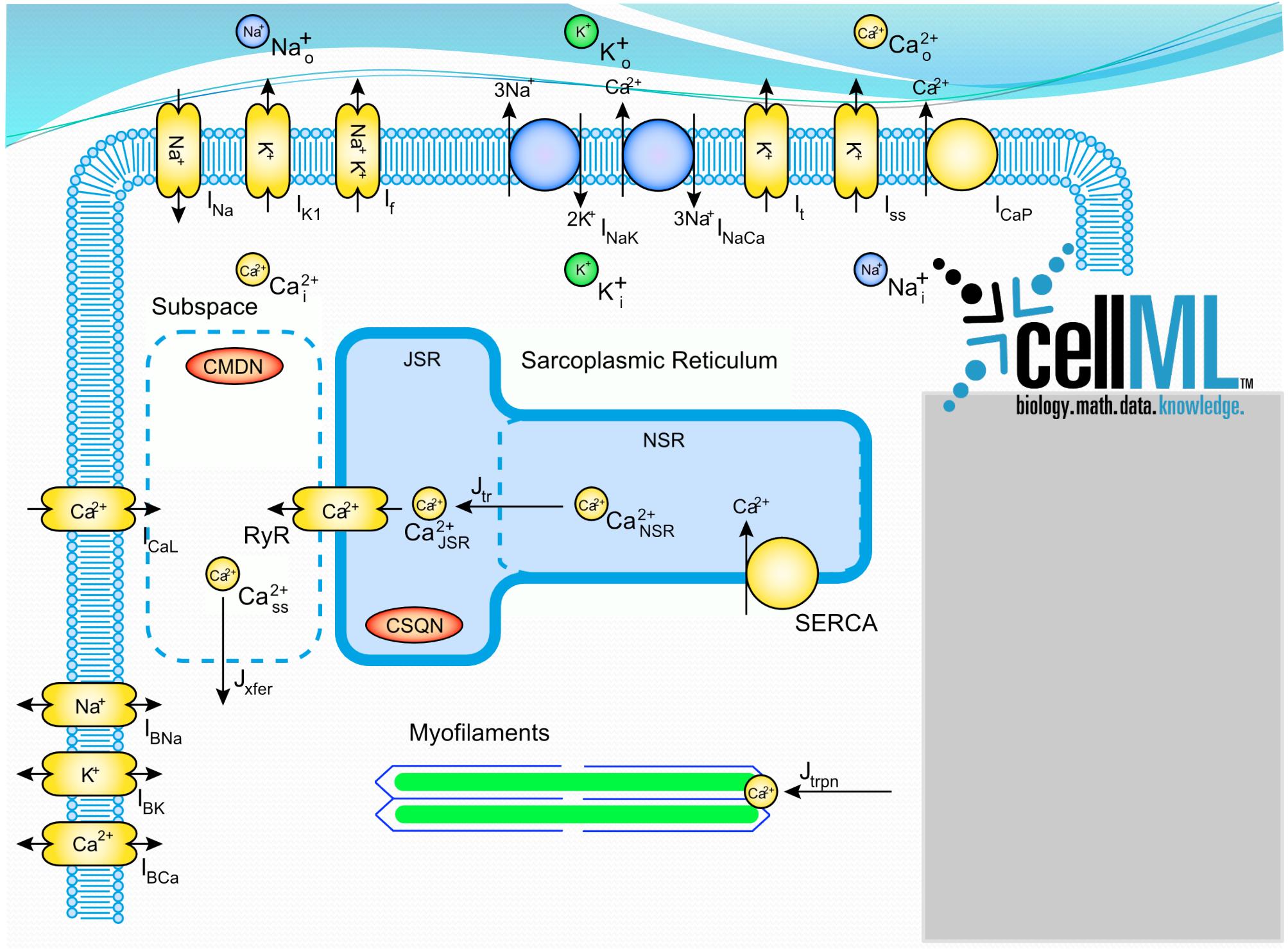


From model to modelsl

Constructing libraries of modular CellML models

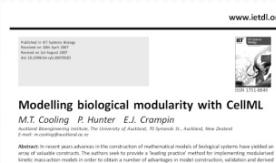
Mike Cooling, February 2010
Auckland Bioengineering Institute



cellML
biology.math.data.knowledge.TM

Modular Models

- Construction with recombination in mind
- Fine-grained reuse – mathematical equation level



ology

472

Experimental Physiology – Research Paper

Facilitating modularity and reuse: guidelines for structuring CellML 1.1 models by isolating common biophysical concepts

S. M. Wimalaratne, M. D. B. Halstead, C. M. Lloyd, M. T. Cooling, E. J. Crampin and P. F. Nielsen
Auckland Bioengineering Institute, The University of Auckland, 70 Symonds Street, Auckland, New Zealand

The CellML language was developed in response to the need for a high-level language to represent and exchange mathematical models of biological processes. The flexible structure of CellML allows modellers to construct mathematical models of the same biological system in many different ways. However, some modelling styles do not naturally lead to clear abstractions of the biophysical concepts and produce CellML models that are hard to understand and from which it is difficult to isolate parts that may be useful for constructing other models. In this article, we advocate building CellML models which isolate common biophysical concepts and, using standardization of biological parts presents an opportunity to develop

