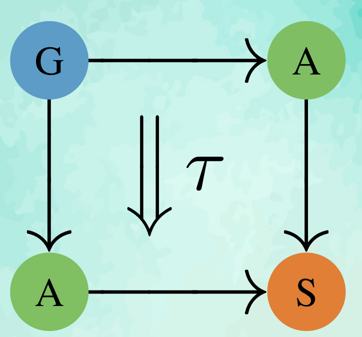
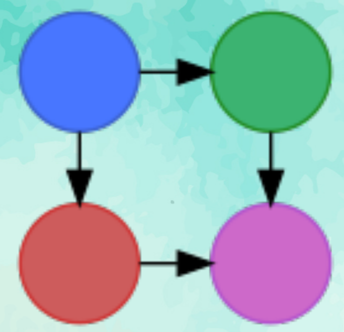
Diagrammatic differential equations

Formal categorical framework and applications to multiphysics simulation

DOI: 10.3934/mine.2023036

E Patterson, A Baas, **T Hosgood**, J Fairbanks





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hidden Markov model, linear recurrence, …

Diagrammatic differential equations

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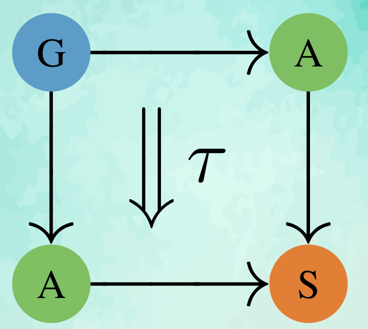

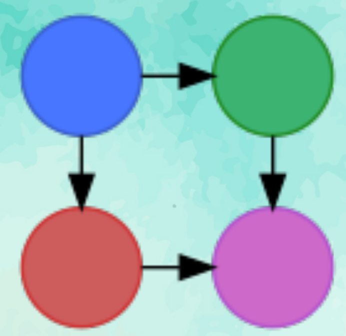

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1. What is multiphysics?

Doing two things at once

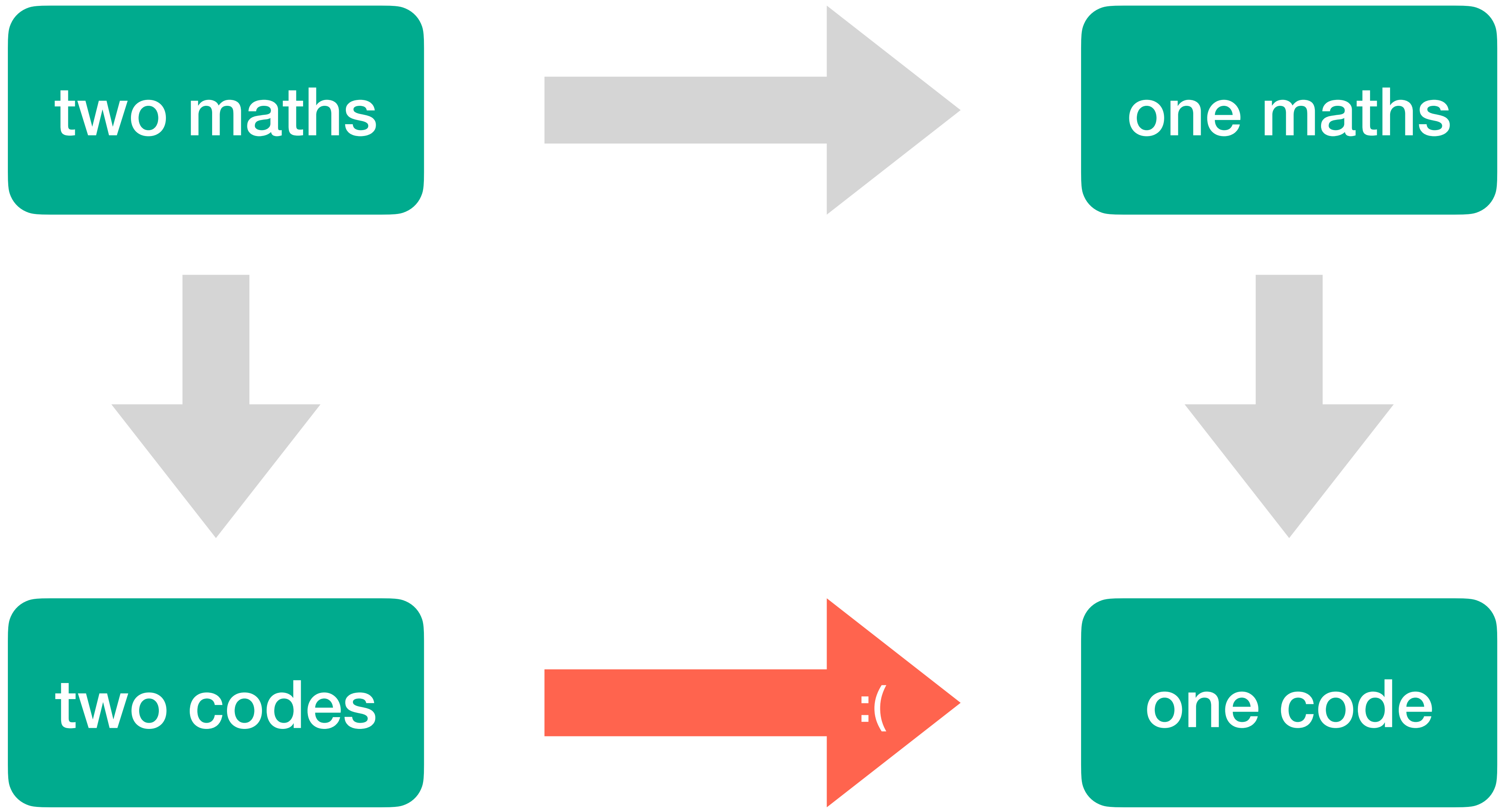
is sometimes harder than just doing two things at once

- Multiphysics is *the simultaneous simulation of different physical aspects of a single system*
- Example: **conjugate convective heat transfer**
  - a solid body sitting inside a moving fluid, to which we introduce a heat source
  - heat transfer is modelled by e.g. the Laplace equation
  - fluid convection is modelled by e.g. Navier–Stokes and energy equations
  - but these two physical phenomena *interact*

Doing two things at once

is sometimes harder than just doing two things at once

- The problem is that ODE/PDE solvers are often ad hoc and "just code"
  - *the colimit of solvers is not a solver for the colimit of the problems*
- This is the **practical** motivation for the paper



Doing two things at once

is sometimes harder than just doing two things at once

- **Analytic reduction**
  - Sometimes multiphysics problems can be reduced “purely formally”
  - … *sometimes*
  - *The problem of heat exchange between two fluid streams in boundary layer flow separated by a flat plate is considered. A general analysis applicable to cocurrent or countercurrent, laminar or turbulent flow is presented. An exact solution for the temperature distribution and the heat transfer along the plate is obtained* ***for the special case of constant property, cocurrent, inviscid flow****.* (DOI:10.1016/0017-9310(71)90180-3)

Doing two things at once

is sometimes harder than just doing two things at once

- **Naive numerical method**
  - Solving just for the body (resp. just for the fluid) gives a boundary condition for the fluid (resp. for the body)
  - Guess some initial boundary conditions, and use to solve for one part, then use the solution to solve for the other part, giving new boundary conditions, and… iterate
  - Problem: rate of convergence depends on initial guess, and there is no systematic way beyond trial and error

Doing two things at once

is sometimes harder than just doing two things at once

- **Category theory**
  - … just use a limit or something?

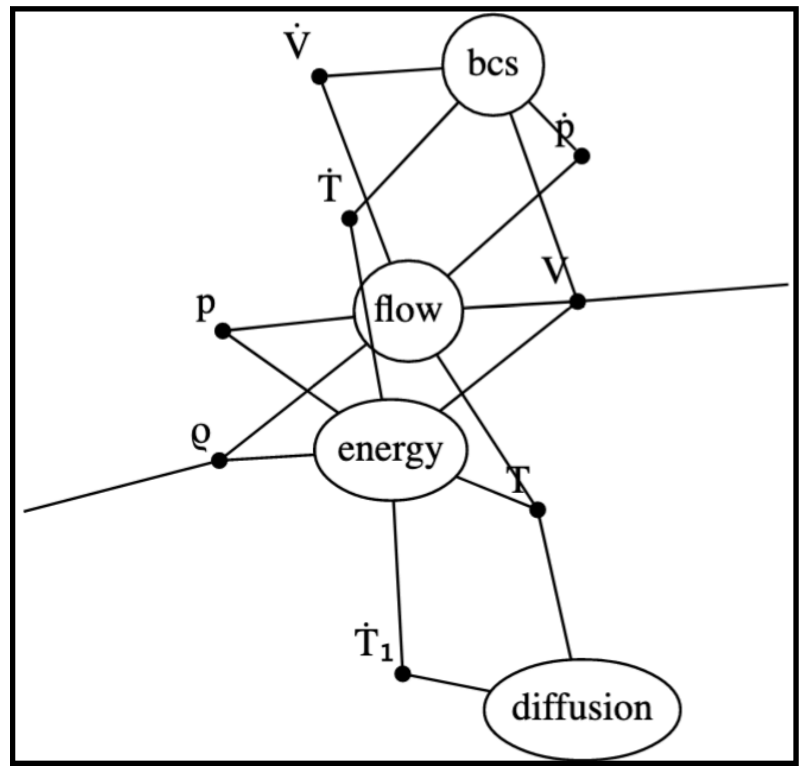
Doing two things at once

is sometimes harder than just doing two things at once

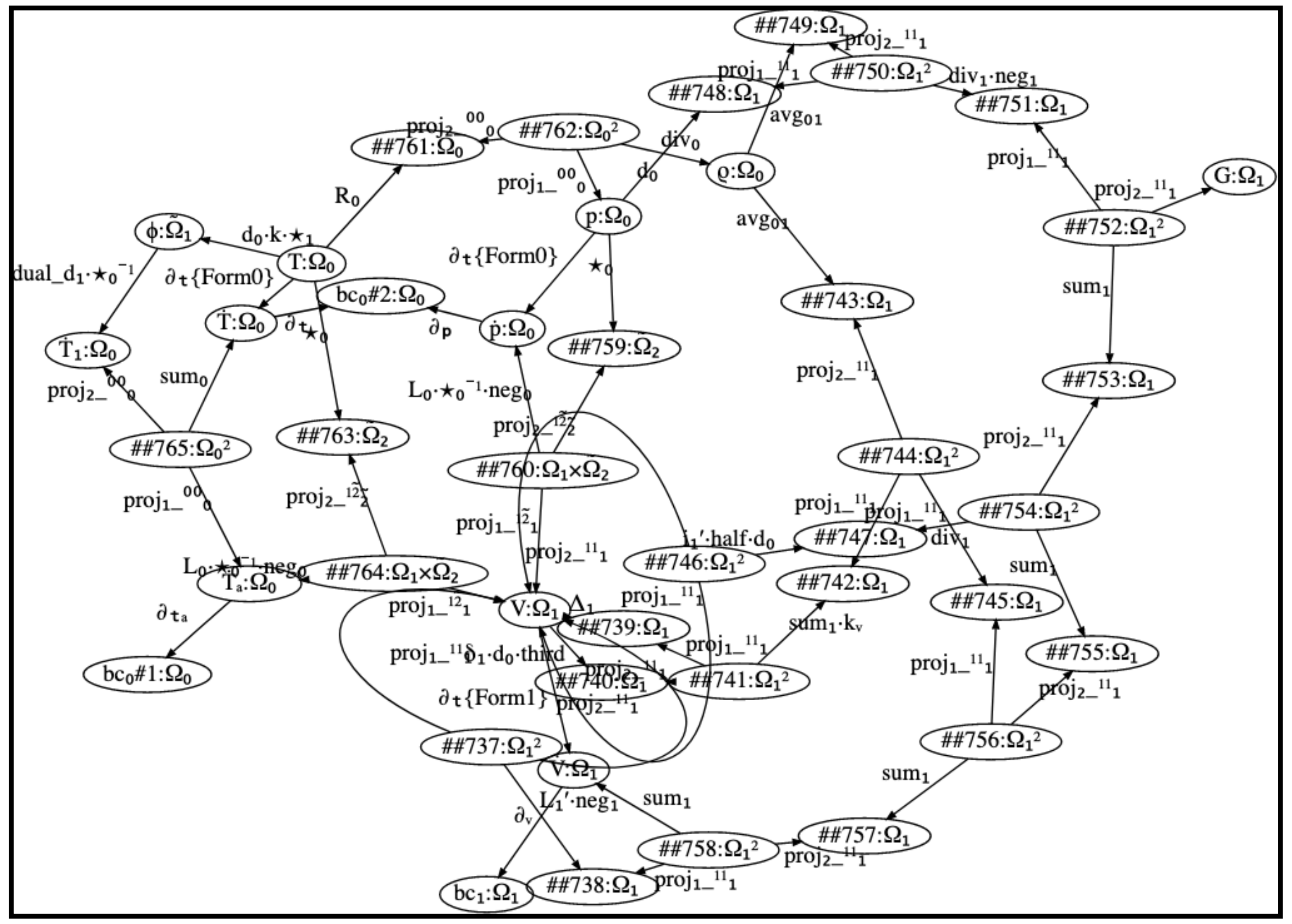
- We will see that limits (e.g. equalisers) are too blunt
    - they give *universal* solutions, whereas we care about *specific* solutions
    - also force us to work in sufficiently nice categories (e.g. diffeologies instead of smooth manifolds)
- This is the **theoretical** motivation for the paper

