Bond Graph Clinic: Part 1

Peter Cudmore

Systems Biology Lab, The University of Melbourne

March 20, 2018

Meta-modelling

Bond Graphs

Summary

Assertions

I hope to convince you that:

- Bond Graphs are a general purpose modelling language for energetic systems.
- Bond Graphs (or something equivalent) emerge naturally from modelling energy distribution networks.
- Bond Graphs are a meta-modelling [3] tool, and hence most powerful when considering multiple physical domains.

Domain Specific Language

Domain-specific languages (DSL) are computer (programming, scripting or mark-up) languages specific to a particular application domain.

Examples include:

- *CellML* and *SBML*
- *Matlab*'s scripting language
- *VHDL* or *Verilog* (for hardware design)
- LaTeX

General Purpose Language

In contrast, general-purpose languages are designed to be applicable in a wide variety of domains

Examples include:

- Assembly, C, C++
- Python
- XML, json
- ASCII

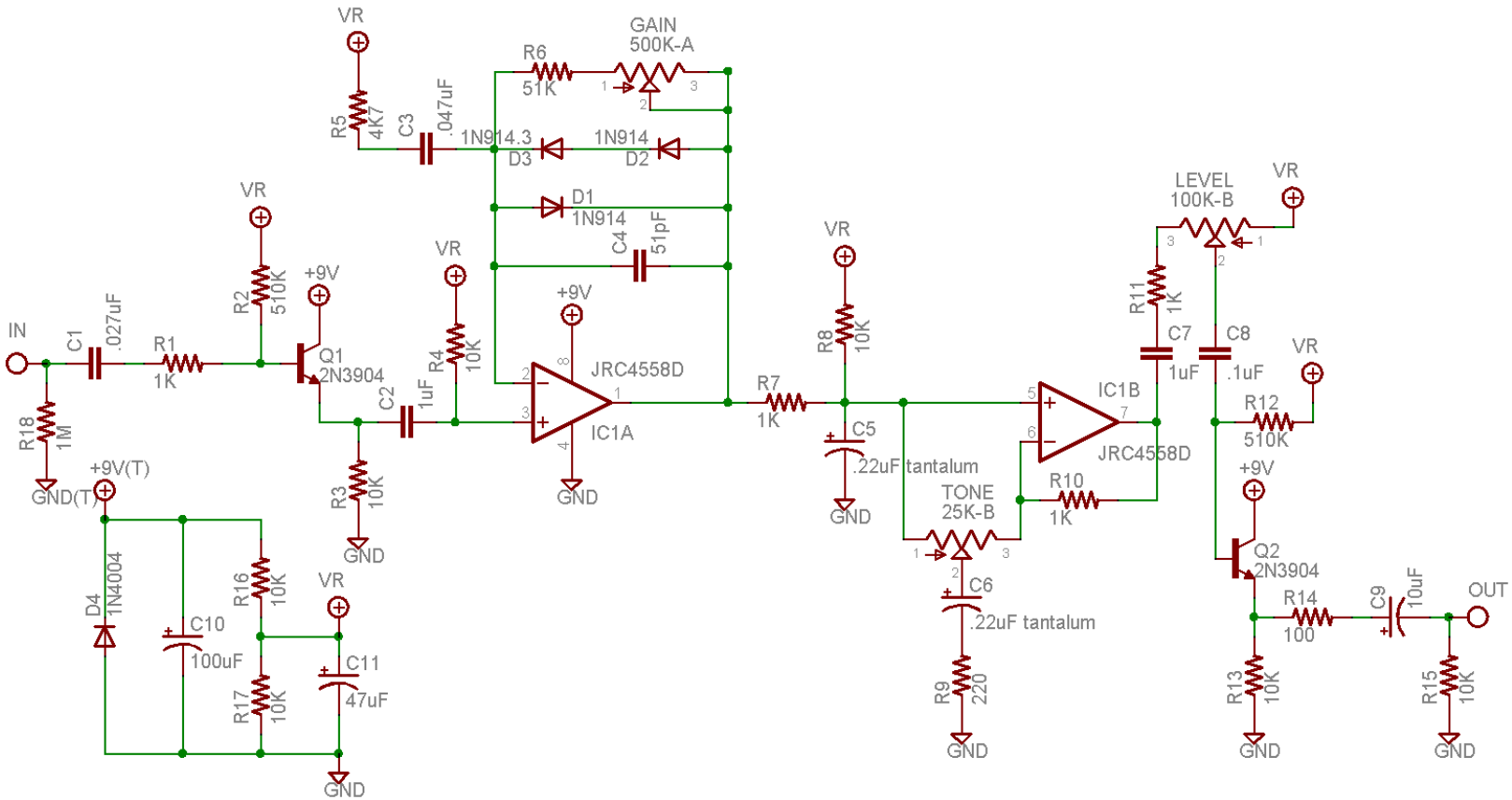
DSL's are not unique to software development.