www.ietdl.org

Exp Physiol 94.5 pp 472-485

rt: A Repository of Modular Model-Biology

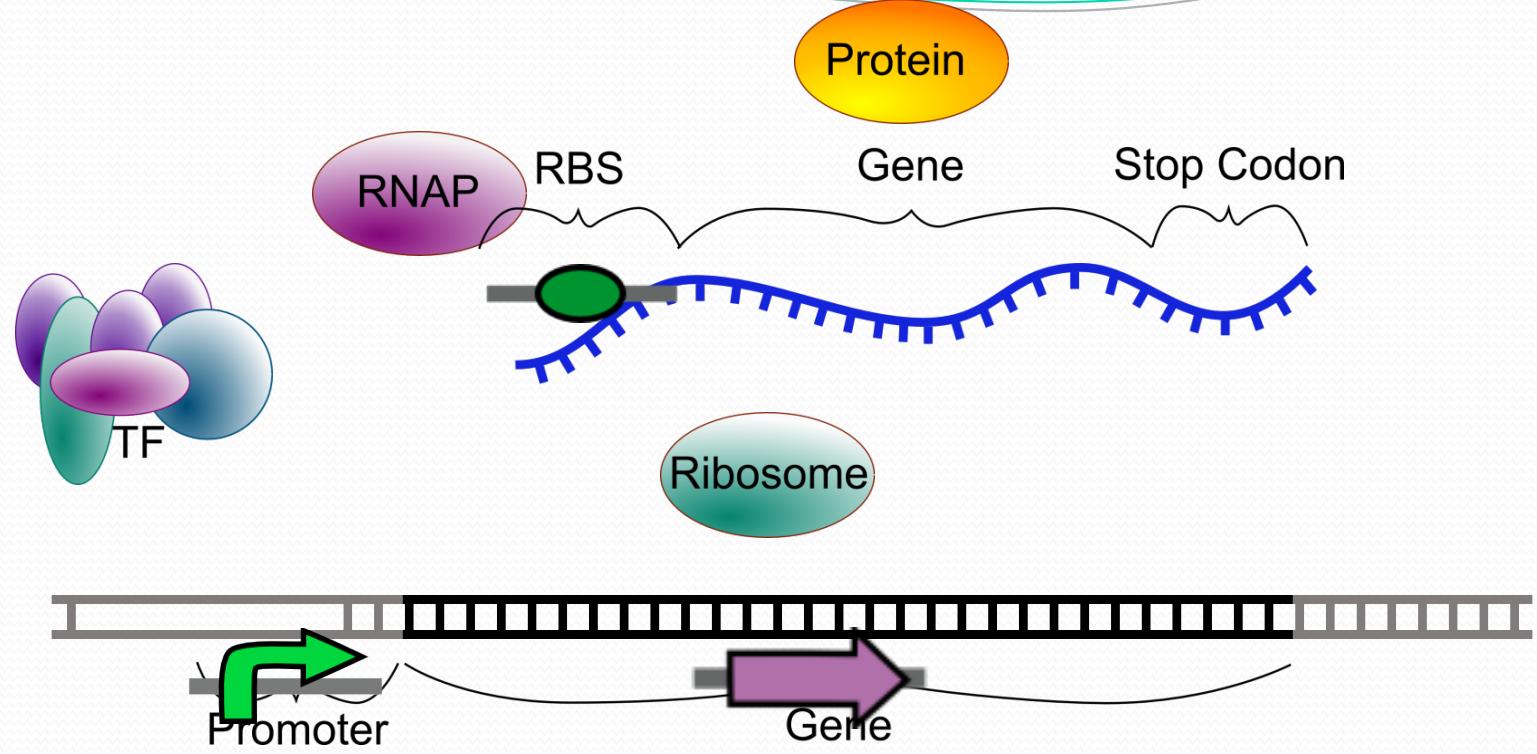
Lawson¹, T. Yu¹, J. Hallinan² and A. Wipat²

and, Auckland, New Zealand

ewcastle upon Tyne NE1 7RU, United Kingdom

n, London SW7 2AZ, United Kingdom

principles such as abstraction, standardization, and characterization to biology [Endy, 2005]. These concepts have proven to be crucial in other engineering disciplines in order to mature from 'dedicated craftsmanship' to successful industrial solutions. Arguably, to date in synthetic biology, the best example of such an approach is the



Registry of Standard Parts

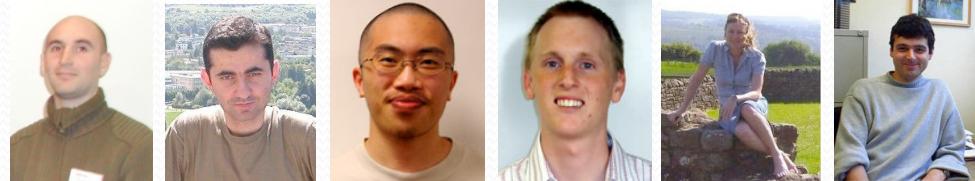
Constitutive *E. coli* σ^{70} promoters

This section lists promoters that are recognized by *E. coli* σ^{70} RNAP. σ^{70} is the major *E. coli* sigma factor so there should be RNAP present to transcribe these promoters under most growth conditions (although maximally during exponential growth).

[More...](#)

-?-	Name	Description	Promoter Sequence	Positive Regulators	Negative Regulators
1★	BBa_I14018	P(Bla)	... gtttatacataggcgaggtactctgttatgg		
1★	BBa_I14033	P(Cat)	... agagggttccaaacttcaccataatgaaaca		
1★	BBa_I14034	P(Kat)	... taaacaactaacggcaatttacccataaca		
	BBa_I732021	Template for Building Primer Family Member	... acatcaagccaaattaaacaggatcacac		
	BBa_I742126	Reverse lambda cl-regulated promoter	... gaggtaaaaatagtcaacacgcacgggtta		

Our goal



- Registry of Standard *Virtual* Parts to complement the Registry of Standard Biological Parts

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This article is part of the supplement: [BioSysBio 2007: Systems Biology, Bioinformatics, Synthetic Biology](#).

