

Distributed computing for systems biology

Douglas Kell & Peter Li

School of Chemistry, University of Manchester,
MANCHESTER M60 1QD, U.K.

{dbk,peter.li}@manchester.ac.uk

<http://dbkgroup.org/>

<http://www.mib.ac.uk> www.mcisb.org



MANCHESTER
1824

The University of Manchester



VISUALISE

Layouts and views

SBGN

Overlays, dynamics

Model merging: (not)
LEGO blocks

Cheminformatic
analyses

Integrate various
levels

LINK WORKFLOWS

Soaplab, Taverna,

Web services, etc.

create

edit

Literature mining

Store in dB

Compare with
other models

METABOLIC MODEL (assumed to be in SBML)

Run, analyse
(sensitivities, etc)

Compare with and fit to **real**
data (parameters and
variables) with constraints

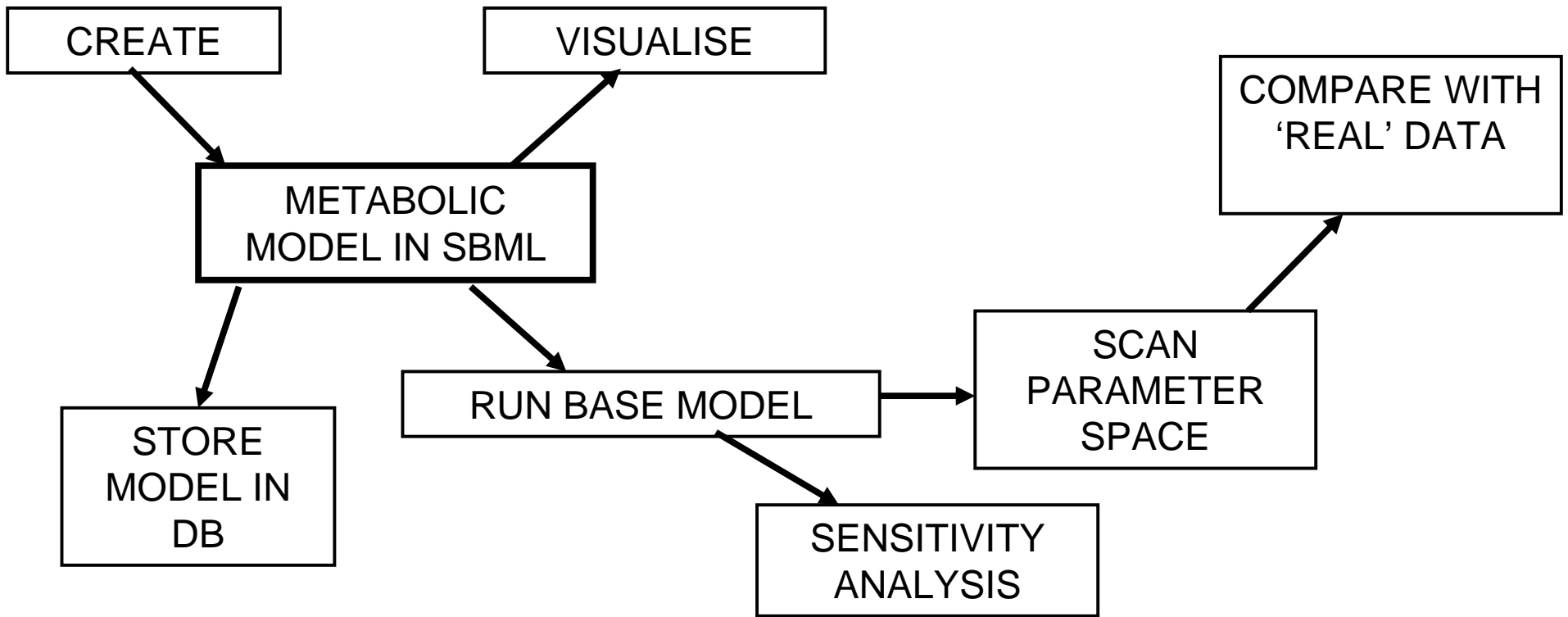
Store results of
manipulations

Network Motif
discovery

How to deal with fitting,
including as $f(\text{global}$
parameters like pH)