Multiphysics simulation with Decapodes.jl

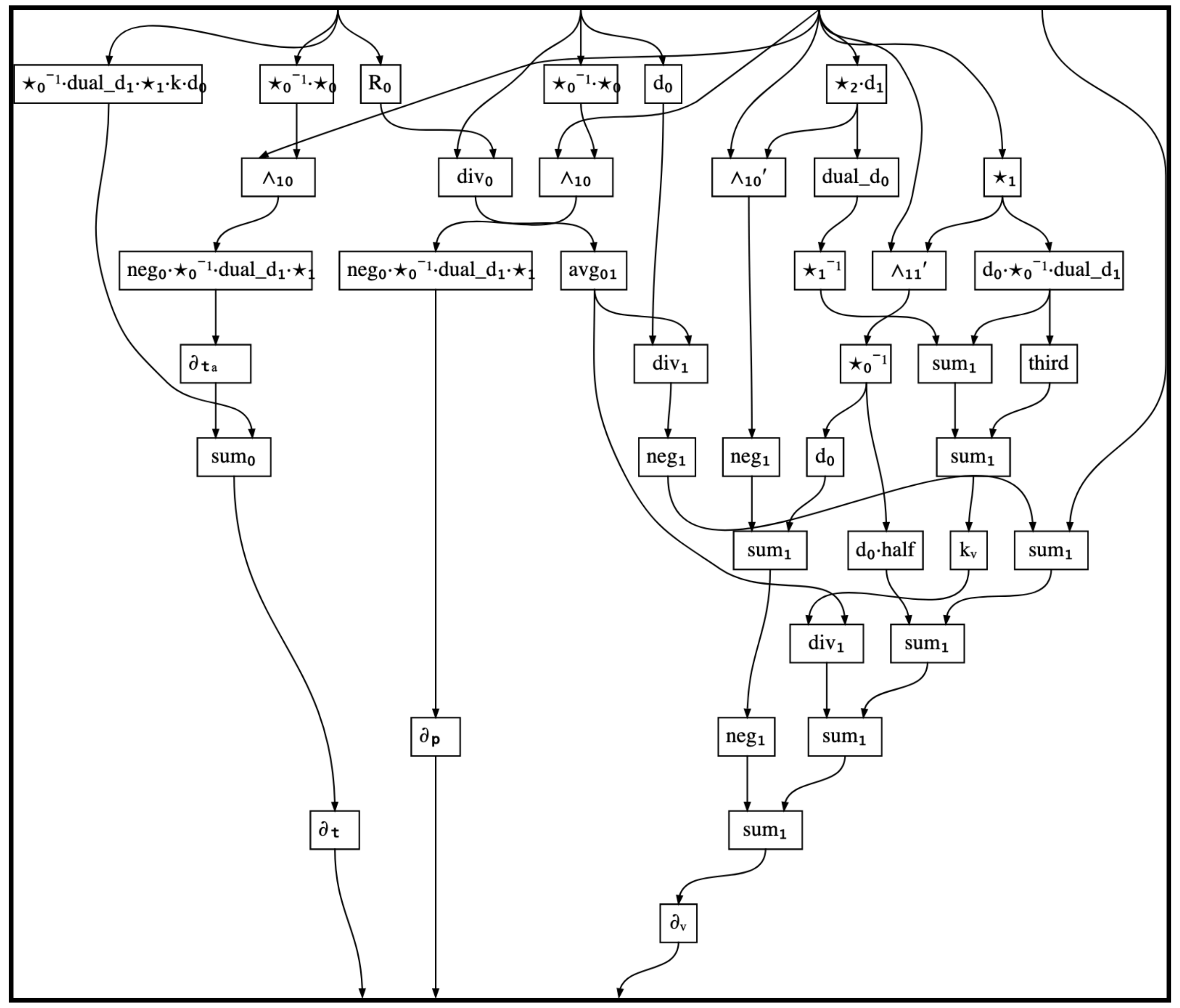
All the stuff I’m going to talk about has *actually been implemented*