Poster presentation

Registry of BioBricks models using CellML

Vincent Rouilly¹ , Barry Canton², Poul Nielsen³ and Richard Kitney¹

¹ Department of Bioengineering, Imperial College, London, SW7 2AZ, UK
² Division of Bioengineering, MIT, Cambridge, MA 02139, USA
³ Bioengineering Institute, University of Auckland, Auckland, New Zealand, 92019

 author email  corresponding author email

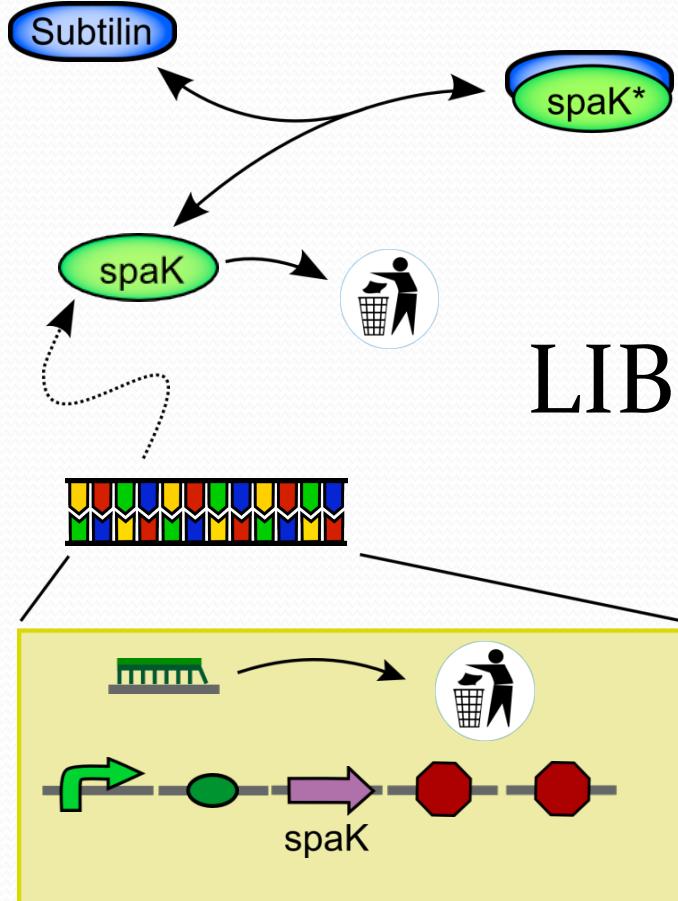
from BioSysBio 2007: Systems Biology, Bioinformatics and Synthetic Biology
Manchester, UK. 11-13 January 2007

BMC Systems Biology 2007, **1**(Suppl 1):P79 doi:10.1186/1752-0509-1-S1-P79

Published: 8 May 2007

- Composition of models to provide *in silico* simulations

Example

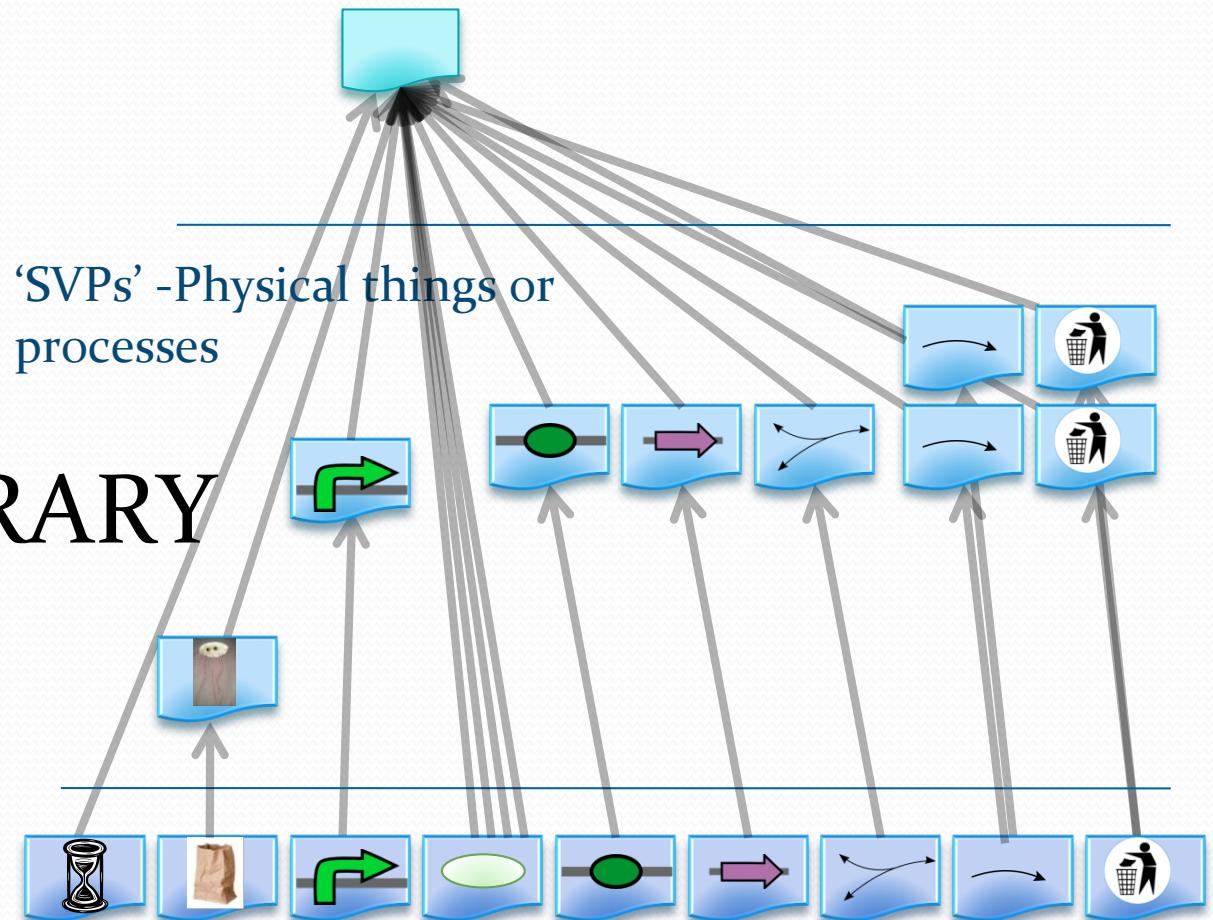


'System Models'

