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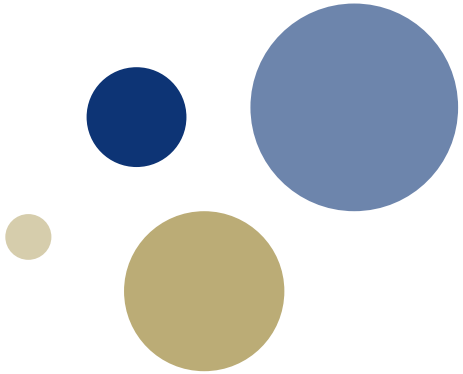


Ontology of Molecular Dynamics

- Johan Christian Edvardsen

Topics

- Introduction
- The original ontology
  - Model, mathematics, and ontology
    - Physical control volumes and signals
- The new ontology
  - Model, mathematics, and ontology
    - Newtonian mechanics and molecular dynamics
- The extended ontology
  - Original + new ontology
- Possibilities and problems

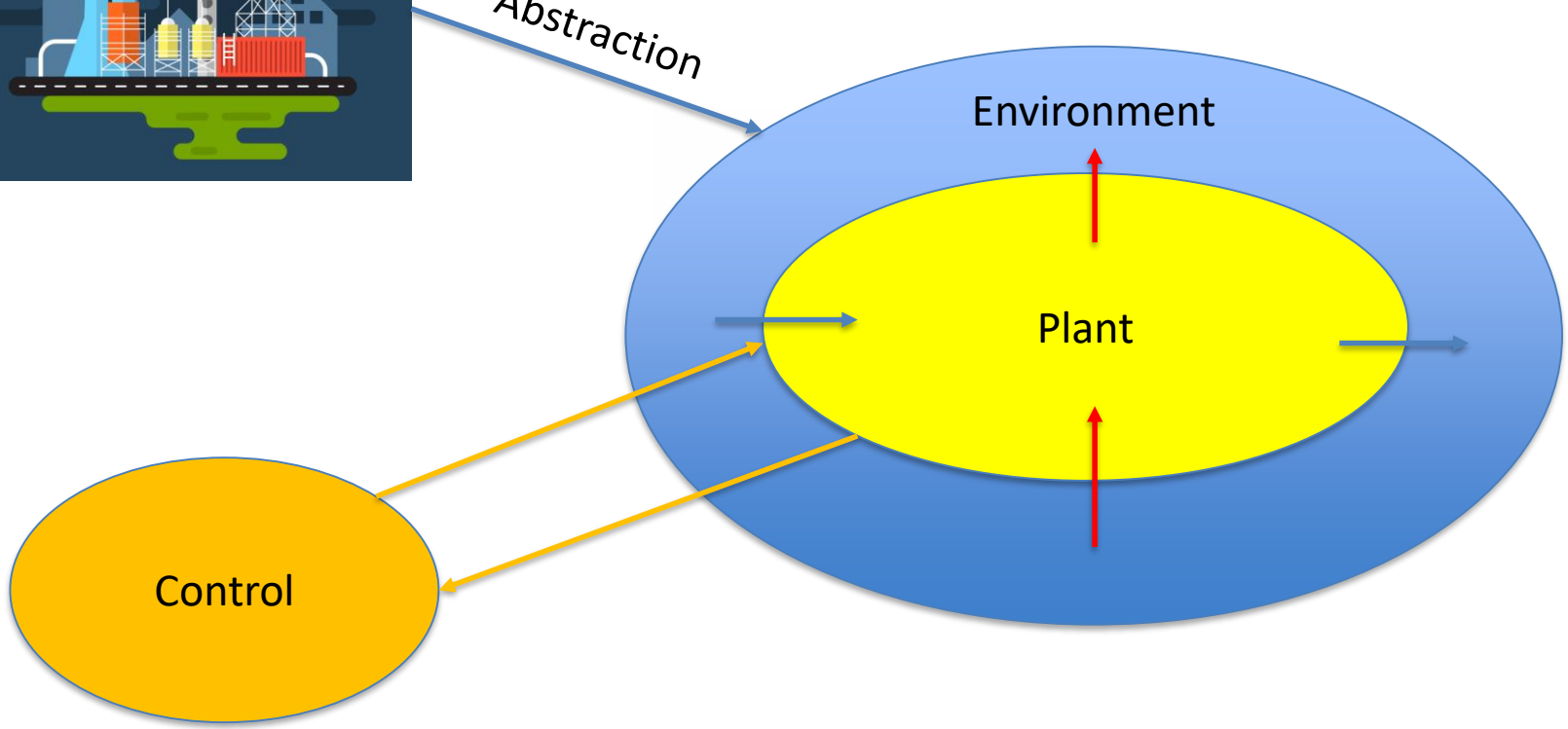
Introduction

- Ontology is an **explicit**, **formal** specification of a **shared conceptualization**.
  - **Explicit:** All relevant concepts must be defined.
  - **Formal:** Machine understandable.
  - **Shared conceptualization:** Consensus about how concepts are related within the relevant domain.
- Ontological maxims:
  - "*Be consistent.*"
  - "*Be general and minimal.*"
    - "*Track only things that matter.*"
- "Ontology is a model toolbox, where the tools and their applications are defined."