Graphical DSL's can be found in the natural sciences:

- Feynman diagrams,
- Circuit schematics,
- Chemical reaction notation,
- Gene regulatory network diagrams,

Here we're focussing on dynamic systems.

Example: Schematic



Example: CRN

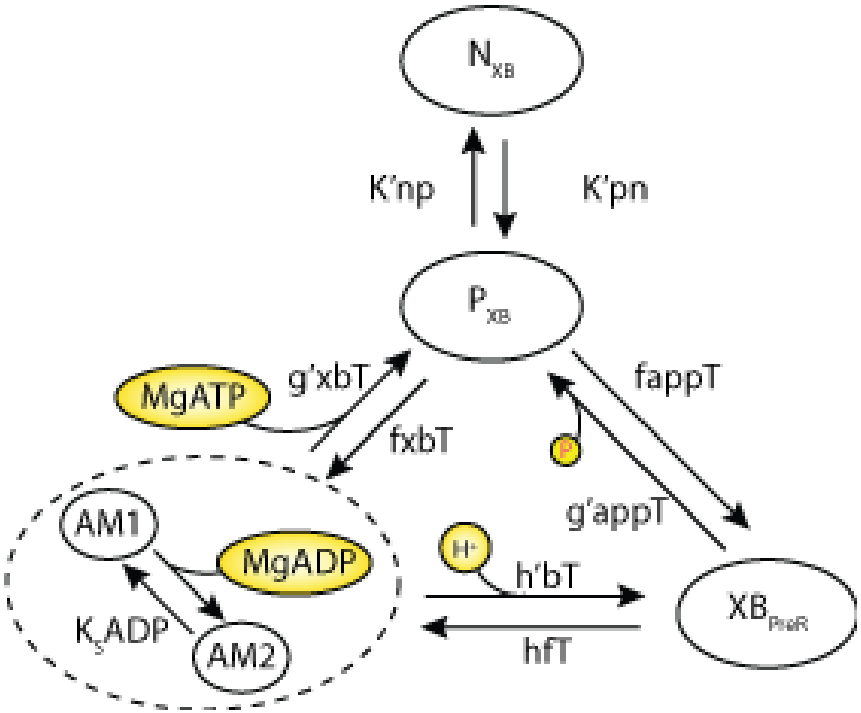


Figure: Tran. *et al.* [1]

General Purpose Modelling

How to represent systems across multiple domains?

General Purpose Modelling

If physics and mathematics are the 'machine language' of physical systems modelling,

What's the equivalent of C?

General Purpose Modelling

Bond Graphs

General Purpose Modelling

Bond Graphs*

*Conditions Apply

Law of Conservation of Energy

> *There is a fact, or if you wish, a law, governing all natural phenomena that are known to date. There is no known exception to this law—it is exact so far as we know. The law is called the conservation of energy.*

- Richard Feynman, 1961 [2].