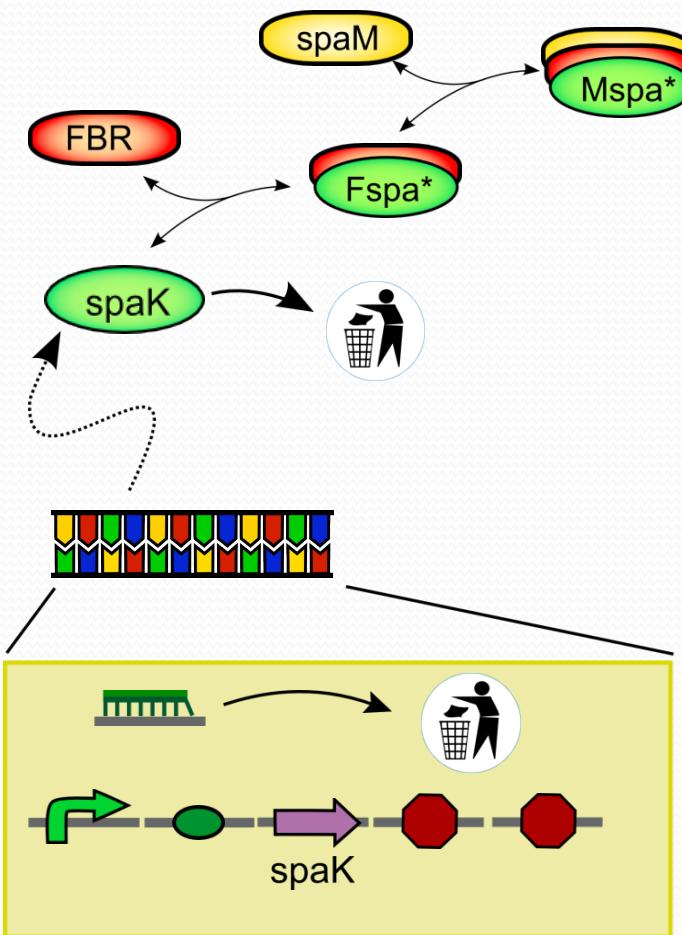
'SVPs' -Physical things or processes

LIBRARY

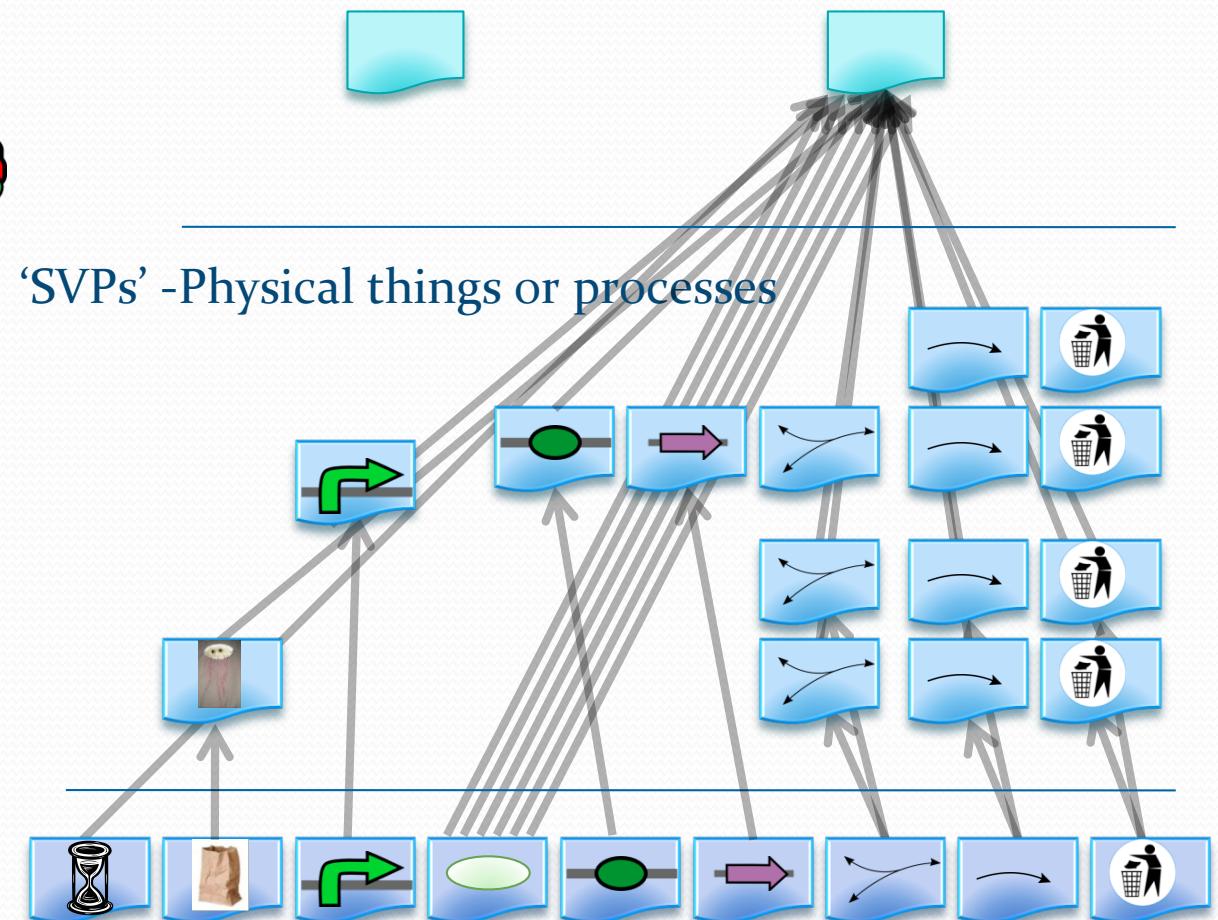
'Templates' – Mathematical structures



Example



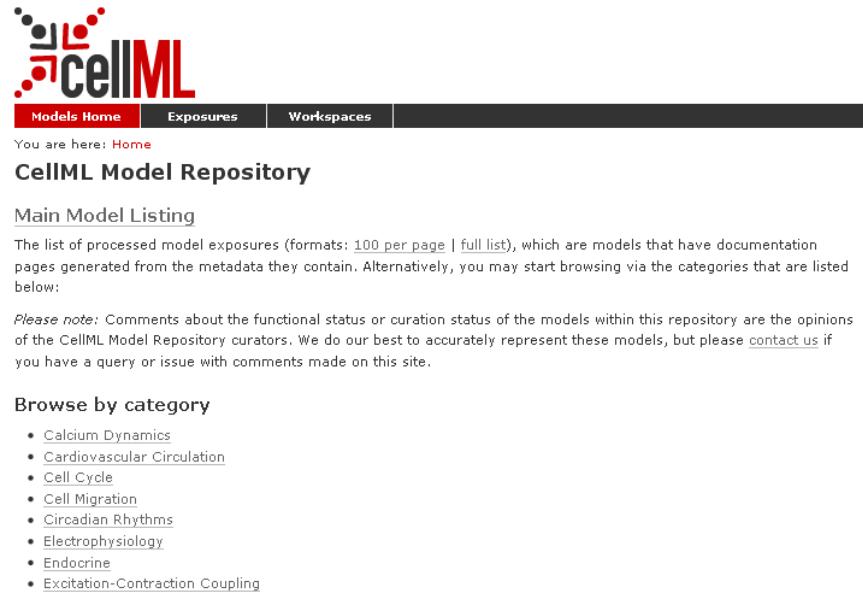
‘System Models’



‘Templates’ – Mathematical structures

<http://models.cellml.org>

- Support for v1.1 models (multi-file, imports)
- ‘Sharing’ of models between projects through ‘embedded workspaces’
- Collaborative options
- (Distributed) version control



The screenshot shows the homepage of the CellML Model Repository. At the top is a navigation bar with links for 'Models Home', 'Exposures', and 'Workspaces'. Below the navigation bar, a breadcrumb trail indicates the user is at 'Home'. The main title is 'CellML Model Repository'. Underneath the title is a section titled 'Main Model Listing' with a descriptive paragraph about the list of processed model exposures. A note below states that comments are opinions of the curators and encourages users to contact them if they have a query or issue. At the bottom of the page is a section titled 'Browse by category' with a list