

An Introduction to Bond Graph Modelling

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Introduction



Power Networks



Common Components



Bond Graphs @ SBL



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Goals of this talk

My first aim is to convince you that:

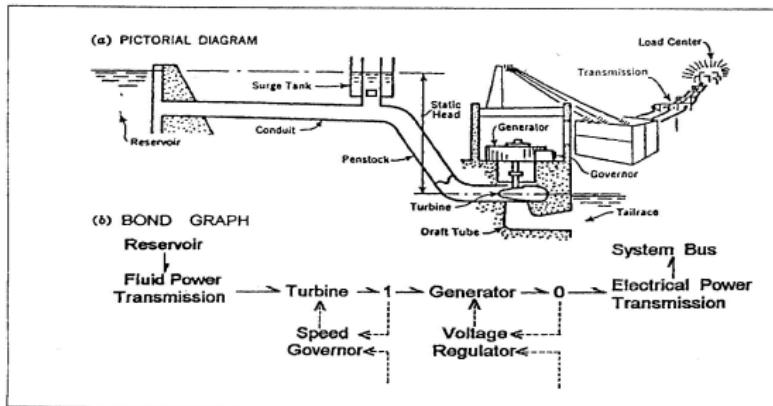
- ▶ Bond graphs are a ‘natural’ way to model energy distribution across networked systems
- ▶ Bond graphs are very useful for modelling multi-domain systems.

I will then introduce some basic bond graph components.

Finally, I will talk briefly about bond graph research at the Systems Biology Lab.

Slides are online: <https://github.com/peter-cudmore/>

Bond Graph History



Hydroelectric plant.

Bond graphs were invented by Henry Paynter [7] in 1959.

Bond Graphs Today

Bond graph modelling (or variants) are established techniques in:

- ▶ power systems engineering
- ▶ mechatronics,
- ▶ control theory,
- ▶ aerospace,
- ▶ automotive design.

Bond graphs have recently been used to model biochemical systems [4, 5, 6].

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The Fundamental Law: 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 [1].

Energy Networks

Bond Graphs model systems that:

- ▶ use energy as the core currency.
- ▶ can be decomposed into functionally discrete subsystems.
- ▶ transfer of energy between subsystems.

Hence Bond Graphs have a network structure!

Implied Network Structure

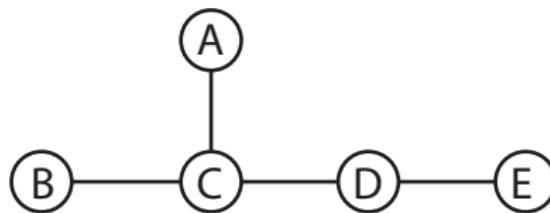
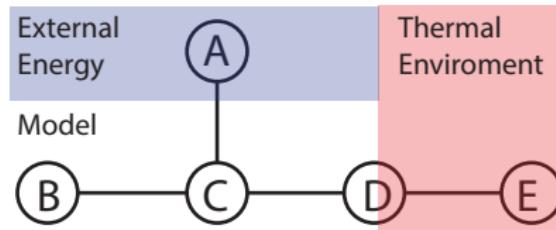


Figure: An Energy Network

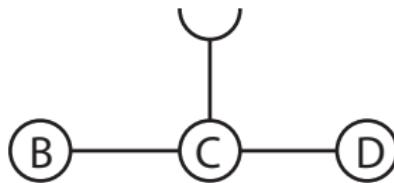
Nodes represent subsystems that act upon energy.

Edges represent transfer of energy between subsystems.

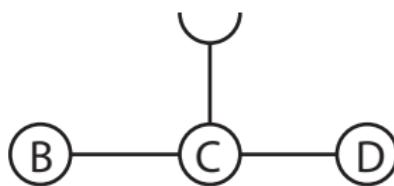
Open Systems



is modelled as



Power



Power is exchanged between subsystems B, C, D .