Core Modelling Assumptions

A general purpose physical modelling language must

- use energy as the core currency.
- decompose a physical system into functionally discrete subsystems.
- describe the transfer of energy between subsystems.

These assumptions imply a network structure!

Implied Network Structure

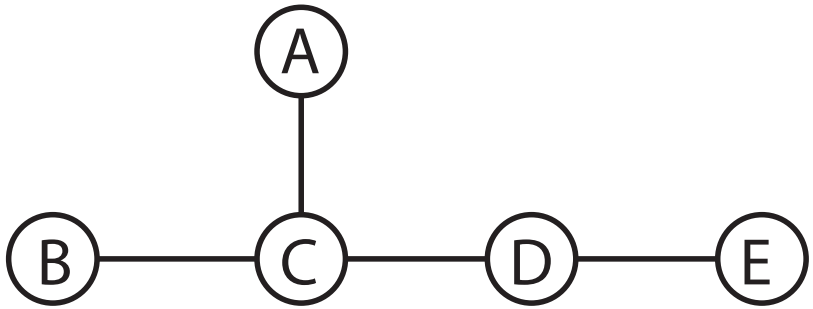
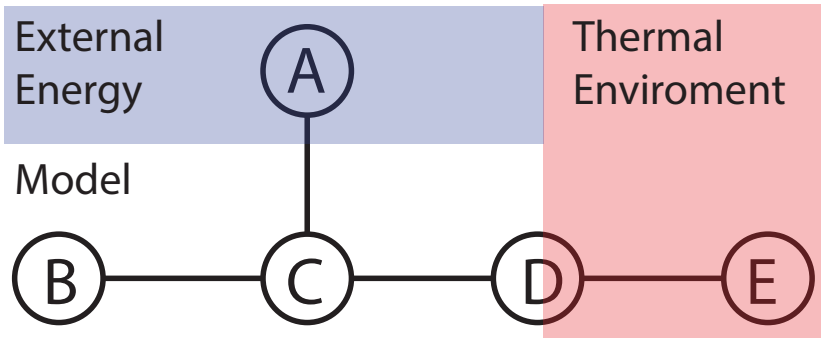


Figure: An Energy Network

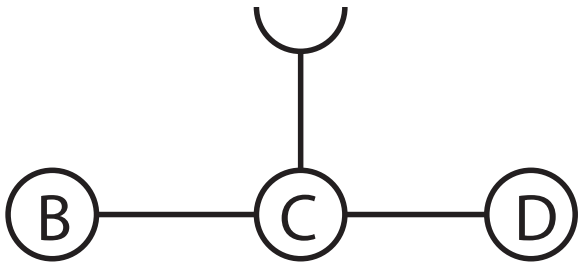
Nodes represent energetic subsystems.

Edges represent transfer of energy between subsystems.

Open Systems



is modelled as



A brief aside: Classical Mechanics

Energy is formally defined as the temporally invariant quantity of a closed system.

Energy comes in two forms, *Potential Energy* and *Kinetic Energy*.

A brief aside: Classical Mechanics

Energy is formally defined as the temporally invariant quantity of a closed system.

Energy comes in two forms, *Potential Energy* and *Kinetic Energy*.

Potential Energy fundamentally depends on something like position q. Examples Include;

- Gravitational potential energy $V(q_1, q_2) \propto -\frac{1}{|q_1 - q_2}$, where q_1, q_2 are the spatial location of a point-masses.
- Elastic potential energy $V = \frac{1}{2}kq^2$ where q is the displacement from equilibrium of a spring.

A brief aside: Classical Mechanics

Energy is formally defined as the temporally invariant quantity of a closed system.

Energy comes in two forms, *Potential Energy* and *Kinetic Energy*.

Kinetic Energy fundamentally depends on motion.
The most common example is the newtonian kinetic energy of a mass m in motion $T = \frac{1}{2m}p^2$, where p is the momentum of the moving object.