of categories including Calcium Dynamics, Cardiovascular Circulation, Cell Cycle, Cell Migration, Circadian Rhythms, Electrophysiology, Endocrine, and Excitation-Contraction Coupling.

Models Home Exposures Workspaces

You are here: Home

CellML Model Repository

Main Model Listing

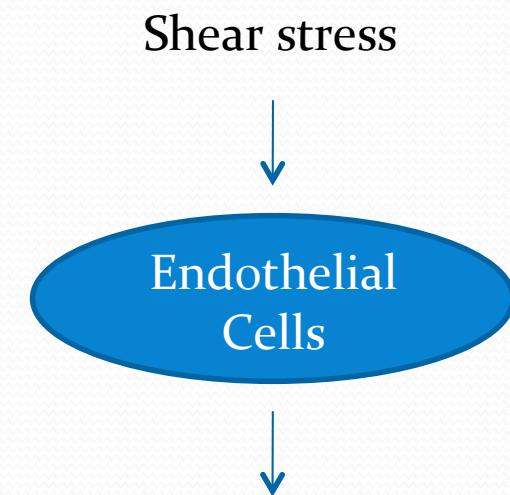
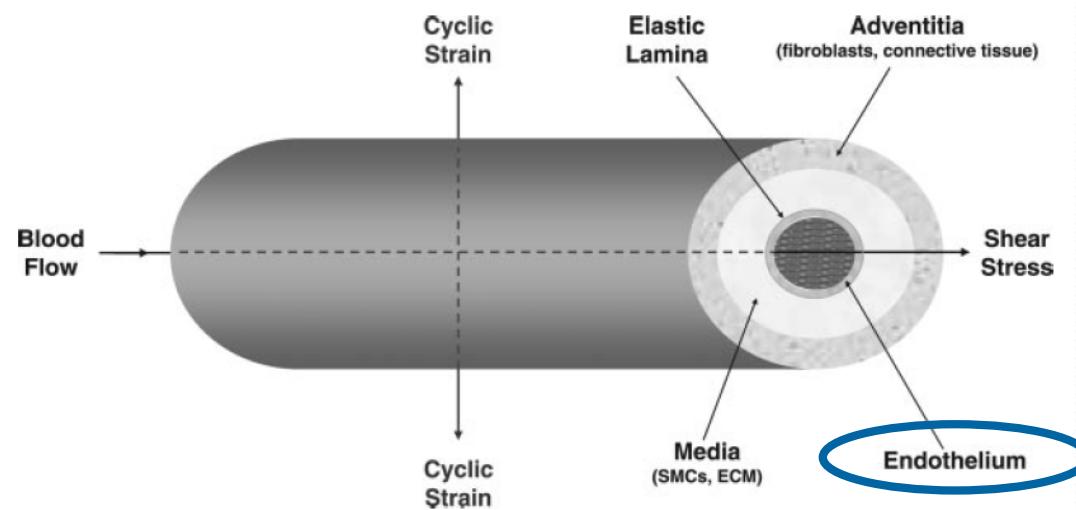
The list of processed model exposures (formats: [100 per page](#) | [full list](#)), which are models that have documentation pages generated from the metadata they contain. Alternatively, you may start browsing via the categories that are listed below:

Please note: Comments about the functional status or curation status of the models within this repository are the opinions of the CellML Model Repository curators. We do our best to accurately represent these models, but please [contact us](#) if you have a query or issue with comments made on this site.

Browse by category

- Calcium Dynamics
- Cardiovascular Circulation
- Cell Cycle
- Cell Migration
- Circadian Rhythms
- Electrophysiology
- Endocrine
- Excitation-Contraction Coupling