Optimal DoE for
Sys Identification,
incl identifiability

Automatic characterisation
of parameter space and
constraint checking



Need the glue to paste together and enact the workflows using suitably configured ('exposed') resources

BIOINFORMATICS

Vol. 20 no. 17 2004, pages 3045–3054
doi:10.1093/bioinformatics/bth361



Taverna: a tool for the composition and enactment of bioinformatics workflows

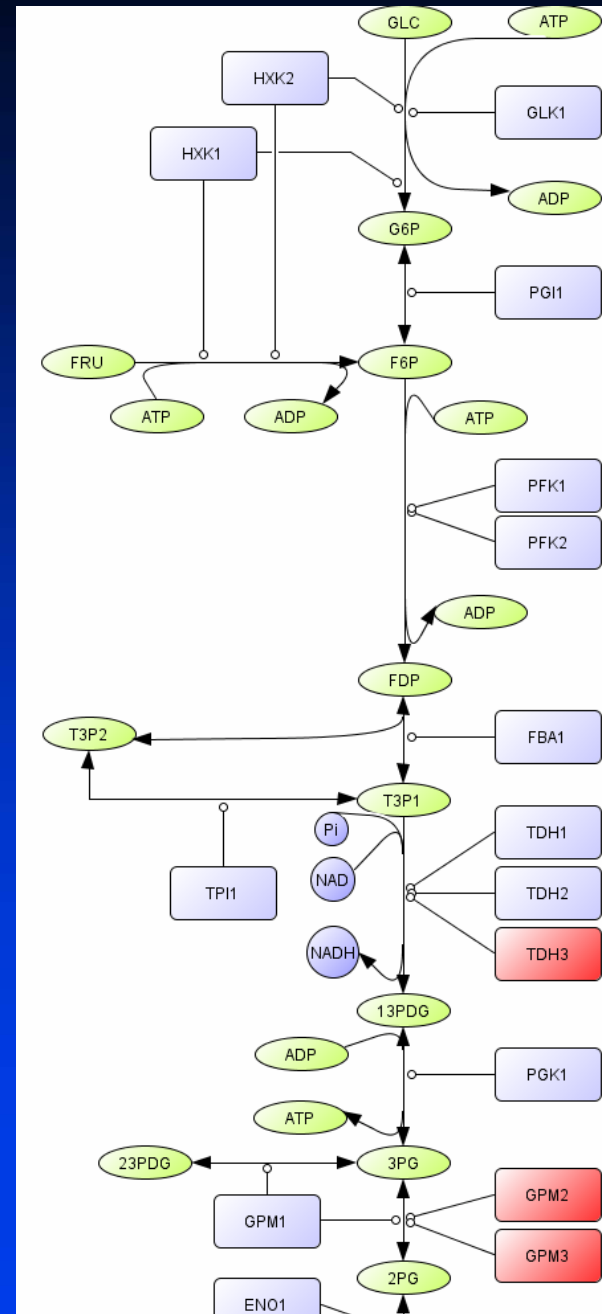
*Tom Oinn¹, Matthew Addis², Justin Ferris², Darren Marvin²,
Martin Senger¹, Mark Greenwood³, Tim Carver⁴, Kevin Glover⁵,
Matthew R. Pocock⁶, Anil Wipat⁶ and Peter Li^{6,*}*

SBGN from a user's perspective

- **MCISB focus: modelling the glycolysis pathway**
- **Used SBGN as implemented by Cell Designer to visualise reactions in glycolysis**