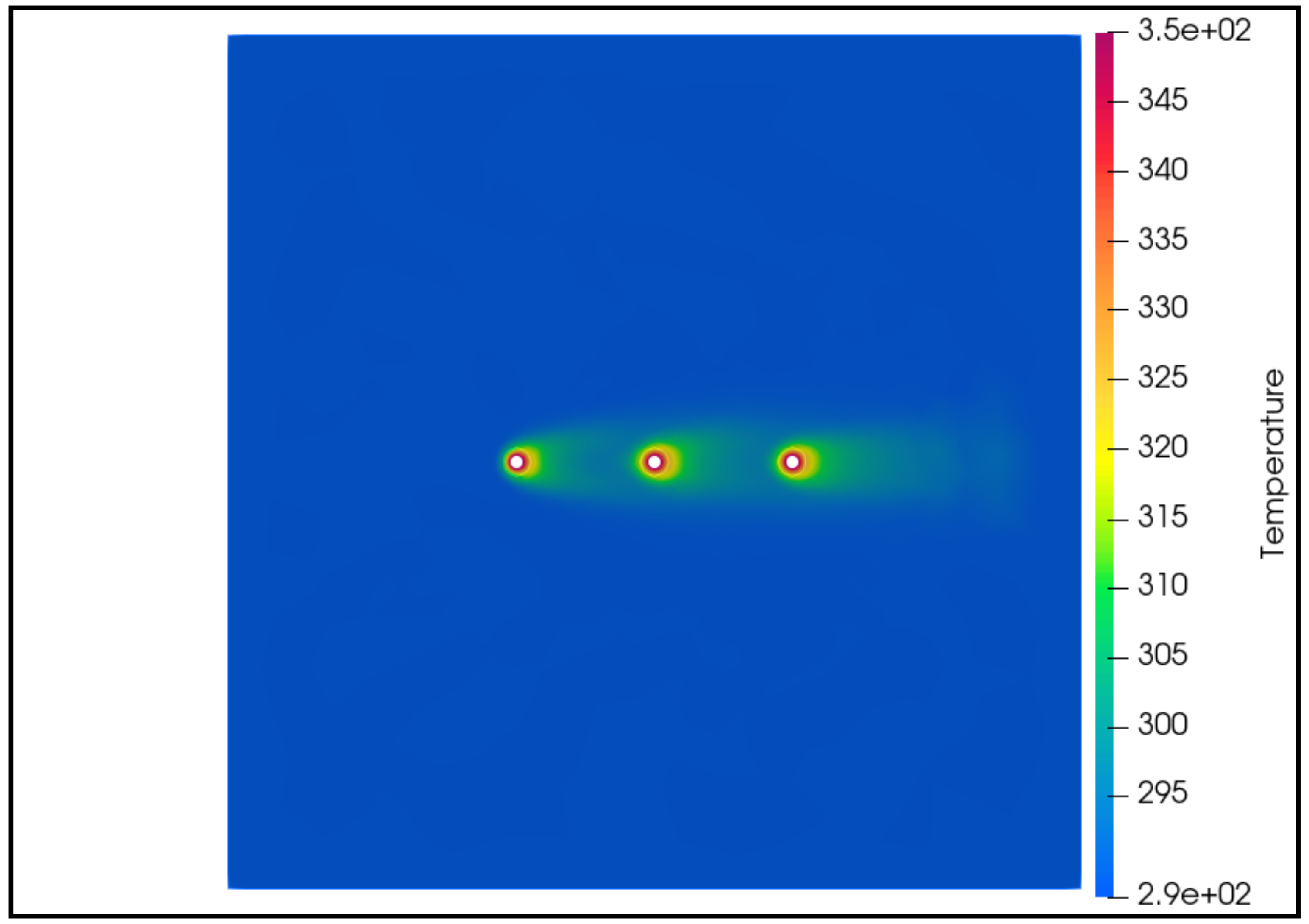
1. Theory



2. Equations



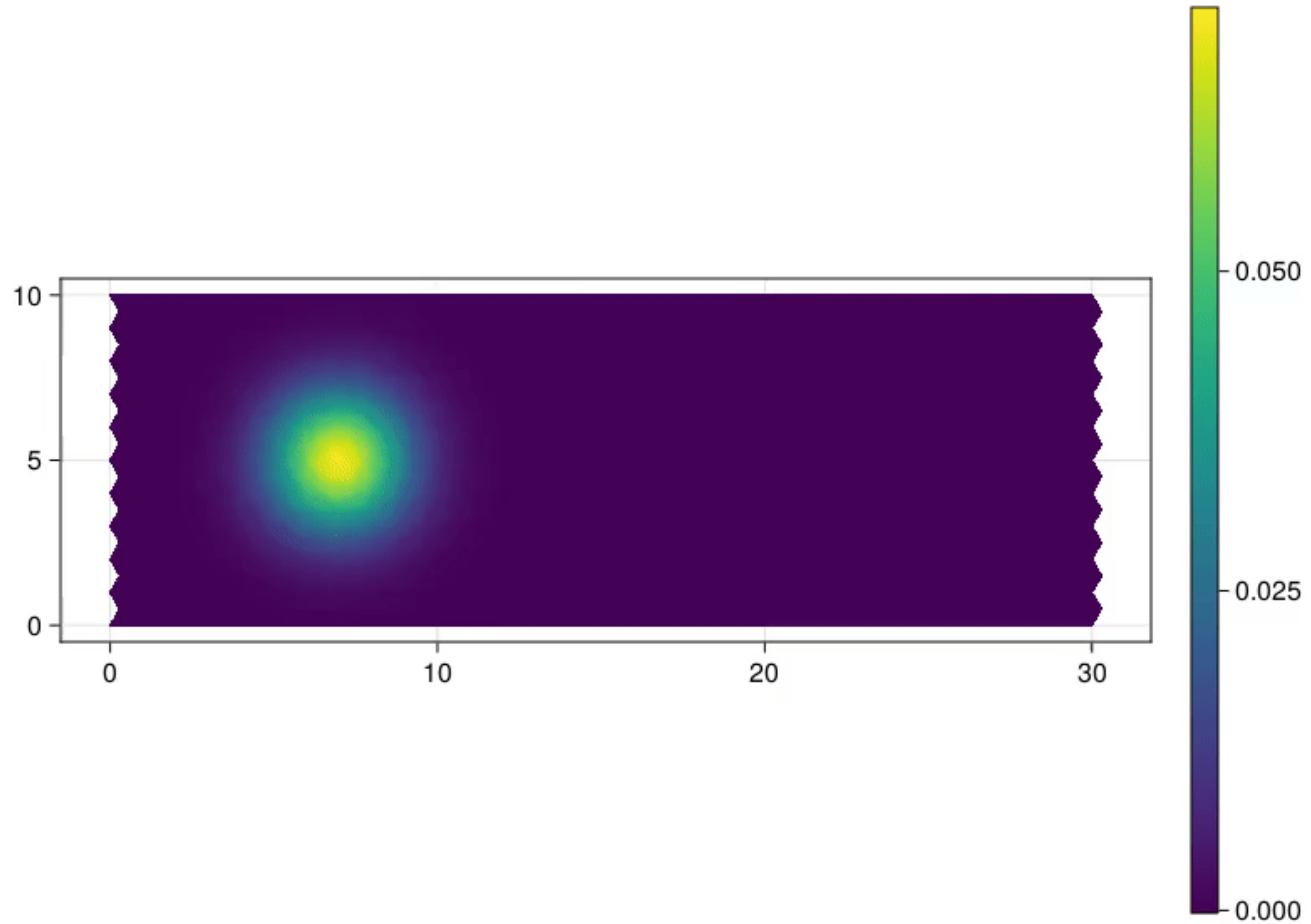
3. Implementation



4.Solution

Multiphysics simulation with Decapodes.jl

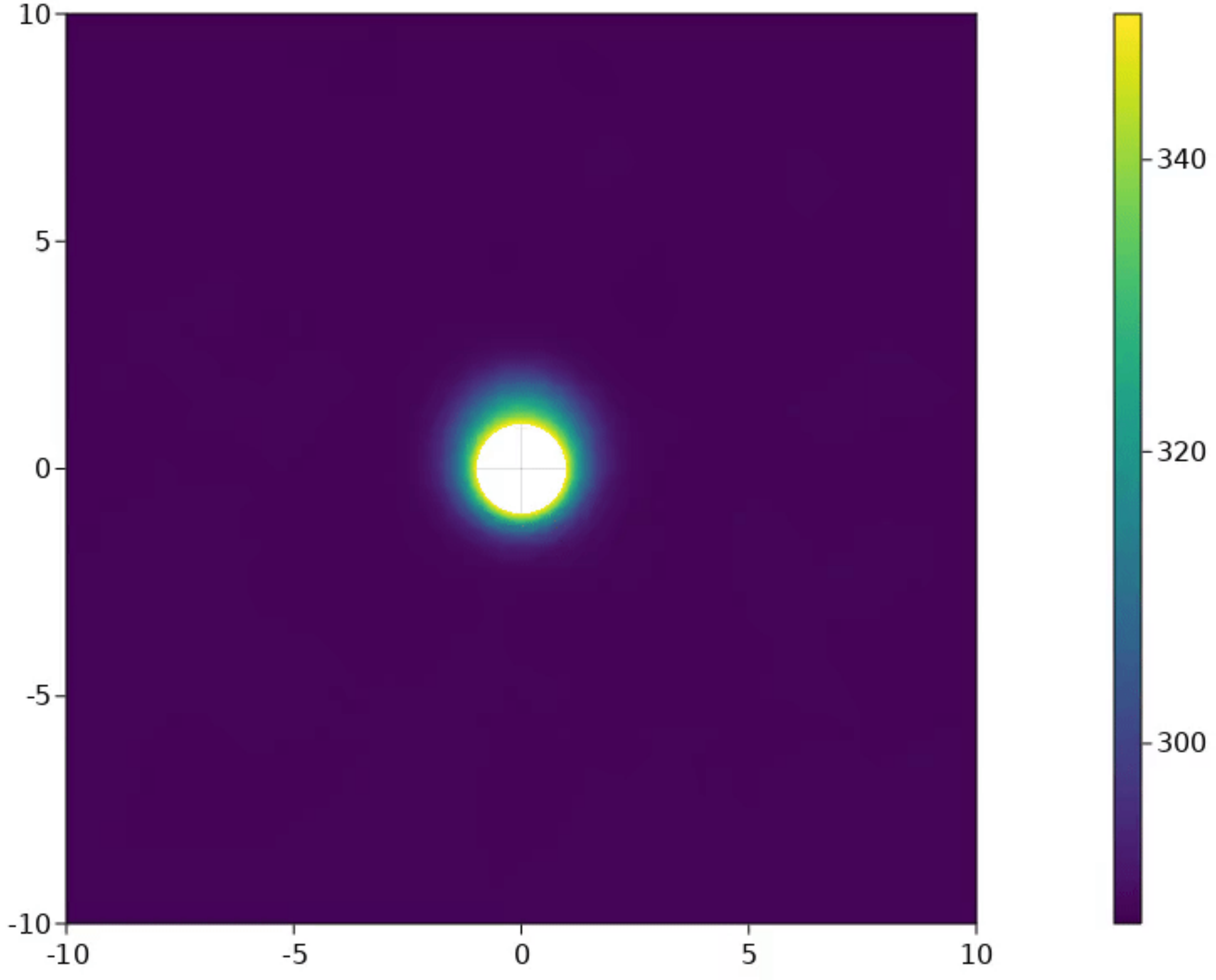
All the stuff I'm going to talk about has *actually been implemented*



Diffusion advection on a torus

Multiphysics simulation with Decapodes.jl

All the stuff I'm going to talk about has *actually been implemented*



Heated rod with fluid flow, ideal gas, and gravity

2. Can we do multiphysics "compositionally"?

Constituent components of diffusion

Understanding equations as conjunctions of principles

- Diffusion of a substance on a 3-manifold is governed by physical quantities
    - concentration $C \in \Omega_t^0$
    - (negative) diffusion flux $\phi \in \widetilde{\Omega}_t^2$
    - diffusivity $k \in \Omega^0$
- … which satisfy
    - $\partial_t C = \star\, \mathrm{d}\phi = \star\, \mathrm{d}(k\star)\mathrm{d}C$

Constituent components of diffusion

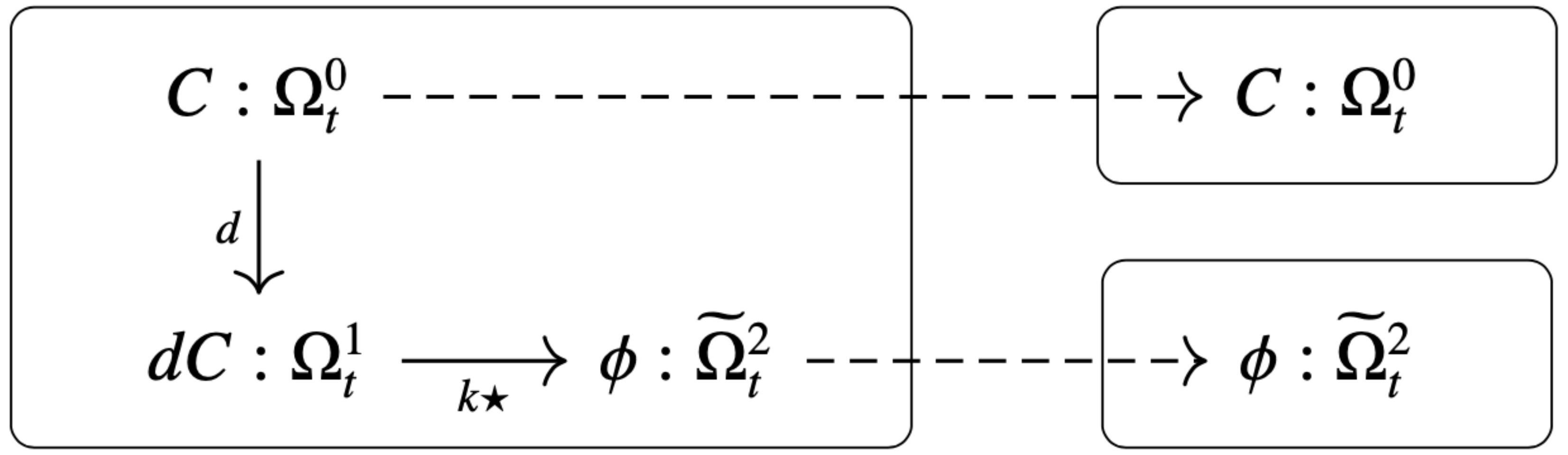
Understanding equations as conjunctions of principles

- $\partial_t C = \star\, \mathrm{d}\phi = \star\, \mathrm{d}(k\star)\mathrm{d}C$
- This is really the conjunction of two physical principles:
  - **Fick's first law**: $\phi = k \star \mathrm{d}C$
  - **Conservation of mass**: $\partial_t C = \star\, \mathrm{d}\phi$
- Informally, both of these give us holes in which we can plug the same two variables: C and ϕ
- We can formalise this using **decorated multispans** and **undirected wiring diagrams**

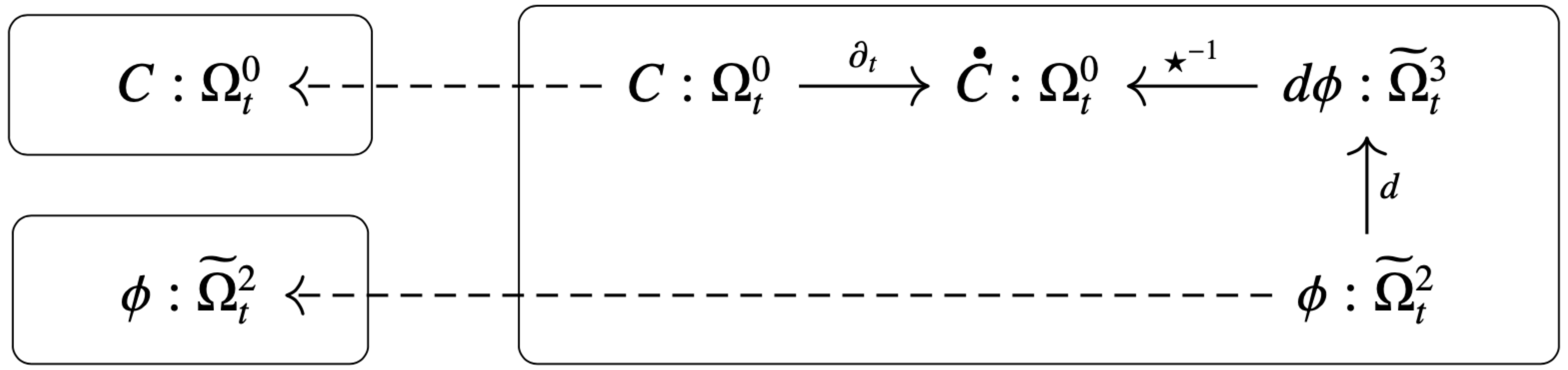
Constituent components of diffusion

Understanding equations as conjunctions of principles

Decorated multispans (components)