A brief aside: Hamiltonian Mechanics

In a closed system, the total energy $T + V$ is conserved.
Hence, we can define a energy function (called a Hamiltonian) $H : X \times X \to \mathbb{R}$ satisfying

$$H(q,p) = T(p) + V(q) \implies \frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial p}\dot{p} + \frac{\partial H}{\partial q}\dot{q} = 0.$$

We can easily recover Hamiltons equations:

$$e = \dot{p} = -\frac{\mathrm{d}H}{\mathrm{d}q}(q,p), \qquad f = \dot{q} = \frac{\mathrm{d}H}{\mathrm{d}p}(q,p)$$

The derivatives e, f are *effort* and *flow* variables!

Phase Space and State Space

Notice

- $H(q,p) = T(p) + V(q)$ has units of energy.
- $\frac{\mathrm{d}H}{\mathrm{d}t}(q,p)$ and hence $\dot{p}\dot{q} = ef$ has units of power (rate of change of energy).

Power can always be factorised into a pair $P = ef$.

For any subsystem, the energy should always satisfy

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\mathrm{d}H(q,p)}{\mathrm{d}t} + D(q,\dot{q}) + P_{\mathsf{in}} = 0 = \Phi(q,p,e_{\mathsf{in}},f_{\mathsf{in}})$$

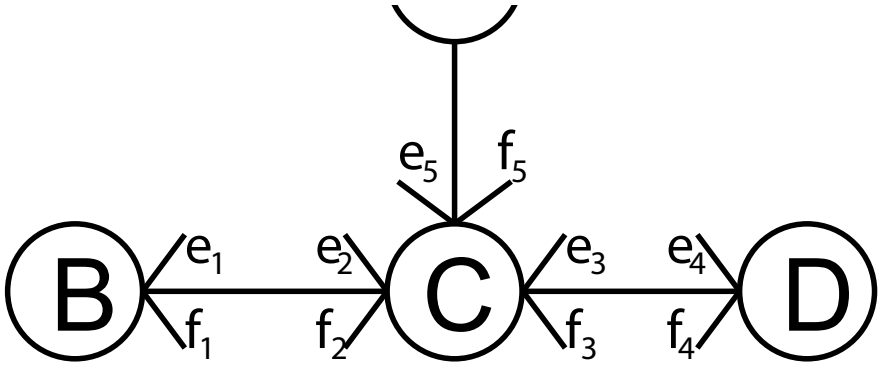
Φ is called the *constitutive relation*. (D is dissipation)

Domain Specific Power

Domain	q	f	p	e
Translational Mechanics	position	velocity	momentum	force
Rotational Mechanics	angle	angular velocity	angular momentum	torque
Electronics	charge	current	flux linkage	voltage
Hydraulics	volume	flow	pressure momentum	pressure
Thermodynamics	entropy	entropy flow	temperature momentum	temperature
Chemistry	moles	molar flow	chemical momentum	chemical potential

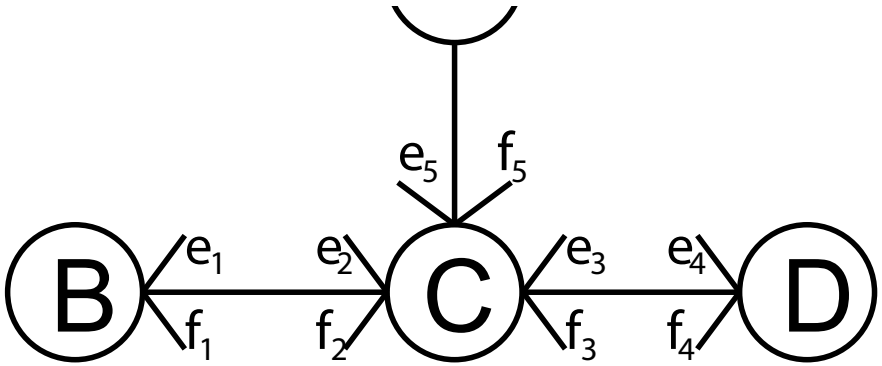
Network Structure with 2-variable Edges

System is represented by



with the energtic behaviour of the B subsystem is specified by $\Phi_B(p_B, q_B, e_1, f_1) = 0$. Similarly for the C and D subsystems.

