“How do these things compose?”
Modularity in materials, databases, and dynamical systems
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Principal Investigator: David I. Spivak
Senior Personnel: Patrick Schultz

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Outline

Composition is everywhere

One of our best tricks is composing and decomposing things.

- Almost any thing we can think of is a composite of other things.
  - A computer or an animal's body,
  - a person's life story or a task,
  - a society or an economic system, etc.
- The system behavior is dictated by the interaction among sub-systems.
- I like when I can view the system and subsystems as having a common type (data-structure).
  - Consider what this would mean for things in the list above.
  - If a domain has such commonality across scales, I call it *operadic*.

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From this point of view, how can we model the really interesting things?

- Can we find a compositional (operadic) structure for *life*, or *mind*?
  - Suppose we want a compositional model of life and evolution.
  - Or of mind and learning. Or of society and culture?

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    - Suppose we want a compositional model of life and evolution.
    - Or of mind and learning. Or of society and culture?
- Let's consider the "common data structure" requirement.
    - We want to capture the interesting aspects of life (or mind).
    - We want it to be composed of proto-systems of the same type.
    - A big question: What might that data structure be??

Use of category theory

My field of expertise is category theory.

- Since it's invention in the 1940s it's revolutionized pure math.
  - It's branched out into CS, physics, linguistics, manufacturing, ...
  - Reason: it connects rather than "unifying" disparate fields.
- Why is category theory (CT) useful for this project?
  - Its primary principle is compositionality.
  - It studies everything in terms of composable relationships.
  - Objects are known by their behavior, not by their implementation.

Outline

Toward modeling thought

I started with a belief that knowledge was networked data.

- CT suggests a way to communicate (transfer data) between such networks.
- The emphasis is on data migration: from my brain to yours.
  - Communication requires an "analogy" between conceptual structures.
  - This can be made precise using functors (maps between categories).
  - Given a functor from my schema to yours, we can transfer data.
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From this came an idea of *olog* or "ontology log", like a scientist's log-book.

- It's a categorical knowledge representation system.
- Aside: I've been recently impressed with work by E. Patterson, who has improved upon the original idea.

Questions remained:

- How does the physical brain implement such a knowledge network?
- How do we "communicate" with reality to update our schema/data?

Working with others

I've always felt it was important to work with people in other fields.

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  - We published several papers, but I always felt something missing.
  - We were always forced into static descriptions of dynamic things.

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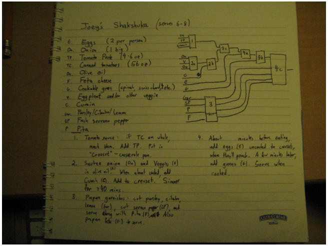
- I worked with materials scientists to represent knowledge as ologs.
  - We published several papers, but I always felt something missing.
  - We were always forced into static descriptions of dynamic things.
- I also worked with informaticists from pharmaceutical companies.
  - The database approach fit well, and we learned from each other.
  - But I felt at a loss when trying to model recipes this way.
    - Pharmaceutical recipes are processes within processes.
    - The database formalism didn't appropriately highlight this.

Outline

Recipes

Pharmaceutical recipes are like recipes we find in cooking.

- A set of steps, combining the outputs of previous steps.



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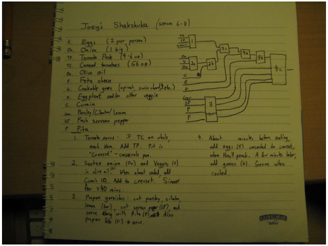

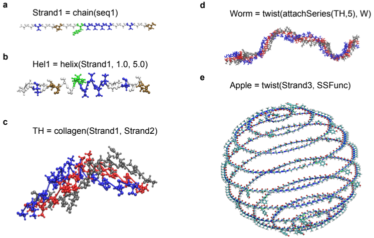

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Recipes are also useful in materials science: hierarchical protein materials.

- We made a program called *Matriarch* for materials architecture.
- Materials like collagen are hierarchical: made from building blocks.

Operads: the mathematics of compositionality

In CT we consider a sort of mathematical object, called an operad.

- Operads are a framework for composing systems of systems.
- Operads are a sort of syntax; their semantics are called algebras.
- Some examples of compositional structures operads can model:
  - Every recipe—as in the pharmaceutical and materials science examples above—is an operad.
    (Performance plans might constitute an algebra for it.)

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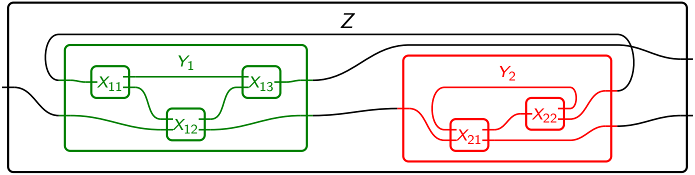
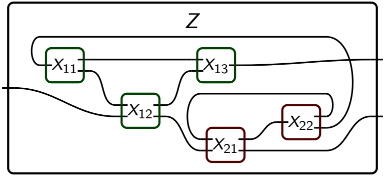
  - Every sort of wiring diagram, as in electric circuits or signal flow.
    (We'll discuss several different algebras for wiring diagrams.)
- I'll describe operads of wiring diagrams next.