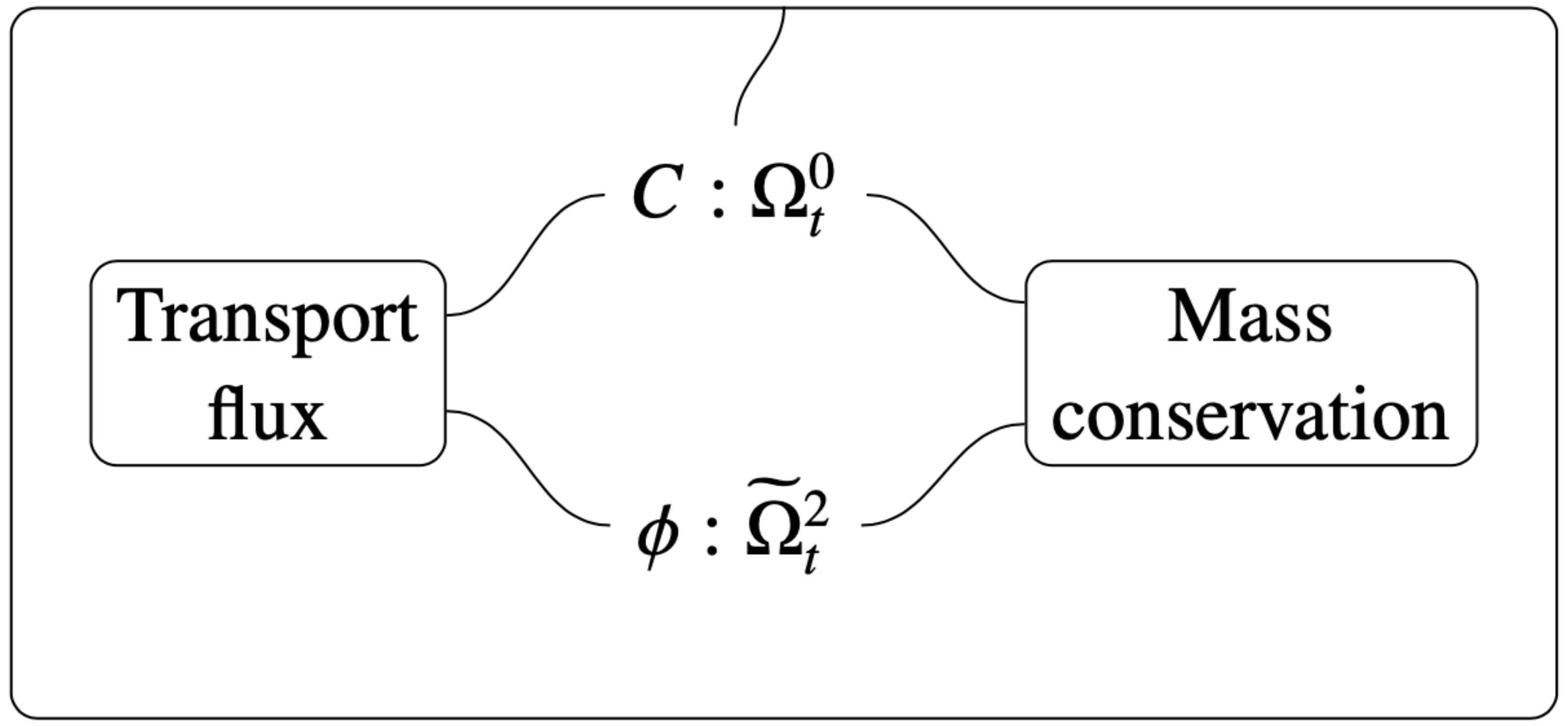


Fick's first law



Conservation of mass

UWD (schema)



Composition pattern for diffusion

Constituent components of diffusion

Understanding equations as conjunctions of principles

- Now we can extend or replace *individual components*

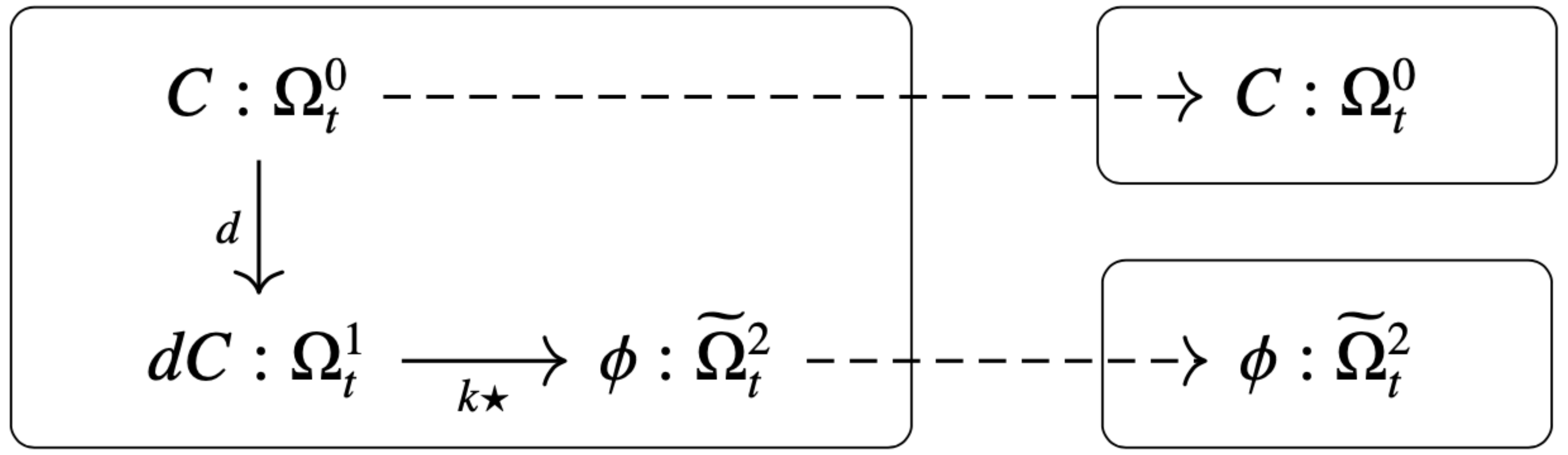
- E.g. to describe advection instead of diffusion, we can just plug a different diagram into the “Transport flux” box: replace Fick’s first law with one that describes flux due to advection along a moving field

$$
\begin{array}{ccc}
C : \Omega^0_t & \xrightarrow{\;\star\;} & \widetilde{C} : \widetilde{\Omega}^3_t \\
 & & \big\downarrow{\scriptstyle -\iota_{\mathbf{v}}} \\
 & & \phi : \widetilde{\Omega}^2_t
\end{array}
$$

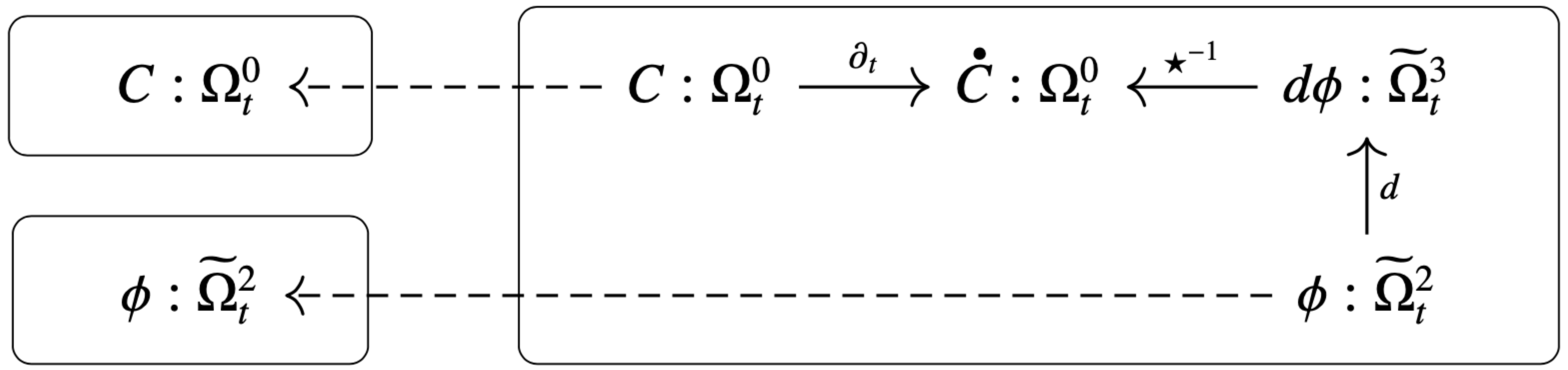
Constituent components of diffusion

Understanding equations as conjunctions of principles

Multispans (components)

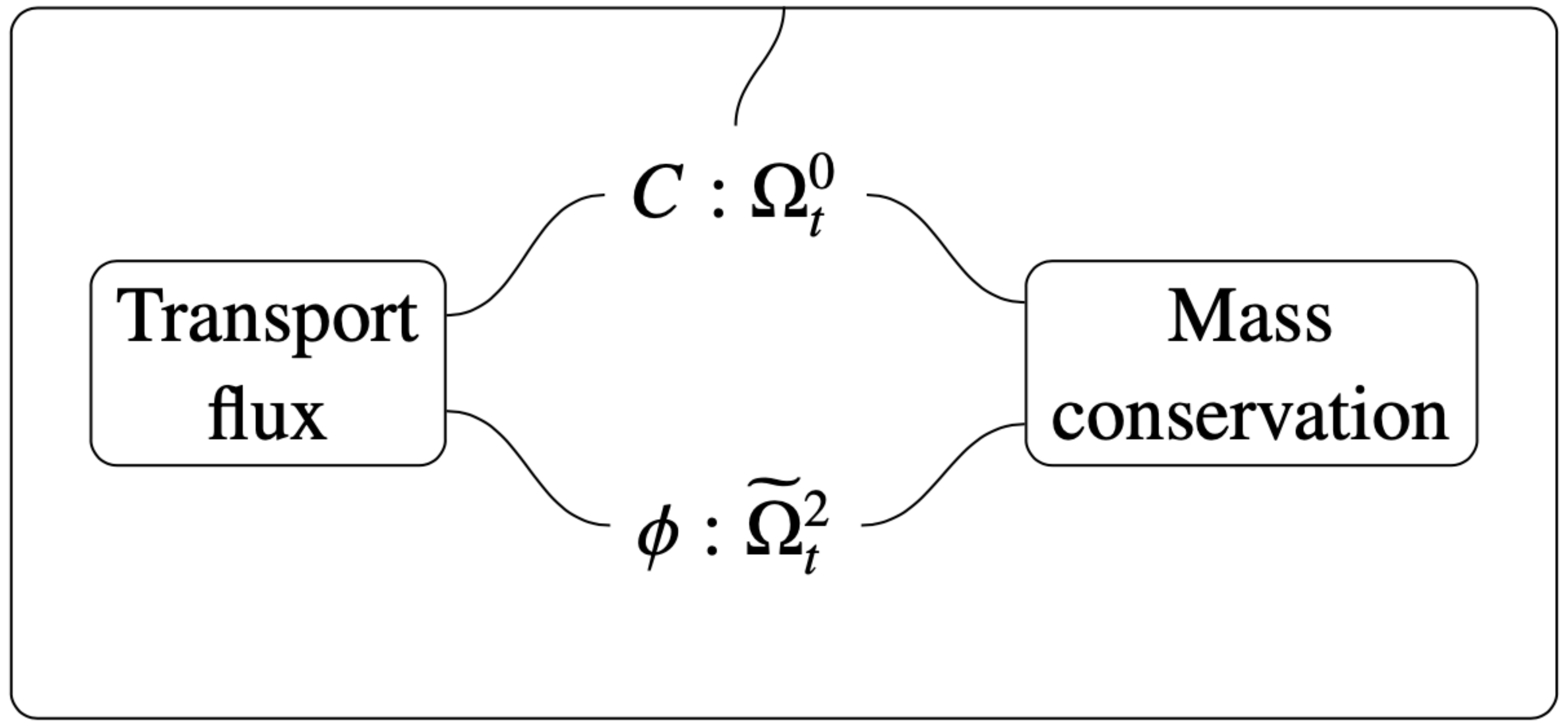


Fick's first law



Conservation of mass

UWD (schema)