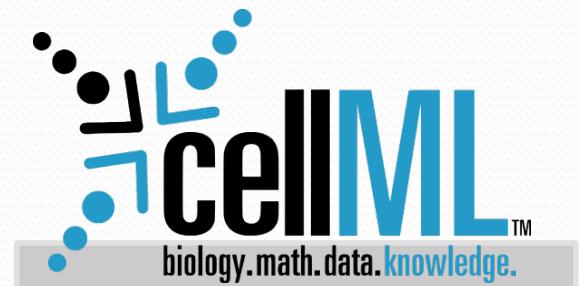
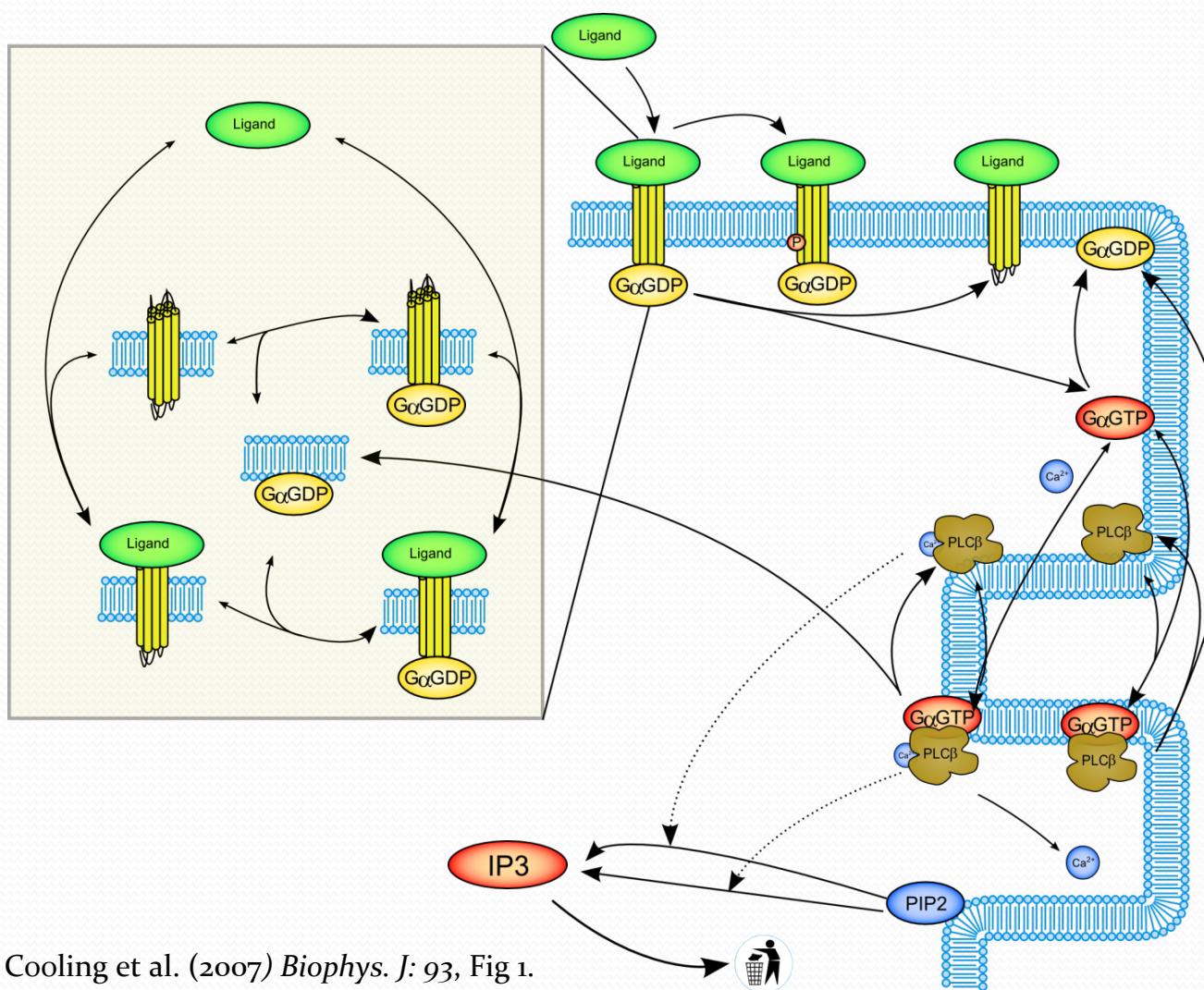
Next: Biomedical Applications



Cummins et al. (2007) *Am J Physiol Heart Circ Physiol*:292, Fig 1.

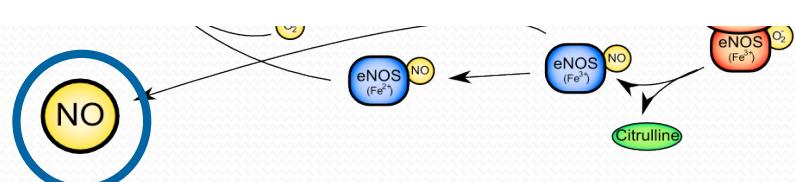
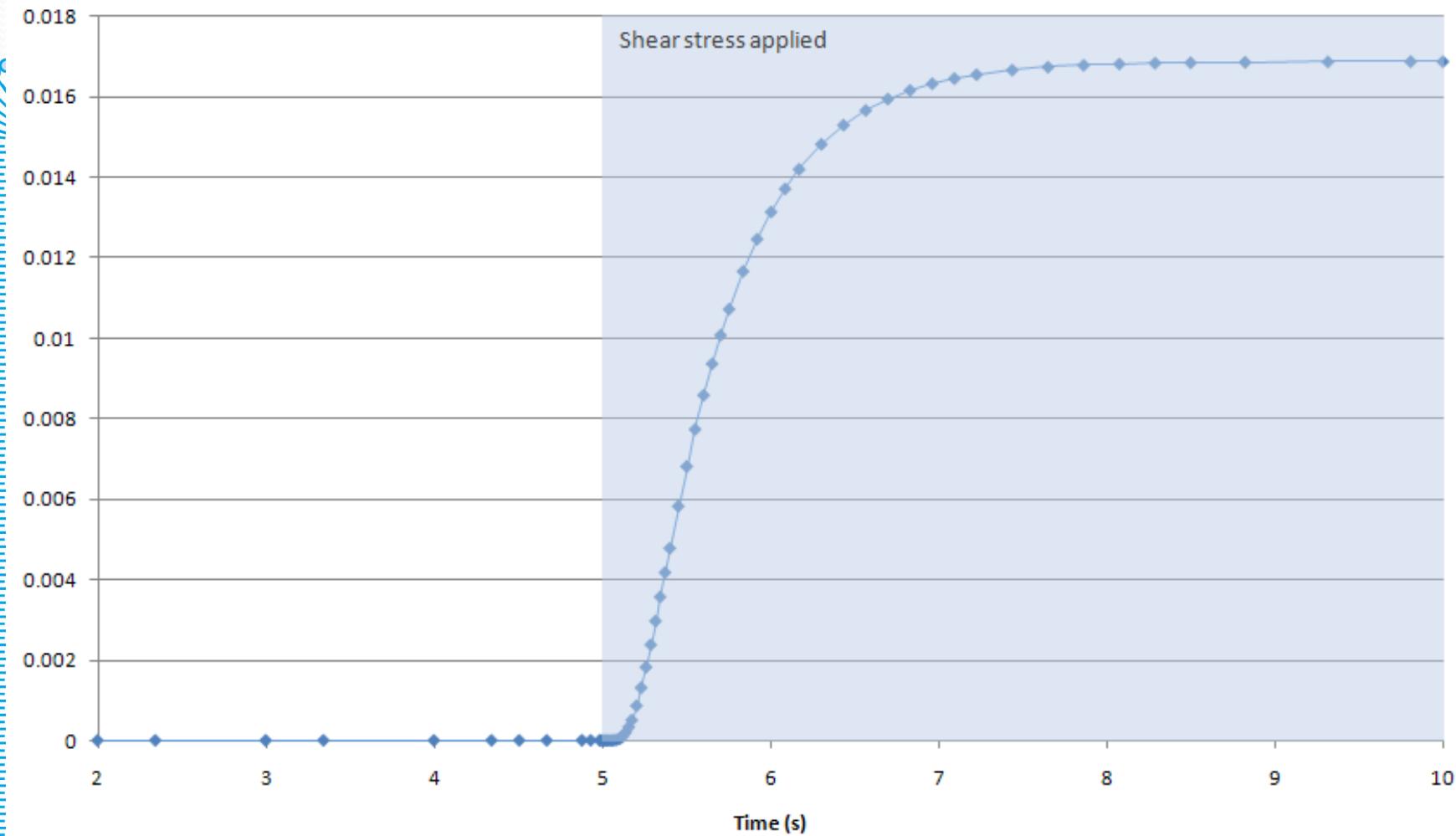
NO