Power is represented in terms of *effort* e and *flow* f such that

$$\text{Power} = \text{effort} \times \text{flow} \quad \iff \quad P = ef$$

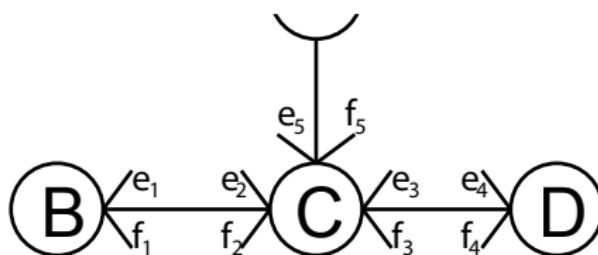
Domain Specific Power

Domain	q	$f = \dot{q}$	p	$e = \dot{p}$
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
Thermo-dynamics	entropy	entropy flow	temperature momentum	temperature
Chemistry	moles	molar flow	chemical momentum	chemical potential

Figure: State space (q, p) and phase space (e, f) variables [2, 3].

Network Structure with 2-variable Edges

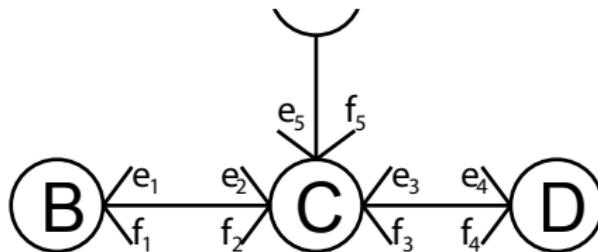
The power transferred into B is given by $e_1 \times f_1$.



Hence the energetic behaviour of the B subsystem can be specified by $\Phi_B(e_1, f_1) = 0$. Similarly for the C and D subsystems.

Φ_B describes some kind of physical process like energy storage or dissipation.

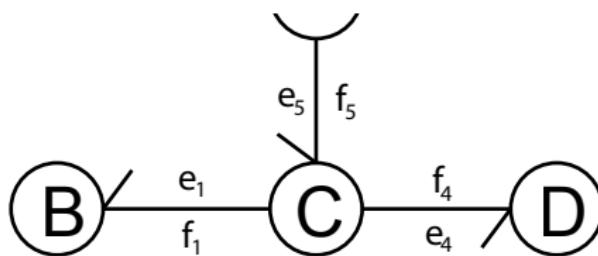
Directed Network Structure



Conservation of Energy must hold across edges, hence

$$e_1 f_1 + e_2 f_2 = 0, \quad e_3 f_3 + e_4 f_4 = 0.$$

Directed Network Structure

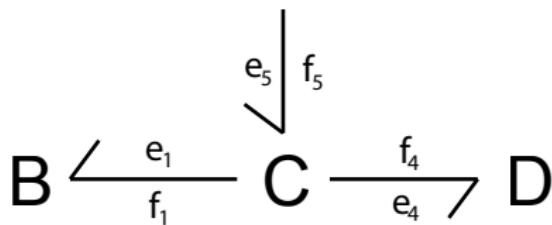


We choose a sign, and denote the direction of positive f by a half-arrow. Hence

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

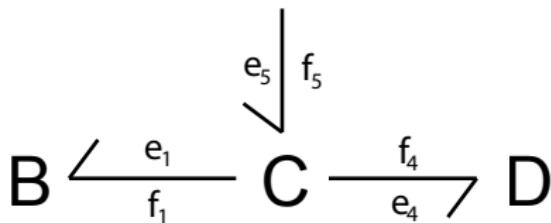
which are used to update the co-ordinates of Φ_B , Φ_C and Φ_D .

Directed Network Structure



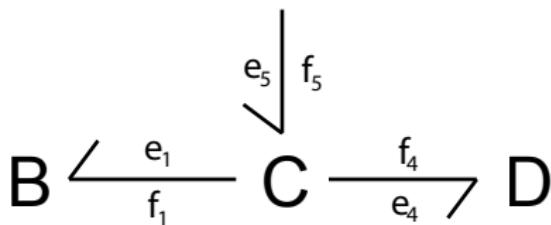
Discard the extra circles, we get an acausal bond graph.

Key Features of a Bond Graph



- ▶ Subsystem defined by constitutive relations $\Phi_B(e_1, f_1) = 0$ etc.
- ▶ Bonds show *shared variables* through which power is balanced.
- ▶ Half arrows indicate positive f (sign convention).

Strengths and Weaknesses

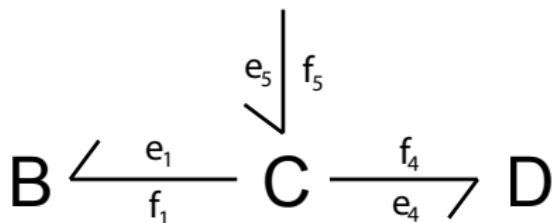


Conservation laws plus networked structure implies that:

A bond graph is physical iff it's subsystems are physical.