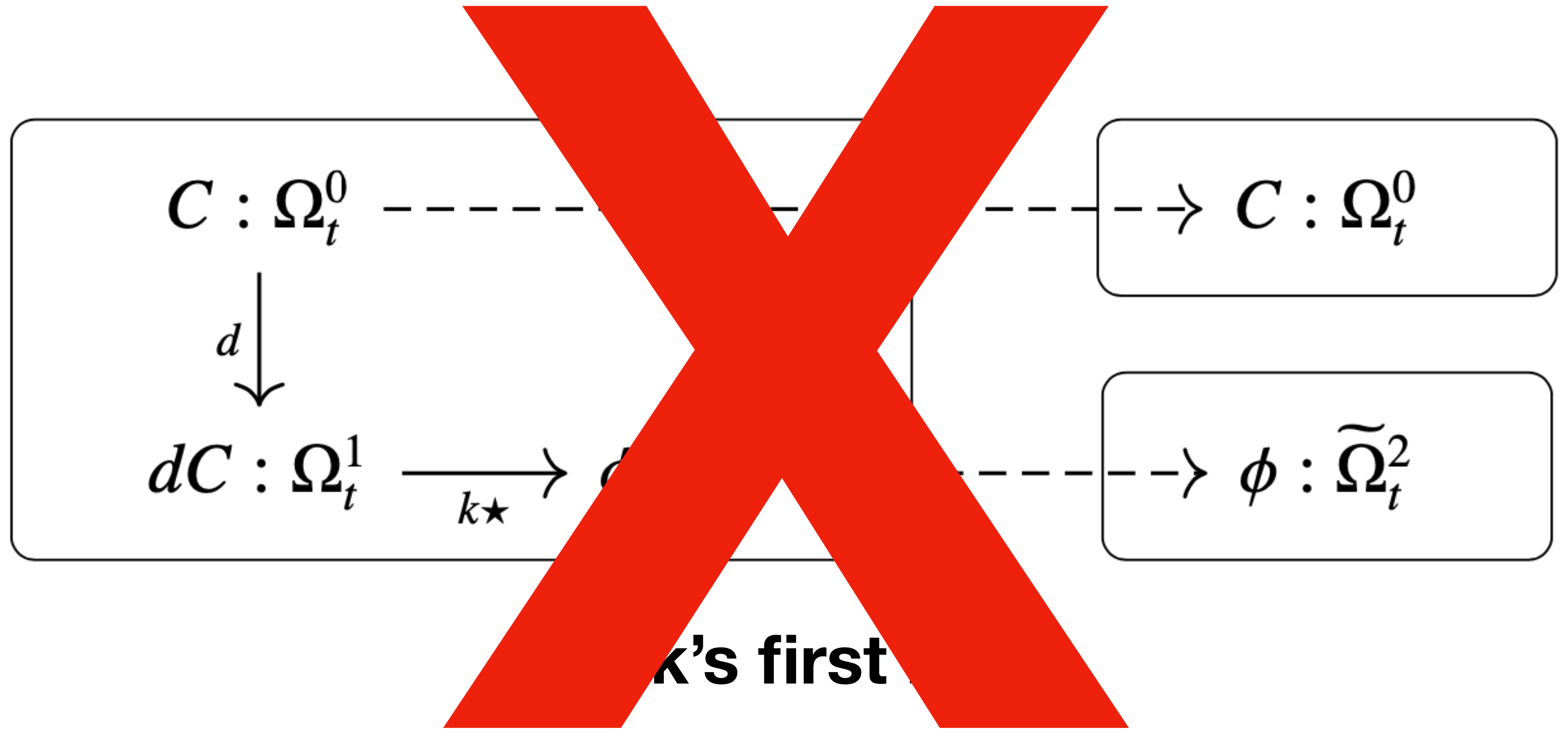


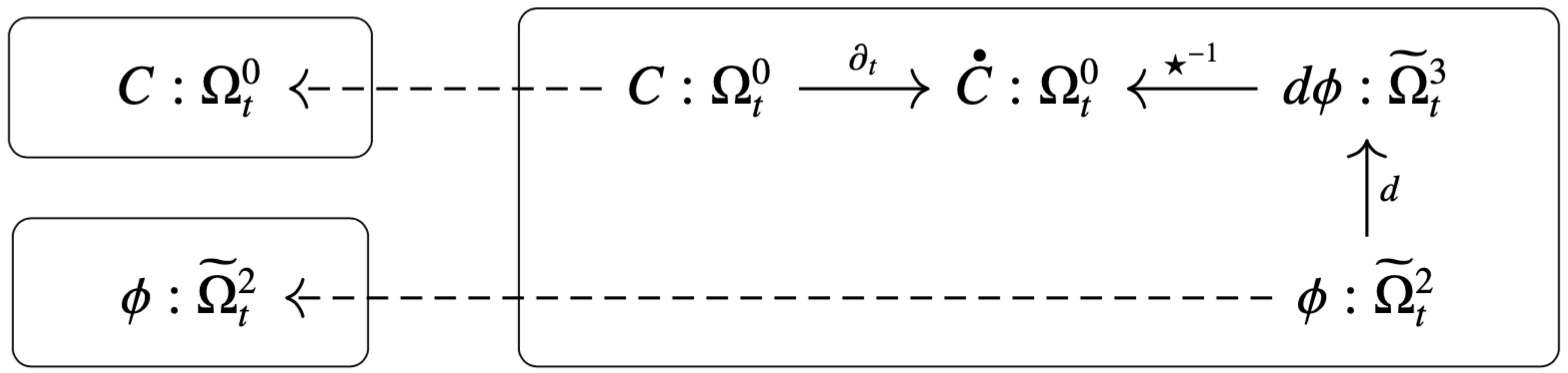
Composition pattern for diffusion

Constituent components of diffusion

Understanding equations as conjunctions of principles

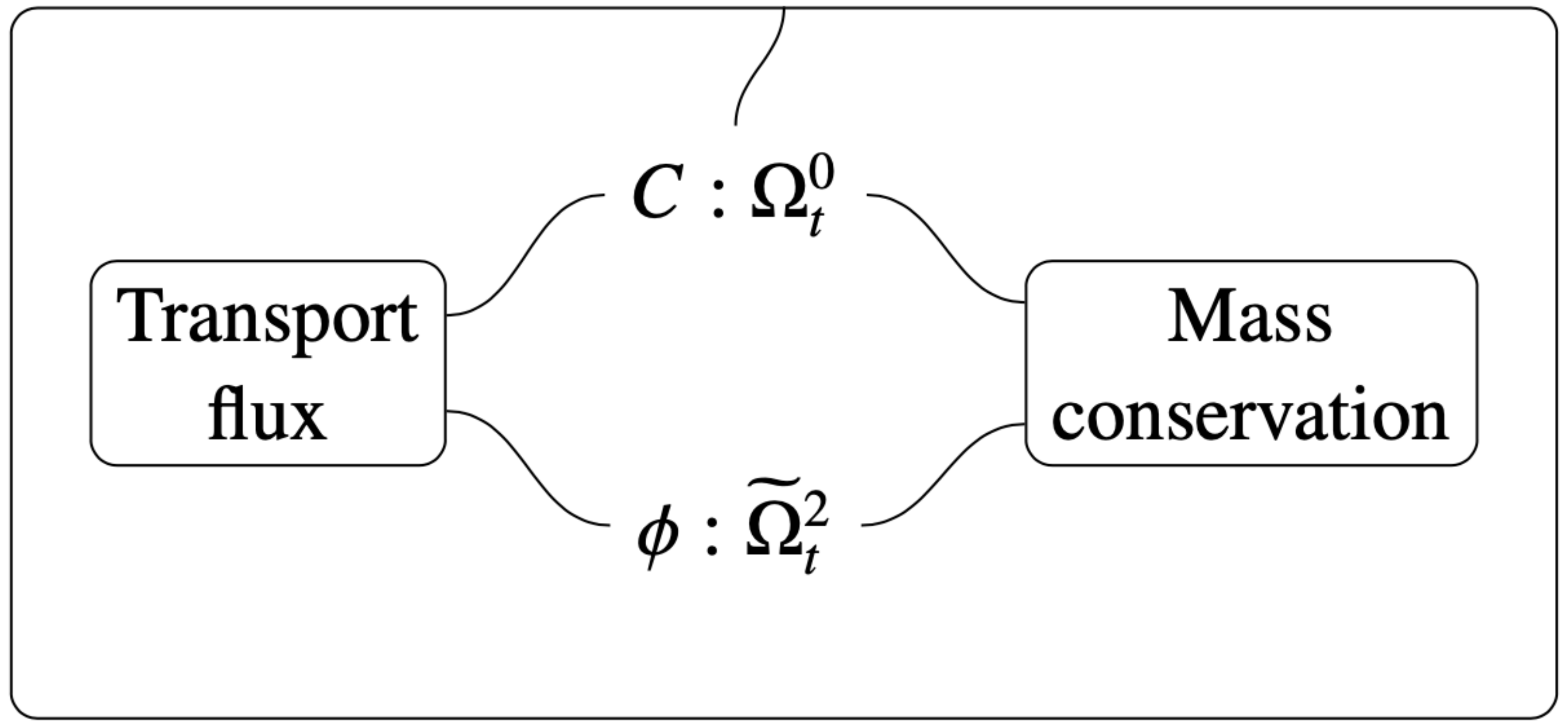
Multispans (components)





Conservation of mass

UWD (schema)