Modular Model Construction



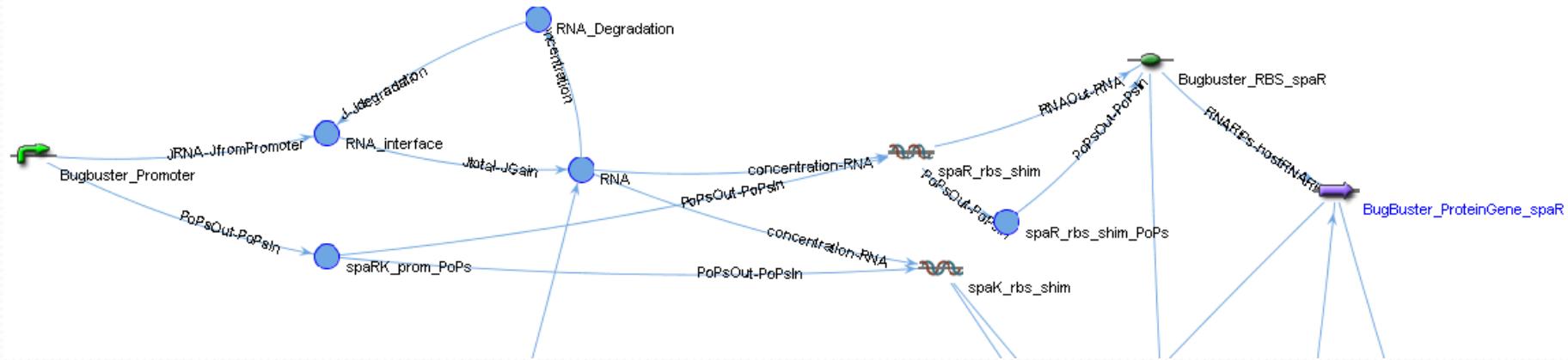
Cooling et al. (2007) *Biophys. J.* 93, Fig 1.

NO Production ($\mu\text{M}/\text{s}$)



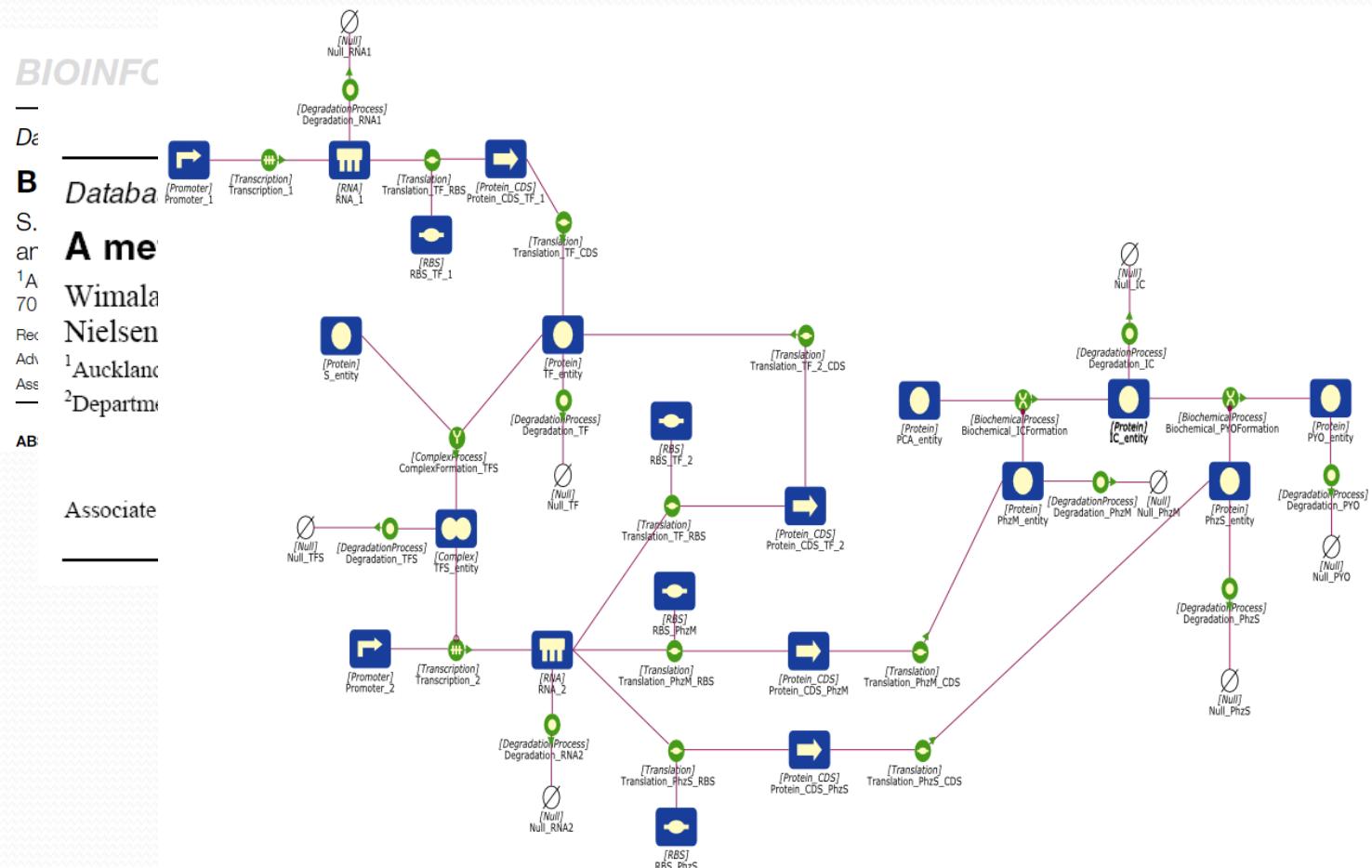
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edge.

