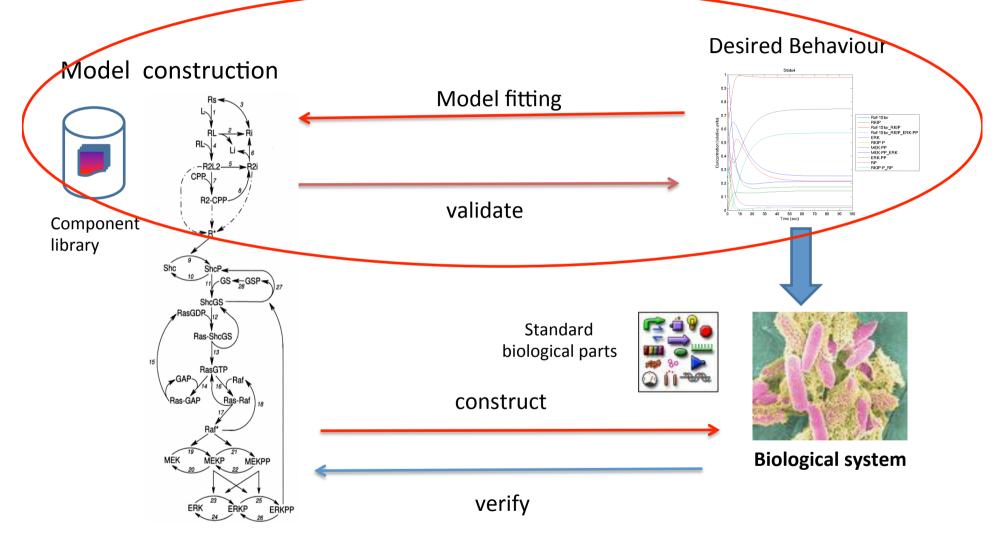


Saccharomyces cerevisiae REMT David Gilbert

Top-down Synthetic Biology development cycle



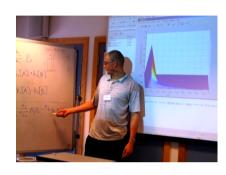
Vision – behaviour driven design



Wu, Gao & Gilbert (CMSB 2010)

Target Driven Biochemical Network Reconstruction Based on Petri nets and Simulated Annealing
RMT David Gilbert Interdisciplinary research









Strategies for integrating disciplines

- Preliminary research phase (open-ended); outcomes:
 - a specification of the range of issues that are central to the research problem
 - how they interact with one another to create or sustain the problem
 - how these interactions can be modified to deliver an implementable, synergistic solution

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Problems

- Interdisciplinary research does not occur automatically by bringing together several disciplines in a research project.
- Extra effort is needed to promote the formation of a cohesive research team involving researchers from different disciplines, to combine expertise from several knowledge domains and to overcome communication problems among researchers from different disciplines.
- Perceived problems in conducting interdisciplinary research include:
 - language and communication issues
 - institutional structures and procedures
 - divergences in worldviews across disciplines
- It thus takes longer to bring together an effective interdisciplinary team, the start-up phase of a project will take longer and the demands on the project co-ordinator will be greater.

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Skills needed by interdisciplinary researchers

- Personality and attitudes of researchers are at least as important for success as discipline base and specialisation. Useful characteristics are:
 - flexibility, adaptability, creativity
 - curiosity about, and willingness to learn from, other disciplines
 - an open mind to ideas coming from other disciplines and experiences
 - good communication and listening skills
 - an ability to bridge the gap between theory and practice
 - a good team worker
 - a high tolerance for ambiguity.
- Researchers who have skills and knowledge in more than one discipline are particularly valuable members of interdisciplinary teams, but a mono-disciplinary researcher with most of the above attributes should be capable of learning rapidly to operate in an interdisciplinary environment.

Project management

- understanding (not necessarily in depth) across the project's main discipline domains
- understanding application areas, in industry or the public sphere, for project outcomes
- focus on team work and on practical results, to overcome differences in disciplinary orientation and between, say, participants from public and private sectors
- respect for other disciplines and some understanding of their general principles
- expertise in their own discipline(s), but not necessarily a strong ambition to pursue acareer in that discipline which would inhibit their willingness to invest attention elsewhere
- balancing openness to new ideas with maintaining the progress of the project
- skills in building relationships, trusting the judgement of others, good interpersonal and diplomatic skills and a pro-active approach to interaction with partners
- a clear vision of the project and what it is trying to achieve

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Checklist for a good interdisciplinary research proposal

- Specify clearly why an interdisciplinary approach is needed, which type of interdisciplinary approach is envisaged and which disciplines should be involved. (Where this has been based on a formal analysis of the problem domain, describe the process briefly.)
- Describe how the disciplines involved will be integrated and how this relates to the type of interdisciplinarity involved; demonstrate how the quality of integration will be assured
- Describe the leadership role and management strategy to deliver the desired outcomes
- Summarise the interdisciplinary skills of the researchers involved
- Where relevant, develop a clear plan for the involvement of end users and stakeholders in the project, including contingency plans for recognised pitfalls. Indicate clearly the benefits to stakeholders and the roles of stakeholders in contributing to the project
- Budget for, and justify, the additional resources needed
- Describe how interdisciplinarity will be reflected in the project outputs and outcomes

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Monika Heiner