Caveat: Modellers must take care when constructing Φ .

Strengths and Weaknesses



No explicitly defined physical domain implies that:

Bond graphs are useful for cross-domain modelling.

Caveat: **No domain specific encoding.**

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Subsystem Relations

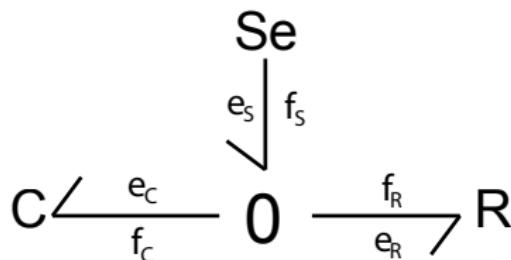


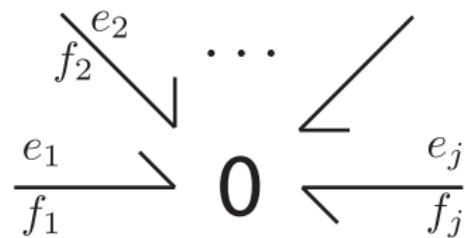
Figure: A simple bond graph

We wish to use this bond graph of as a simple example of how to generate model equations.

We need the constitutive relations for the components.

0-Junction

The 0-Junction, or common effort junction, conservatively balances power across many bonds, with equal effort.



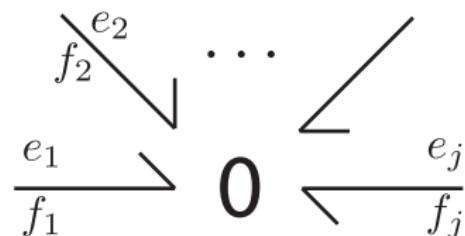
Conservation of Energy implies $\sum_{i=1}^j e_i f_i = 0$.

Equal effort implies $e_1 = e_2 = \dots = e_j$, hence $\sum_{i=1}^j f_i = 0$.

This is Kirchoff's Current Law!

0-Junction

The 0-Junction, or common effort junction, conservatively balances power across many bonds, with equal effort.



$$\Phi_0(e_1, f_1, e_2, f_2, \dots, e_j, f_j) = \begin{pmatrix} e_1 - e_2 \\ \cdots \\ e_{j-1} - e_j \\ f_1 + f_2 + \dots + f_j \end{pmatrix} = 0$$

R component

The R component dissipates power proportionally to f^2 (or e^2).

$$\frac{e}{f} \searrow R$$

The constitutive relation is given by

$$\Phi_R(e, f) = e - Rf = 0.$$

This is both Ohms law and Newtonian friction.

C component

The C component stores potential energy.

$$\frac{e}{f} \searrow C$$

The constitutive relation is given by

$$\Phi_C(e, f) = Ce - \int f dt = 0.$$

This is Hooke's law and the ideal capacitor relation.

Se component

The ideal effort source provides power into the system.

$$\frac{e}{f} \searrow \text{Se}$$

Here f is allowed to vary freely and effort is specified by a control variable u

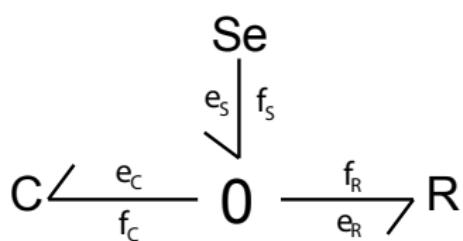
$$\Phi_{\text{Se}}(e, f) = e - u.$$

Table of Constitutive Relations

Node	Constitutive Relation
R	$\Phi_R = e - Rf$
L	$\Phi_L = \int e dt - Lf$
C	$\Phi_C = Ce - \int f dt$
Se	$\Phi_{Se} = e - u$
Sf	$\Phi_{Sf} = f - u$
TF	$\Phi_{TF} = \begin{pmatrix} e_2 - \rho e_1 \\ f_2 + \frac{1}{\rho} f_1 \end{pmatrix}$
GY	$\Phi_{GY} = \begin{pmatrix} e_2 - \rho f_1 \\ f_2 + \frac{1}{\rho} e_1 \end{pmatrix}$
Ce	$\Phi_{Ce} = e - \alpha - \beta \ln \int f dt$