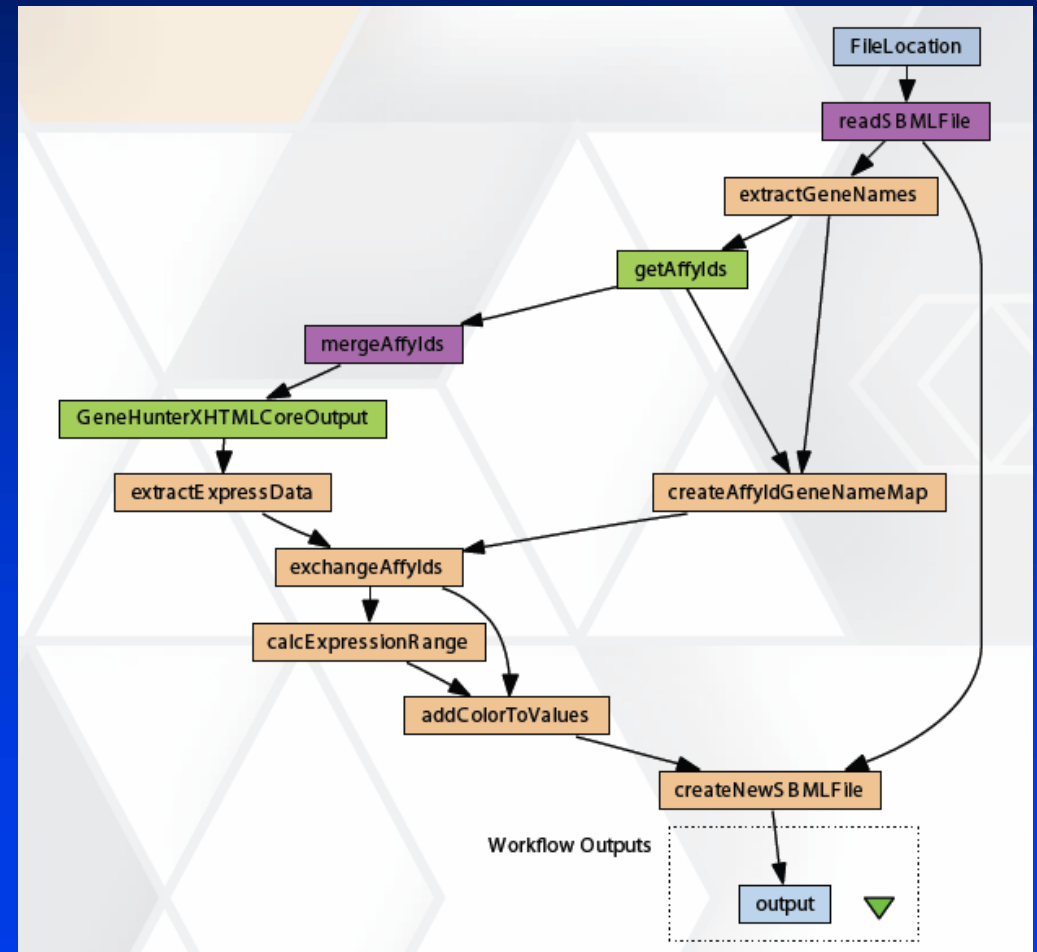
Issues:

- Layout of components that is intuitive to biologists
- Abstraction or nested processes to simplify visualisation of complex pathways
- Visualisation/integration of other types of biological data on pathways