Extensions - Annotations

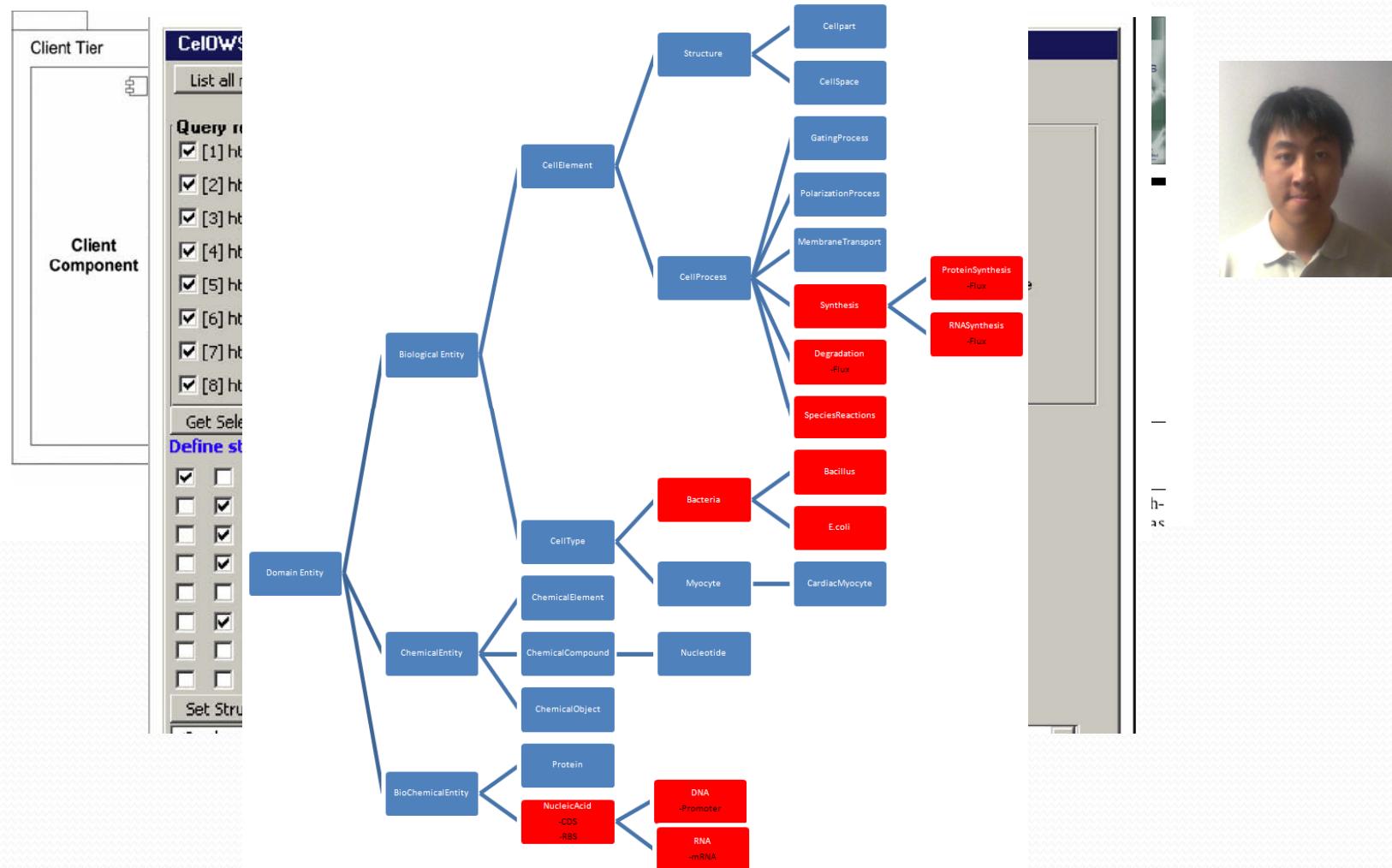


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(Semi-Automated) Visualisation



(Semi-Automated) Composition



Summary

- Constructing libraries of modular reusable components in CellML
- Building larger models from those parts
- Goal: to make it easier to build and understand large models from reusable components.
 - Visualisation
 - Composition
 - Ontologies
 - Tools
- Practices not perfect....

Funding



wellcometrust