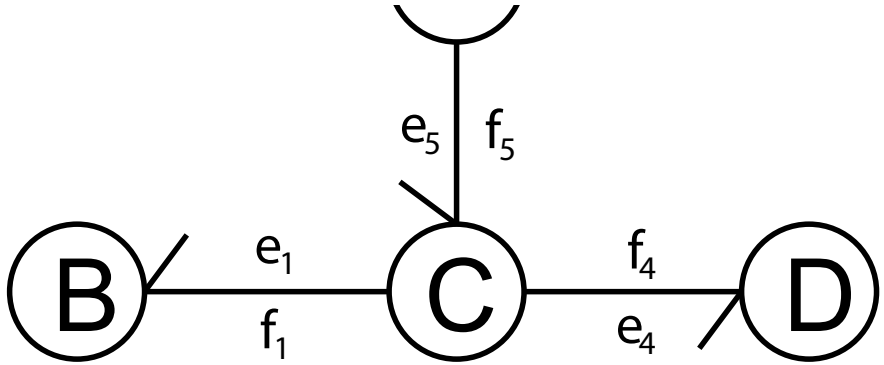
Directed Network Structure



Conservation of Energy must hold across edges, hence

$$e_1 f_1 + e_2 f_2 = 0 \qquad e_3 f_3 + e_4 f_4 = 0$$

Directed Network Structure

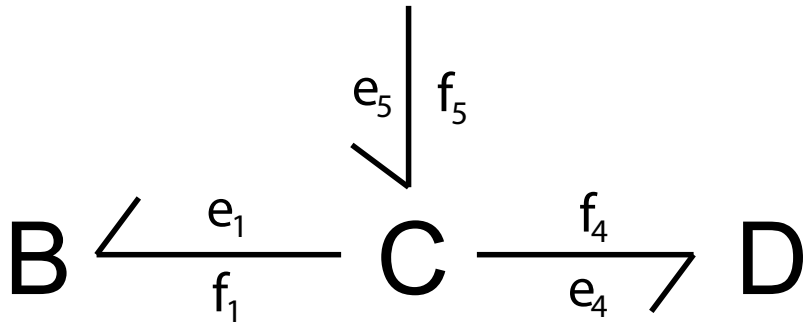


We choose a sign, and denote the direction of positive f by a half-arrow. Hence

$$e_2 = e_1 \quad f_2 = -f_1 \qquad e_3 = e_4 \quad f_3 = -f_4$$

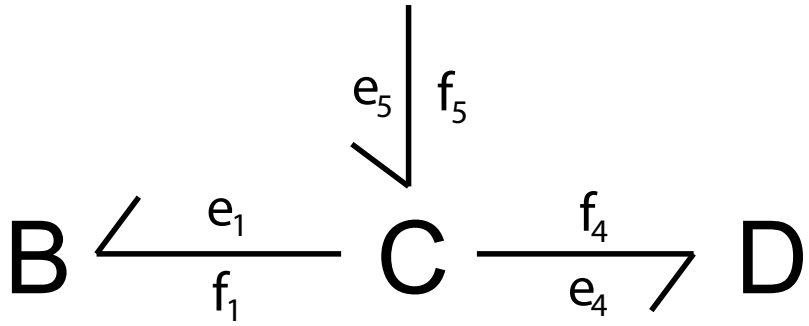
which are used to update the co-ordinates of Φ_B, Φ_C and Φ_D.