An operad of wiring diagrams





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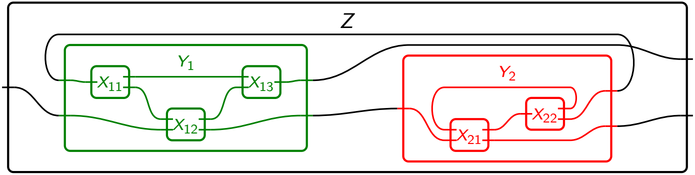

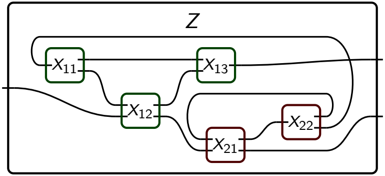

- Wiring diagram operads can have many different semantics (algebras):
  - The boxes can represent arrays or *tensors*.
  - The boxes can represent multi-ary relations.
  - The boxes can represent quantum processes (teleportation, etc.).
  - The boxes can represent open dynamical systems.

Compositional analyses: bifurcation theory

There can be more than one semantics (algebras) for the same operad.

- As mentioned above, wiring diagrams have many semantics.
- One such semantics is that of open dynamical systems. $\mathit{in} \rightarrow \boxed{X} \rightarrow \mathit{out}$
  - These are machines that process input and produce output.
  - A labeled transition system would be such a thing.
  - But so would an ODE with time-varying parameters $\begin{cases} \dot{x} = f(x, \mathit{in}) \\ \mathit{out} = g(x) \end{cases}$
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A *compositional analysis* is a translation, preserving composition structure.

- For example, for each DS take the bifurcation diagram as a tensor.
- Theorem: the bifurcation diagram of a composed system is given by multiplying—as tensors—the bifurcation diagrams of the subsystems.

What else is compositional?

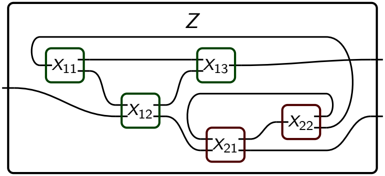
These leads to a research program of finding other compositional analyses.

- Let's summarize what that would mean; maybe you can think of one.
  - Suppose you have a framework in which you can build things.
  - And suppose it's modular: we can nest building blocks.
  - We want to be able analyze systems in a compositional way.
  - Calculate a property of the whole by those of the parts (together with the wiring diagram or "operad morphism" that forms it).

Outline

Mode-dependent wiring diagrams

In wiring diagrams like the above, the interaction pattern is fixed.



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- But not for society, or human interaction, or maybe even brains.
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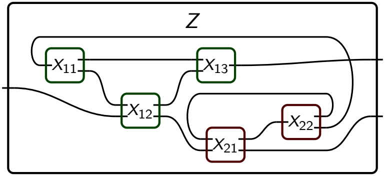

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- We found a neuroscience example, but I'd like to keep working on it.
  - I'd eventually like to see if/how it connects to π-calculus.
  - Or to find a programming language for it.

Evolution and learning

Evolution and learning should also be compositional. How so?

- We look for useful building blocks, and then we reproduce them.
    - For example, logic gates have been very useful.
    - The adder circuit has been very useful.
    - Monitors and CPUs, Arduino, the cloud.
- Whatever works, we repeat it in every conceivable combination.
    - We combine useful building blocks in new ways to solve problems.
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  - But so does nature in evolution, be it for species or ecosystems.
  - You win if you create a building block that gets repeated a lot.

But how to formalize evolution and learning?

I'd like to formalize evolution and learning mathematically. But how?

- What is the data structure that we find at multiple levels?
- I'm thinking "organizations" are a way to think about both.
  - A person is an organization, as is a cell, a company, a society.
  - As is new knowledge: an organized group of ideas or procedures.
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  - How does something become self-sustaining?
- Inspiring authors and thinkers:
  - Been inspired by Minsky, Koestler, Bateson, Maturana, Varela.
  - I'm currently looking with interest at Nikolas Luhmann.
  - What am I doing when I convert other researchers' work into advances in my own thinking. What leads to scientific evolution?

Outline

Project summary

Research Objectives:	Technical Approach:
What sorts of interesting data structures are compositional? Most importantly I want to consider agents (say, things that design custom solutions to problems based on experience). How are experiences, stories, problems, and solutions composed?	Using mathematics to formalize communication and compositionality. Specifically, I use category theory, and within that, operads and sheaves.
Key Findings:	**Benefits to the wider academic or DoD community:**
Databases are good for modeling static structures, and CT builds rigorous "functorial" bridges to connect different worldviews (database schemas). For processes and nestable structures, operads serve much better. Bifurcation diagrams of open dynamical systems are compositional.	The categorical database work (and a KR framework offshoot) has been used by researchers in materials science and at the European Spallation Source. A company was also formed around the categorical data migration technology. Work on composing open dynamical systems led to a NASA grant as well as to a separate DoD grant.

Publications, Awards, Patents, or Transitions Attributed to the Grant

Nine publications have resulted from this grant, published in diverse journals:

- *Mathematical Structures in Computer Science* ('14)
- *Nanotechnology* ('15)
- *ACS Biomaterials Science & Engineering* ('15)
- *Theory and Application of Categories* ('15 and '16)
- *Communications in Contemporary Mathematics* ('16)
- *Journal of Complex Networks* ('16)
- *Journal of Computing and Information Science in Engineering* ('17)
- *Journal of Pure and Applied Algebra* ('17)

A company, called *Categorical Informatics* was spun out of MIT. It involved some work from this grant (though more from a previous ONR grant).

Two new awards have resulted from my work on this grant: NASA NNH13ZEA001N and AFOSR FA9550-17-1-0058.