Node	Constitutive Relation
0	$\Phi_0 = \begin{pmatrix} e_1 - e_2 \\ \dots \\ e_{j-1} - e_j \\ f_1 + f_2 + \dots + f_j \end{pmatrix}$
1	$\Phi_1 = \begin{pmatrix} f_1 - f_2 \\ \dots \\ f_{j-1} - f_j \\ e_1 + e_2 + \dots + e_j \end{pmatrix}$
Re	$\Phi_{Re} = \begin{pmatrix} \kappa e^{\alpha e_1} - \kappa e^{\alpha e_2} - f_1 \\ f_1 + f_2 \end{pmatrix}$

Putting it Together



$$\Phi_C = Ce_C - \int f_C dt \quad (1)$$

$$\Phi_R = e_R - Rf_R \quad (2)$$

$$\Phi_{Se} = e_S - u \quad (3)$$

$$\Phi_0 = \begin{pmatrix} e_S - e_C \\ e_S - e_R \\ f_S + (-f_C) + (-f_R) \end{pmatrix} \quad (4)$$

Goal: Find f_S .

Notice that (3) and (4) give $u = e_S = e_R = e_C$ which when combined with (1) and (2) gives $f_C = C^{-1}\dot{u}$ and $f_R = R^{-1}u$ respectively.

The last equation of (4) then gives our result:

$$f_S = \left(\frac{1}{R} + \frac{1}{C} \frac{d}{dt} \right) u.$$

In Review

Hopefully I've convinced you that bond graphs :

- ▶ 'naturally' model energy distribution across networks
- ▶ are very useful for modelling multi-domain systems.
- ▶ conserve energy when connecting network subsystems.

Network subsystems can be:

- ▶ derived from first principles,
- ▶ defined phenomenologically,
- ▶ constructed hierarchically.

This makes for a powerful, multi-domain and multi-scale modelling tool.

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Bond Graph researchers at the SBL:

- ▶ Prof. Edmund Crampin (Director)
- ▶ Prof. Peter Gauthrop
- ▶ Michael Pan
- ▶ PC

Website: <https://systemsbiologylaboratory.org/>

At the Systems Biology Lab we aim to build ‘comprehensive’ models of cells, with heart cells as our working model.

Bond Graphs play a central role in ensuring our models remain physical.

Cellular Biochemistry and Metabolism

Prof. Peter Gawthrop is working on bond graph models of cellular biochemistry and metabolism.

Website: www.gawthrop.net

Recent Publications:

- ▶ P.J. Gawthrop, E.J. Crampin. 2017. *Energy-based Analysis of Biomolecular Pathways* Proceedings of the Royal Society A, 473:20160825.

- ▶ P. Gawthrop. 2017. *Computing Biomolecular System Steady-states*. IEEE Transactions on NanoBioscience, vol. PP, no. 99, pp. 1-1.

Electrophysiology

Michael Pan is working on bond graph approaches in electrophysiology and ionic homeostasis.

You'll hear more from Michael later in this session.

Forthcoming publications:

- ▶ M. Pan, P.J. Gawthrop, J. Cursons, K. Tran, E.J. Crampin.
*Bond graph modelling of the cardiac action potential:
Implications for drift and non-unique steady states.*

- ▶ M. Pan, P.J. Gawthrop, J. Cursons, K. Tran, E.J. Crampin.
*The cardiac Na⁺/K⁺ ATPase: An updated,
thermodynamically consistent model.*

Synthetic Biology

I joined the System Biology Lab in November, 2017 and am working on:

- ▶ Bond graph techniques for rational design in synthetic biology and bioengineering.
- ▶ Improving the bond graph modelling tool-chain.
- ▶ Investigating the connection between bond graphs, Hamiltonian mechanics, network dynamics, and operator theory applications to stochastic mechanics.

Website: <https://github.com/peter-cudmore/>

Thanks

Thanks to

- ▶ Prof. Edmund Crampin and Prof. Peter Gawthrop
- ▶ Andre, the CellML workshop organisers and the Auckland Bioengineering Institute
- ▶ Systems Biology Laboratory, School of Mathematics and Statistics and Department of Biomedical Engineering, University of Melbourne, Parkville, Victoria 3010
- ▶ ARC Centre of Excellence in Convergent Bio-Nano Science and Technology, Melbourne school of Engineering, University of Melbourne, Parkville, Victoria 3010

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Online Resources

<https://github.com/peter-cudmore/>

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