Directed Network Structure



Discard the extra circles, we get an acasual bond graph.

Acausal Bond Graphs



Hence:

- A Bond Graph models a network of energetic systems.
- A Bond Graph model is not tied to any particular domain.
- A Bond Graph is physical so long as the subsystem models Φ are physical.

These properties make it useful as a general purpose physical modelling language.

Strengths and Weaknesses

Strengths:

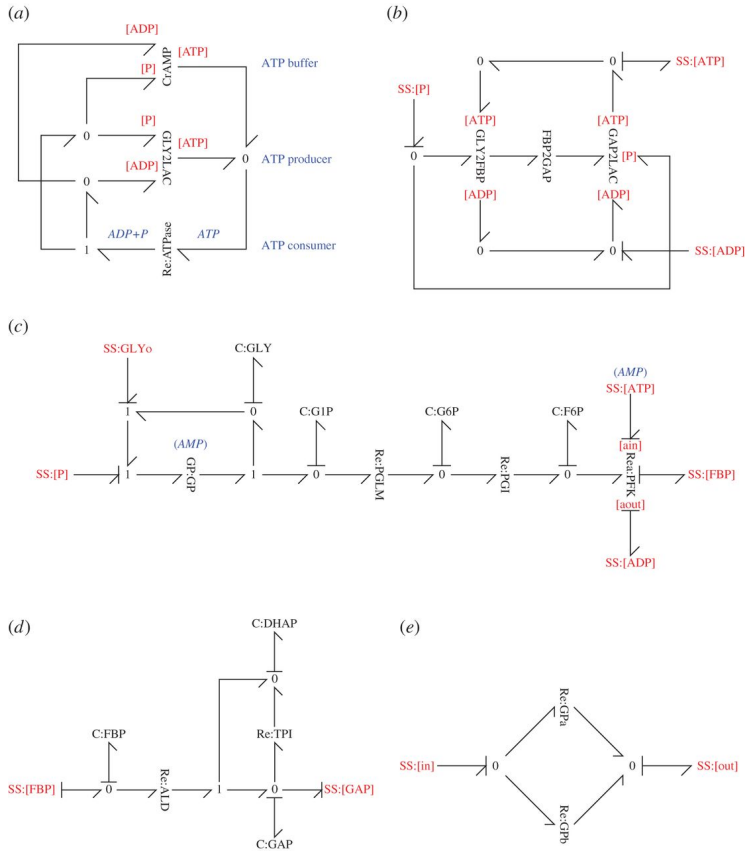
- Cross domain modelling
- Modular systems modelling and design that obeys thermodynamics.
- Designed to be 'easy' to get equations out the other end. (More on this later)

Weaknesses:

- Same as the DSL/GPL tradeoffs in programming.
- Requires a different mindset.
- Lack of software.

Next Time:

Bond Graph Components[4]




A metabolite-sensitive, thermodynamically-constrained model of cardiac cross-bridge cycling: Implications for force development during ischemia, Kenneth Tran, Nicolas P. Smith, Denis S. Loiselle and Edmund J. Crampin, 2009, *Biophysical Journal*, 98, 267-276


Feynman, Richard. The Feynman Lectures on Physics; Volume 1. 1964. U.S.A: Addison Wesley. ISBN 0-201-02115-3.


Gawthrop, Peter, Smith, Lorcan. Metamodelling: Bond Graphs and Dynamic Systems. 1996., Prentice Hall. Hertfordshire UK. 0-13-489824-9


Hierarchical bond graph modelling of biochemical networks Peter J. Gawthrop, Joseph Cursons, Edmund J. Crampin *Proc. R. Soc. A* 2015 471 20150642; DOI: 10.1098/rspa.2015.0642. Published 2 December 2015

http://www.me.utexas.edu/~longoria/paynter/hmp/Bondgraphs.html

http://math.ucr.edu/home/baez/week289.html