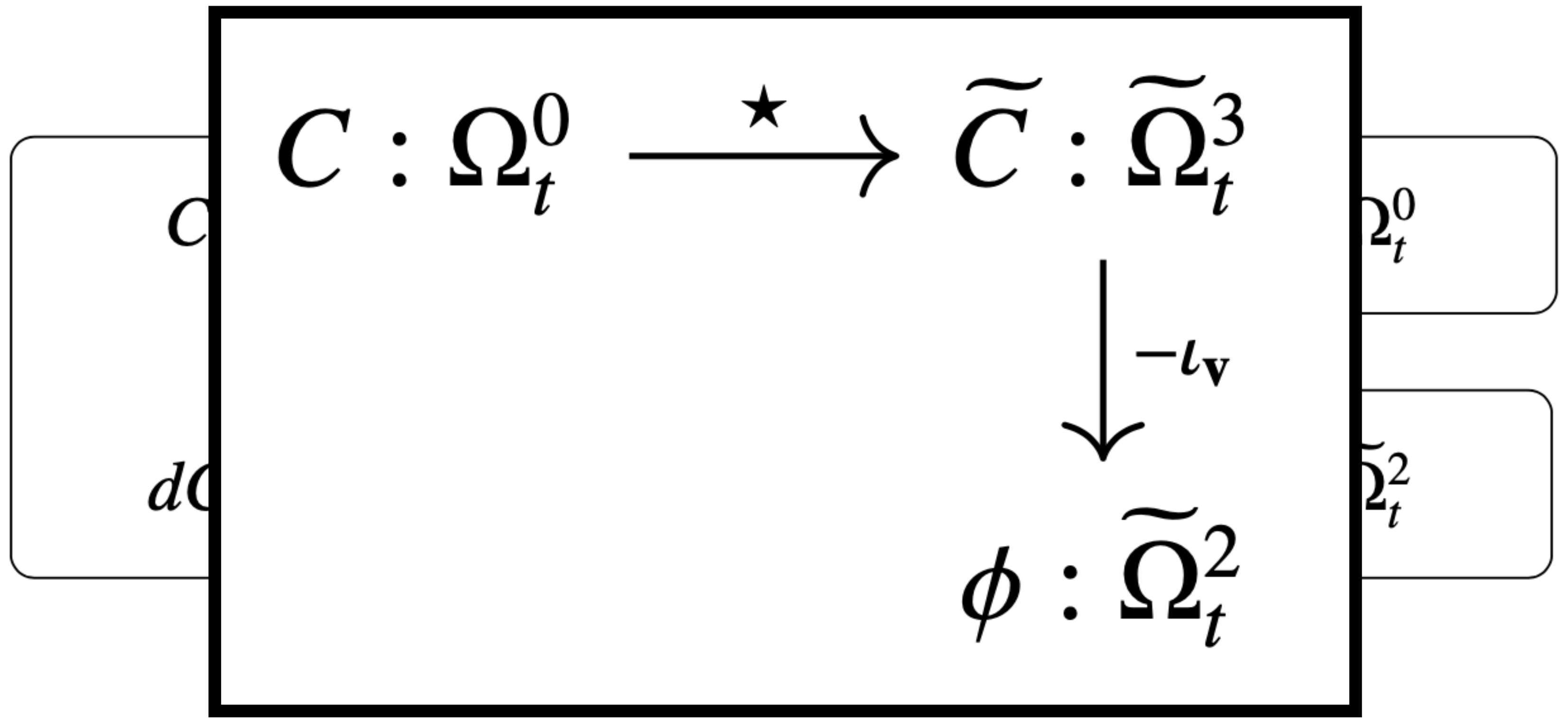


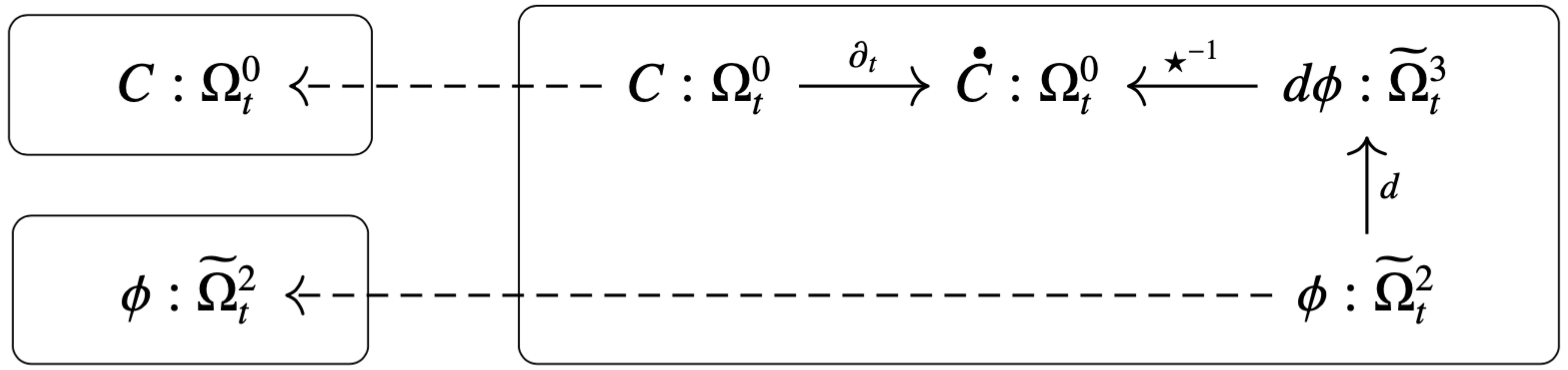
Composition pattern for diffusion

Constituent components of diffusion

Understanding equations as conjunctions of principles

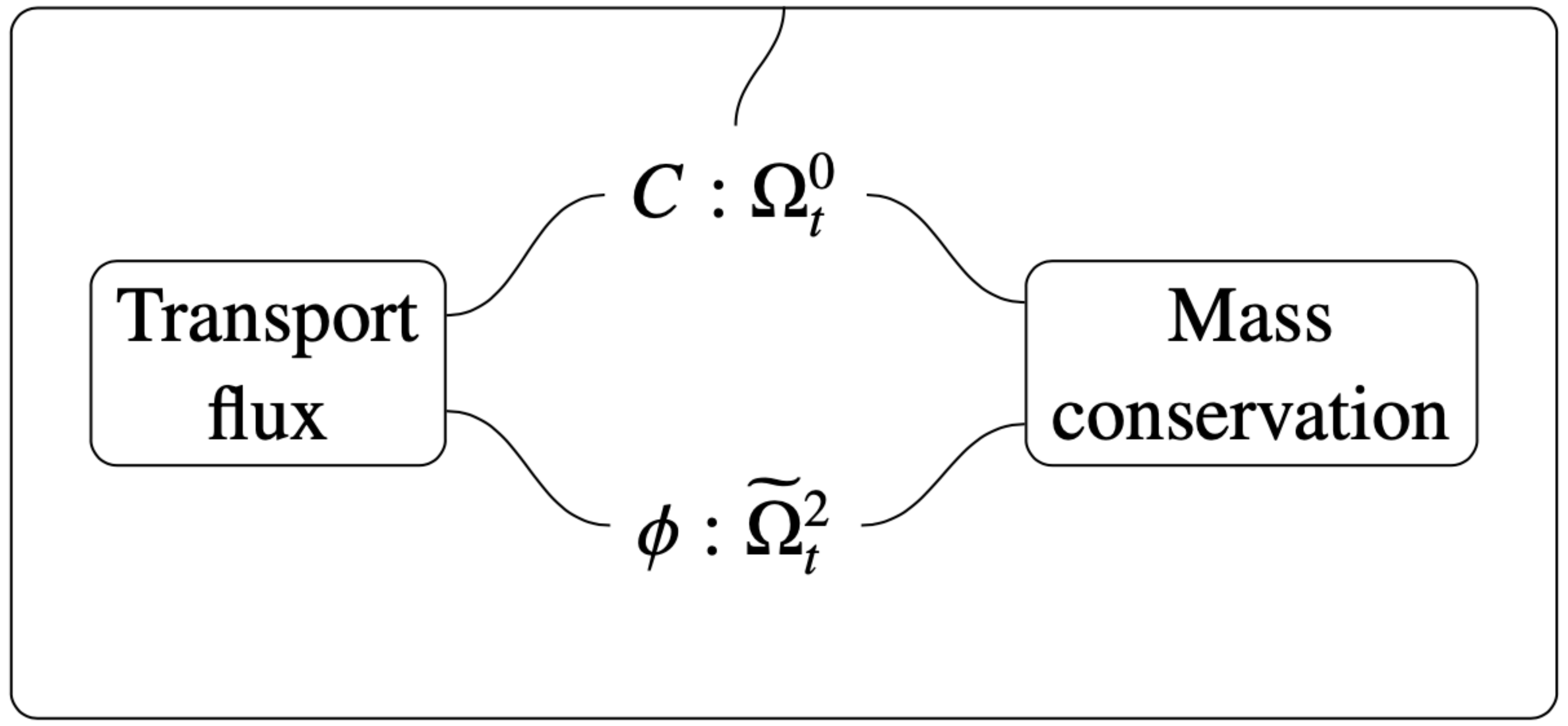
Multispans (components)





Conservation of mass

UWD (schema)

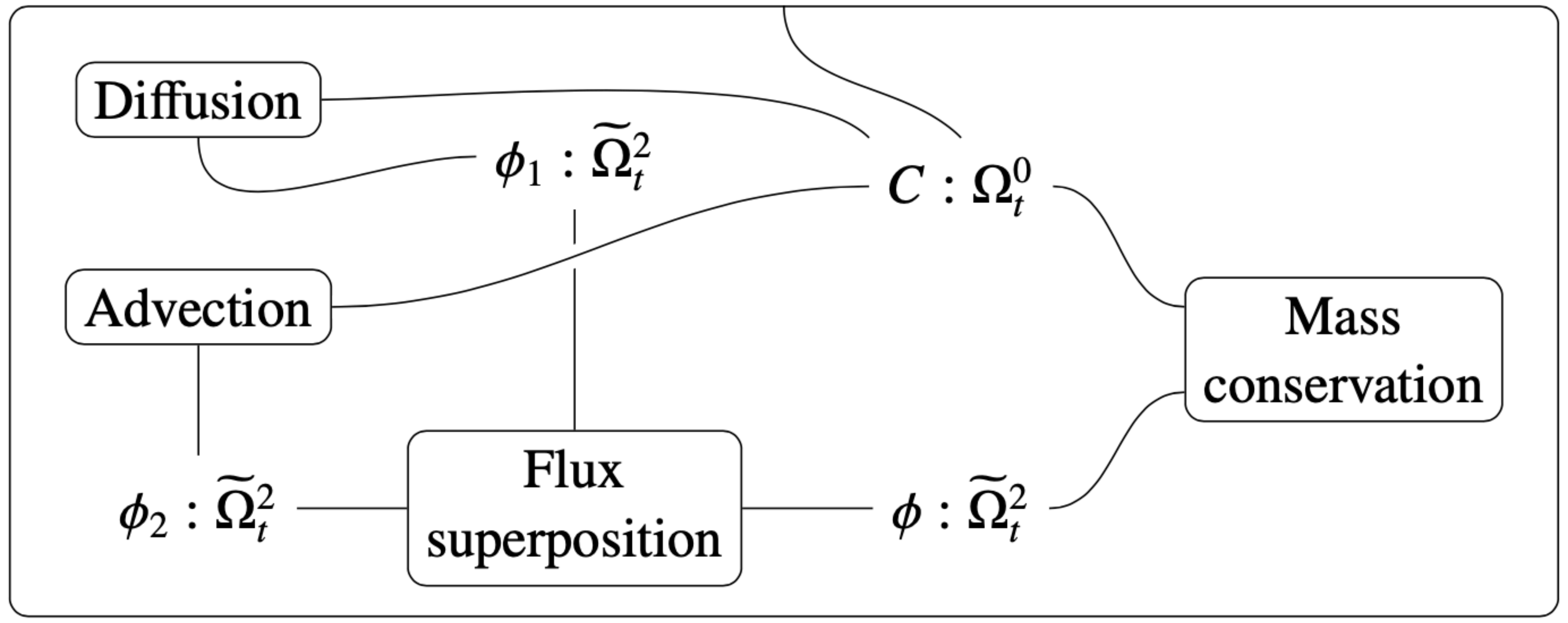


Composition pattern for diffusion

Constituent components of diffusion

Understanding equations as conjunctions of principles

- This modularity is really also *hierarchicality* [sic]
- *Two levels*: combine diffusion with advection by operadic composition of UWDs



Composition pattern for advection-diffusion

- *Three levels*: advection-diffusion-reaction
- *More levels*: operad!