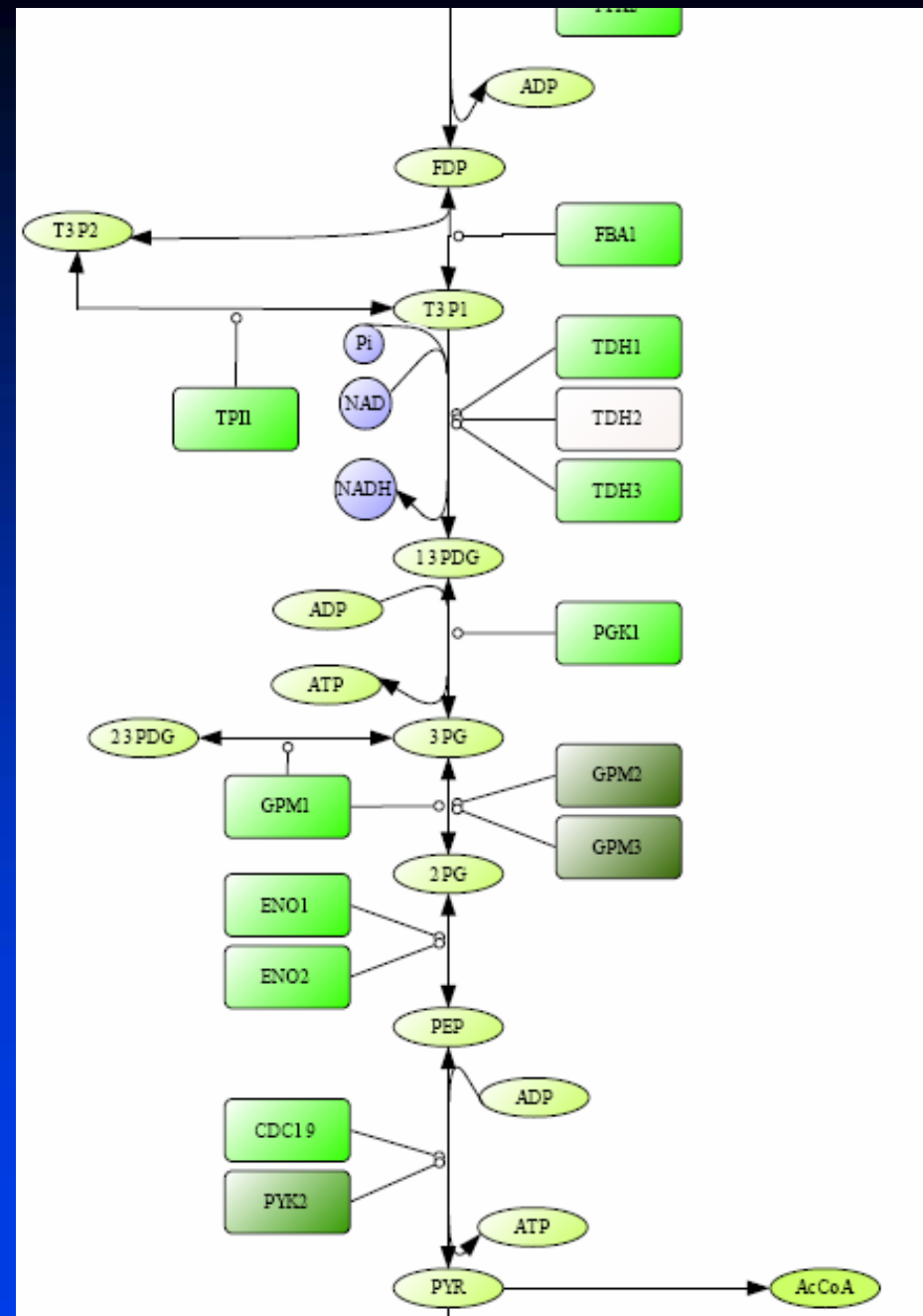


Superimposition of array data onto pathways

- Used Taverna workflows to automate the visualisation of transcriptome data on glycolysis pathway



- Gene expression levels of glycolysis enzymes shown by colour intensity



Wish items

- **An API preferably in the form of a Web service**
- **Open source**

Distributed computing for systems biology

Douglas Kell & Peter Li

School of Chemistry, University of Manchester,
MANCHESTER M60 1QD, U.K.

{dbk,peter.li}@manchester.ac.uk

<http://dbkgroup.org/>

<http://www.mib.ac.uk> www.mcisb.org



MANCHESTER
1824

The University of Manchester