3. What are the building blocks?

Maxwell’s house

The general philosophy of “Tonti diagrams”

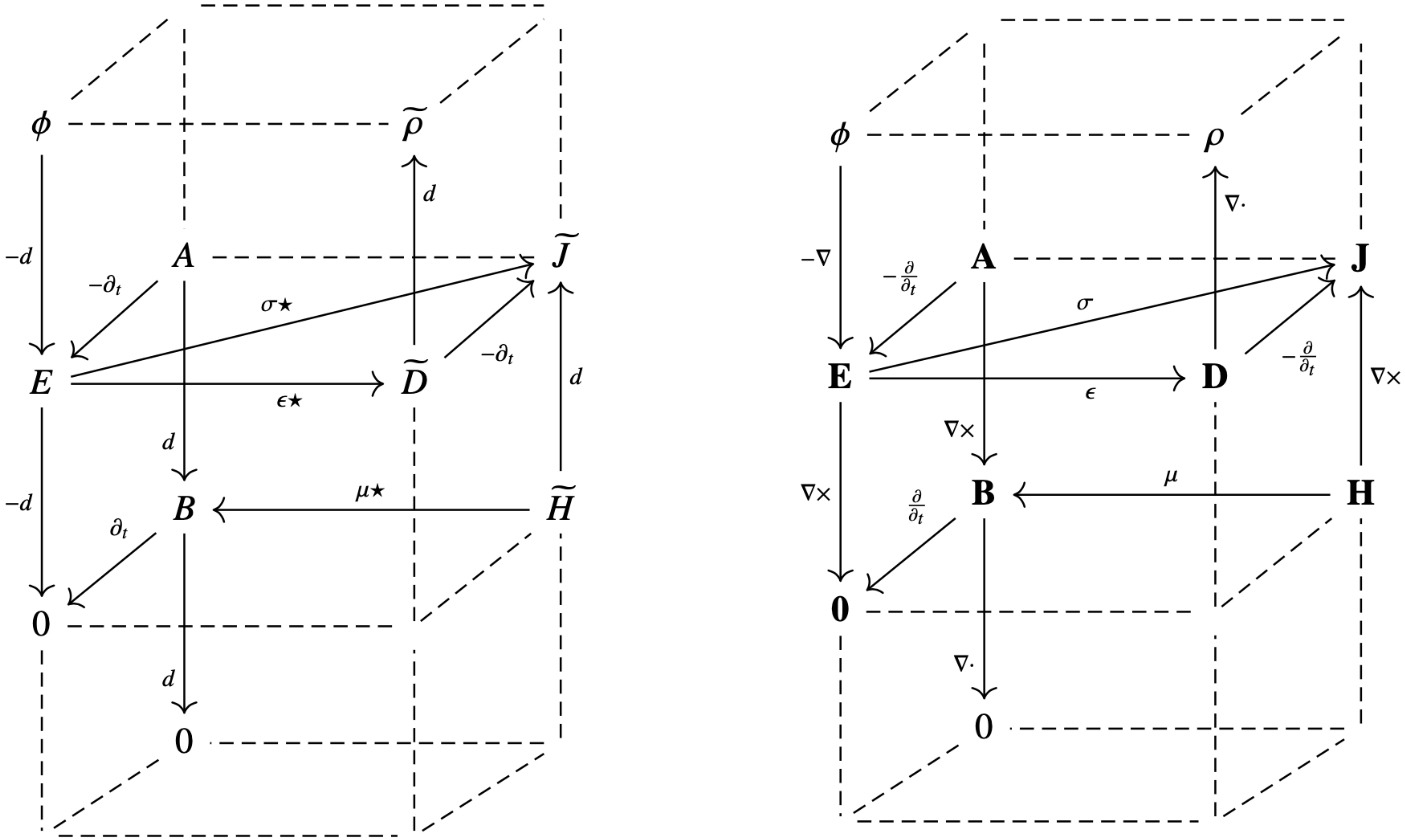
- The main idea: an arrow

$$x \xrightarrow{f} y$$

asserts the equation

$$f(x) = y$$

- The main problem: inconsistent & informal conventions, even within a single diagram



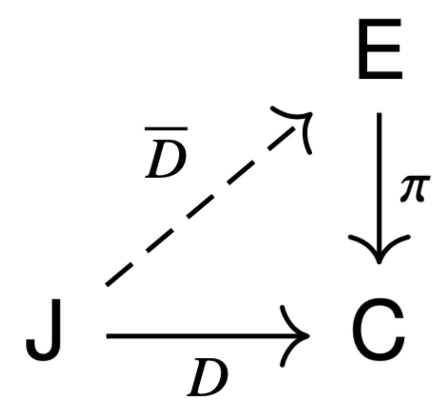
Left: exterior calculus, from Bossavit
Right: vector calculus, from Cortes Garcia et al.

4. Are these building blocks good enough?

Diagrams, formally

Three definitions

- A **diagram** in a category $\mathscr{C}$ is a functor $D\colon \mathscr{J} \to \mathscr{C}$ where the **shape** $\mathscr{J}$ is a small category
  - for our purposes, $\mathscr{C}$ is usually some category of "geometric sheaves" on a space, e.g. wedge products of the (co)tangent bundle of a manifold (so sections are differential forms and vector fields)
- Given a category $\mathscr{C}$ and an object $S \in \mathscr{C}$, the category $\mathsf{El}_S(\mathscr{C})$ of **generalised elements of shape** S is the coslice category $\mathsf{El}_S(\mathscr{C}) = S/\mathscr{C}$
- A **lift** of a diagram $D\colon \mathscr{J} \to \mathscr{C}$ through a functor $\pi\colon \mathscr{E} \to \mathscr{C}$ is a functor $\overline{D}\colon \mathscr{J} \to \mathscr{E}$ such that $\pi \circ \overline{D} = D$
  - we generally take π to be a discrete opfibration



Solutions

Not limits, but lifts

$$C : \Omega^0_t \underset{k\Delta}{\overset{\partial_t}{\rightrightarrows}} \dot{C} : \Omega^0_t$$

The heat equation: $\dfrac{\partial C}{\partial t} = k \nabla C$

- Note that the diagram presenting an equation does ***not*** commute
  - if it did, then this would say that ***everything*** is a solution to the equation!
- Maybe surprisingly, we do ***not*** just take the limit (e.g. equaliser) of a diagram
  - this would give us ***universal*** solutions, but in (P)DEs, we're often just interested in single solutions (by design)
  - (we would also have to leave the categories of classical differential geometry in order for the relevant limits to exist)

Solutions

Not limits, but lifts

$$C : \Omega^0_t \underset{k\Delta}{\overset{\partial_t}{\rightrightarrows}} \dot{C} : \Omega^0_t$$

The heat equation: $\frac{\partial C}{\partial t} = k \nabla C$

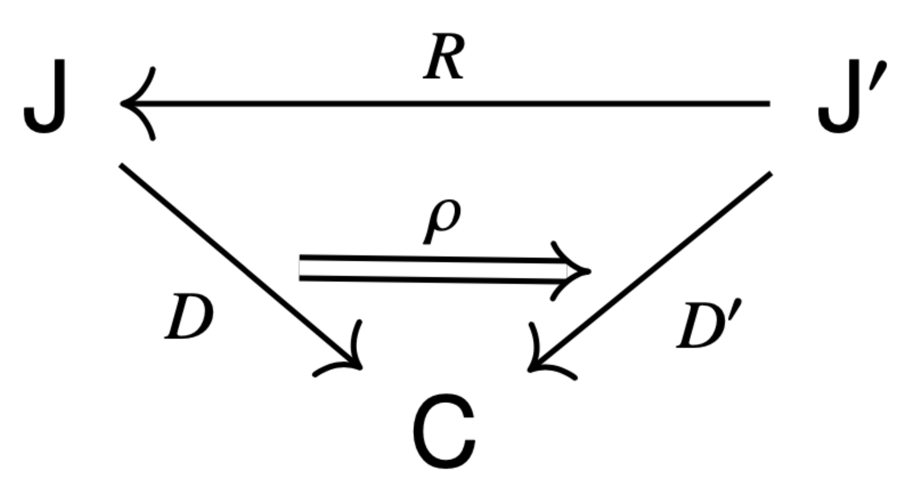
- Instead, *solutions correspond to lifts of the diagram* D *through the codomain functor* $\mathrm{cod}\colon \mathsf{El}_S(\mathscr{C}) \to \mathscr{C}$
    - when working with (P)DEs, we usually take $S = \underline{\mathbb{R}}$ (the constant sheaf of $\mathbb{R}$ on M), since morphisms $\underline{\mathbb{R}} \to \mathscr{F}$ of sheaves (of real vector spaces on M) are in bijection with global sections of $\mathscr{F}$
- Note that we can recover limits from lifts, since a lift through cod is exactly a cone over D with apex S

Morphisms of diagrams

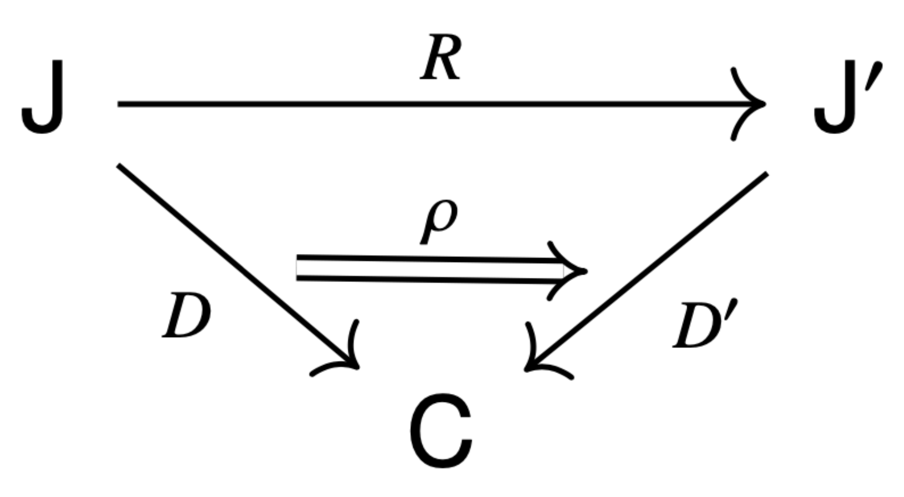
Two constructions

- Given a category $\mathscr{C}$, the **backwards category of diagrams in** $\mathscr{C}$ has objects $(\mathscr{J}, D\colon \mathscr{J} \to \mathscr{C})$ and morphisms $(R\colon \mathscr{J}' \to \mathscr{J}, \rho\colon D \circ R \Rightarrow D')$; the **forwards** category has morphisms $(R\colon \mathscr{J} \to \mathscr{J}', \rho\colon D \Rightarrow D' \circ R)$

cf. Perrone and Tholen



Forwards



Backwards

- If ρ is the identity, then we recover (the opposite of) the slice category $\mathsf{Cat}/\mathscr{C}$
- Morphisms in the *backwards* category send solutions to solutions
  - thus these tend to go in the direction of *increasing generality*, e.g. from static Maxwell–Faraday *with* potentials to static Maxwell–Faraday *without* potentials

Purpose of morphisms

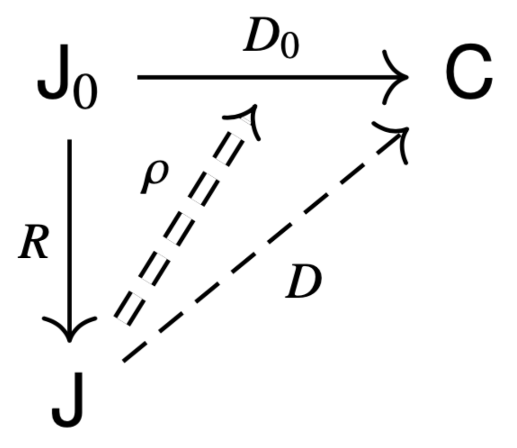
Why care?

- We can use morphisms for a few things, e.g.
  - steady states of diffusion processes
  - different presentations of the same physics (but this is subtle!)
  - boundary (and initial) value problems
    - this is the really nice one!

BVPs (and IVPs)

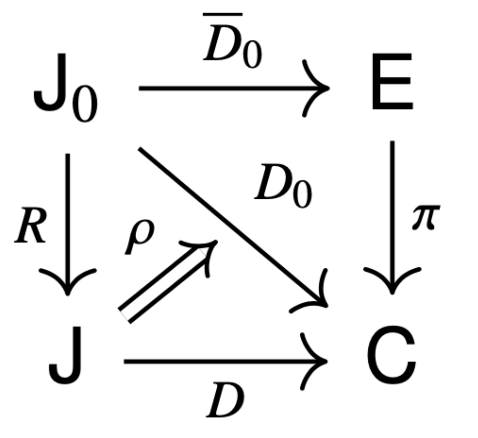
Pretty important for actually solving and modelling stuff

- An **extension** of a diagram $D_0 \colon \mathscr{J}_0 \to \mathscr{C}$ along a functor $R \colon \mathscr{J}_0 \to \mathscr{J}$ is a diagram $D \colon \mathscr{J} \to \mathscr{C}$ and a (backwards) morphism $(R, \rho) \colon (\mathscr{J}, D) \to (\mathscr{J}_0, D_0)$

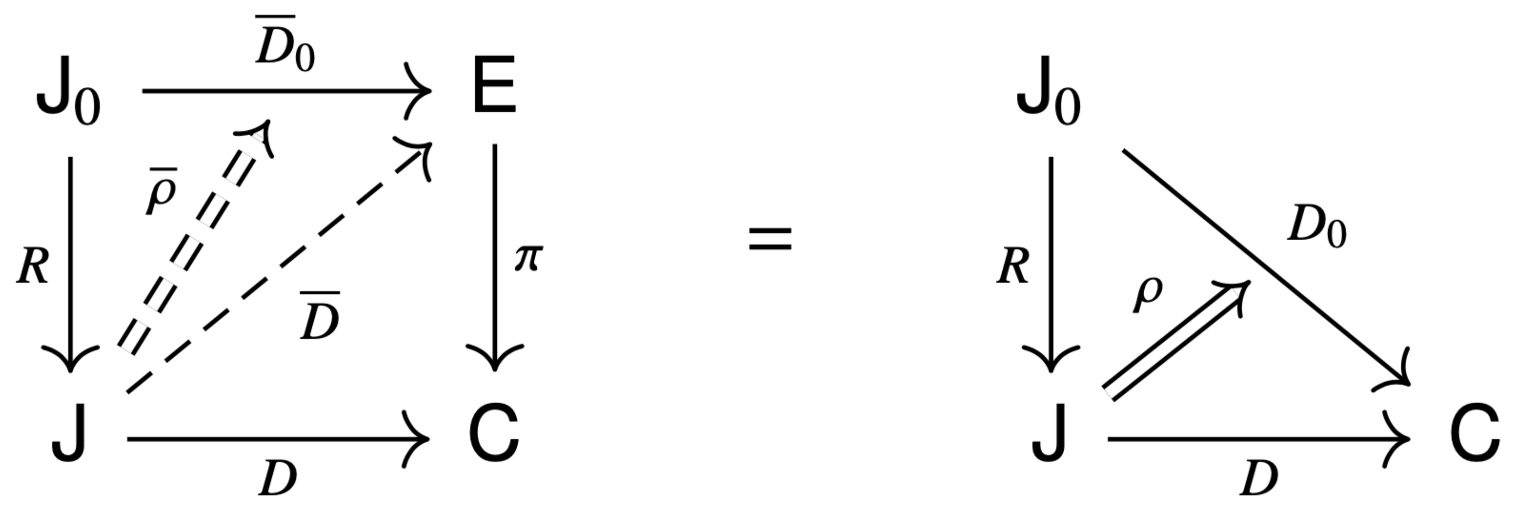


- Given

    1. an extension of D_0 along R
    2. a lift $\overline{D_0}$ of D_0 through some functor $\pi \colon \mathscr{E} \to \mathscr{C}$



the **extension lifting problem** is to find an extension $(R, \overline{\rho}) \colon (\mathscr{J}, \overline{D}) \to (\mathscr{J}_0, \overline{D_0})$ of $\overline{D_0}$ along R such that $\overline{D}$ is a lift of D through π in a "2-compatible way"



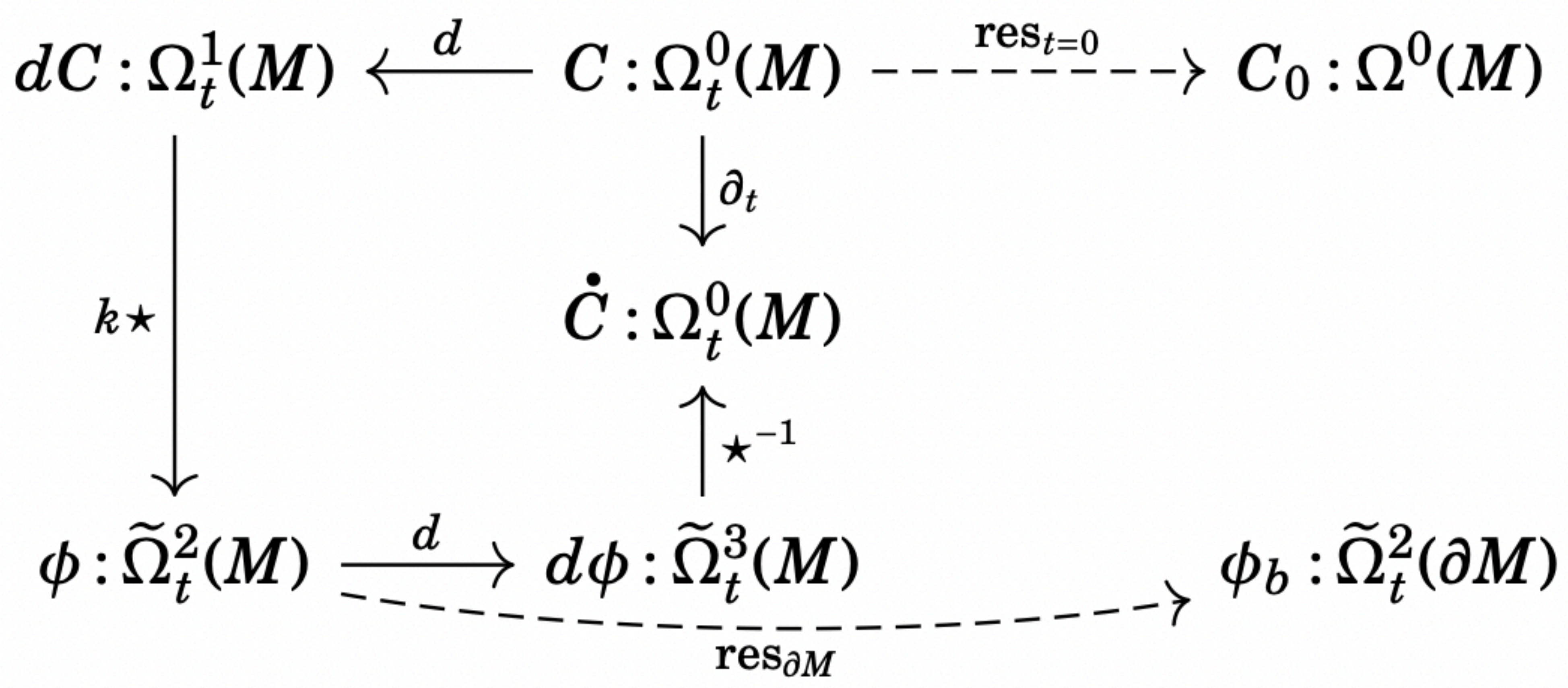
BVPs (and IVPs)

Pretty important for actually solving and modelling stuff

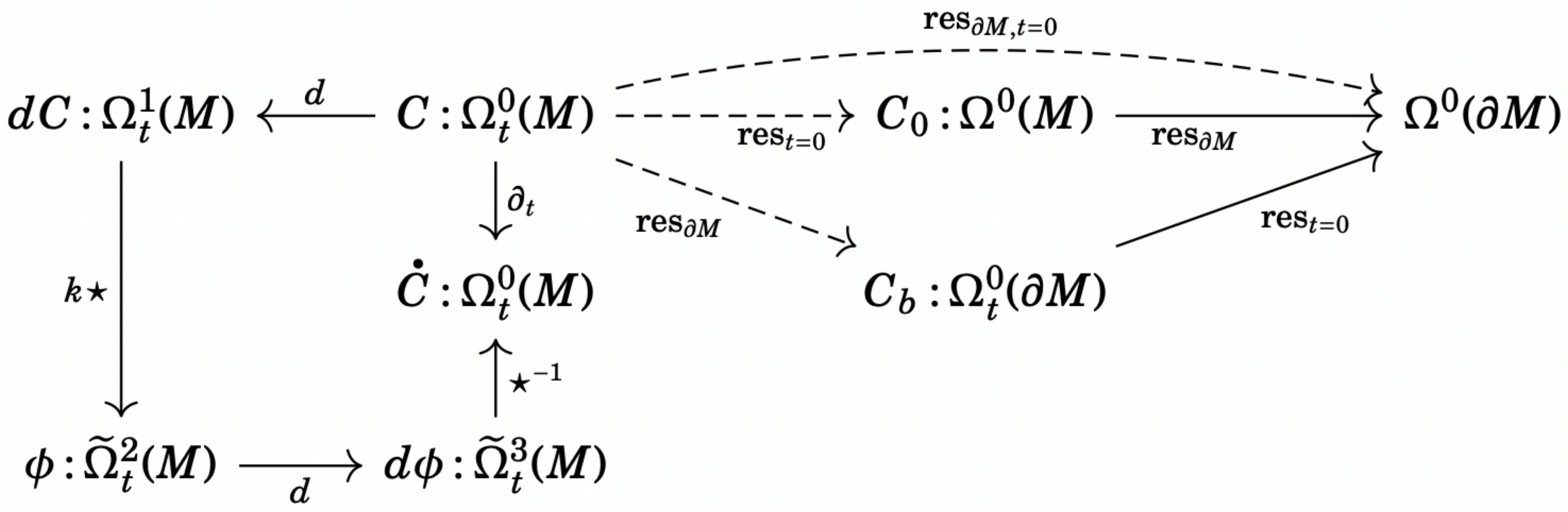
- D represents the whole system
- D_0 represents the boundary of the system
- $D \to D_0$ projects the system onto its boundary
- A lift $\overline{D_0}$ of D_0 is a choice of boundary data
- N.B. unlike in “classical” algebraic topology, we allow extension-lifting problems to be non-strict, i.e. to have non-trivial 2-cells

BVPs (and IVPs)

Pretty important for actually solving and modelling stuff



Neumann BVP for diffusion

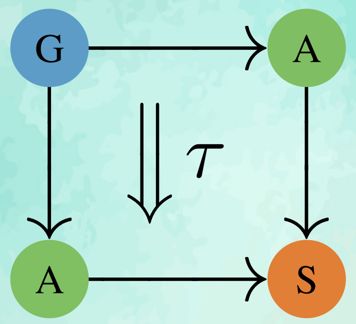


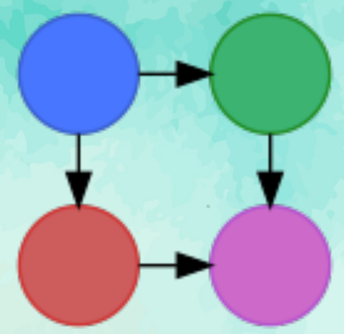
Dirichlet BVP for diffusion

Conclusion

1. Categorical framework for talking about equations and their solutions

2. Julia implementation (+ DEC + simplicial complexes) for multiphysics simulation





5. “I want more category theory”

Some things we use and discuss

And others which we will talk about in future work

- Diagram categories in the presence of cartesian/symmetric monoidal structures
  - these let us talk about more complicated physics, e.g. Maxwell's house, Navier–Stokes
- Homotopical structure of diagram categories
  - weak equivalences of are defined so that "w.e. implies bijective solutions"
  - we give a sufficient (but not necessary) condition in terms of **initial functors**; these generalise to something more 2-categorical: **relatively initial functors**
- The framework is "independent of geometry"
  - most of our examples are in PDEs, but there's nothing stopping us from talking about e.g. finite difference equations, or probabilistic/statistical things (e.g. structural equation models)
- Tonti's desired classification of physical theories?