The Original Ontology: **Model**

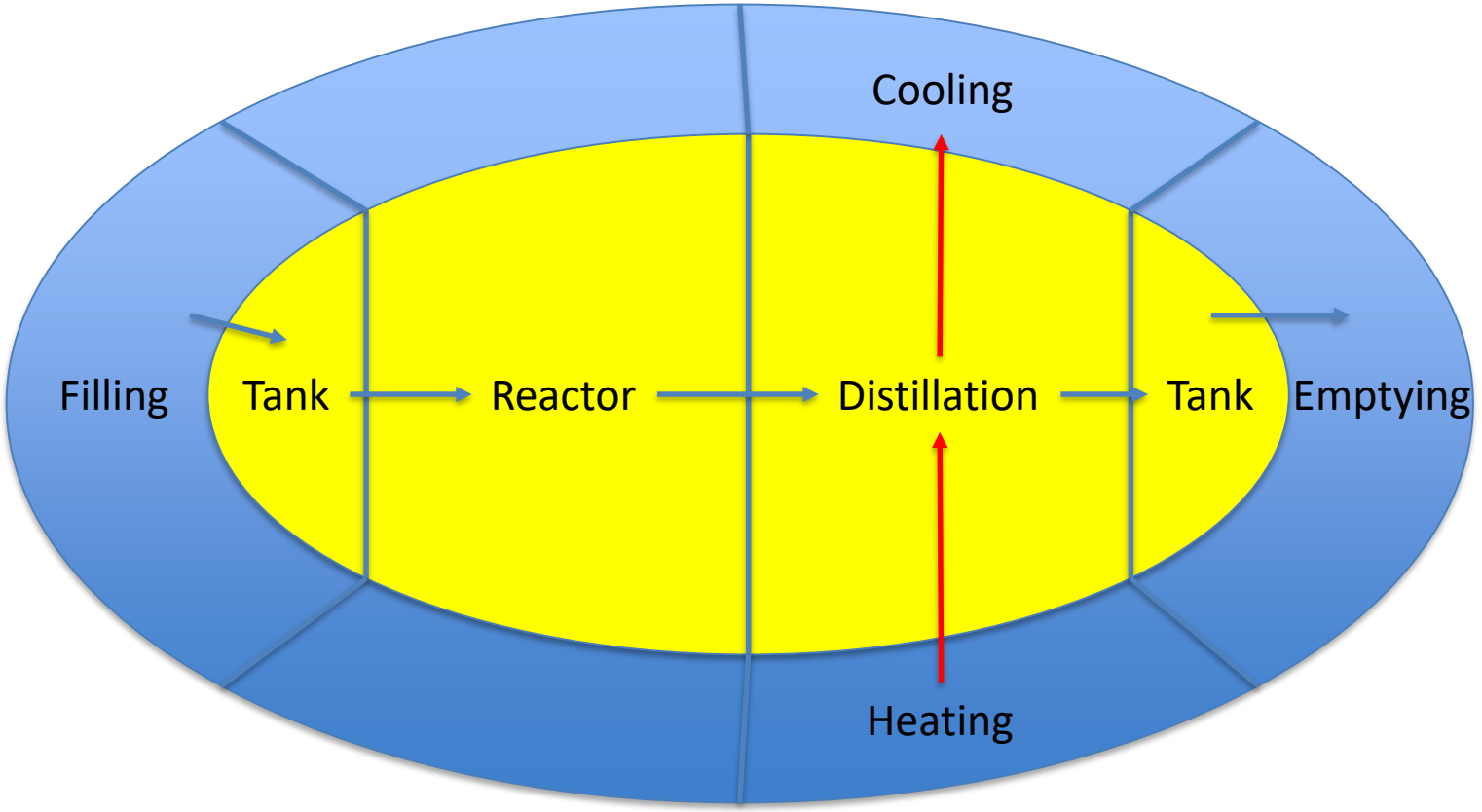
- Important concepts:
  - Physical control volume (CV)
    - Accumulation, transport, and source/sink
  - Signal
    - Manipulation of transport (output) based on CV (input)
  - Network
    - Physical phases, species, and signal information
  - Representation
    - Nodes, arcs, and tokens
  - Scale
    - Time and size

Old Example: **The Plant Model**



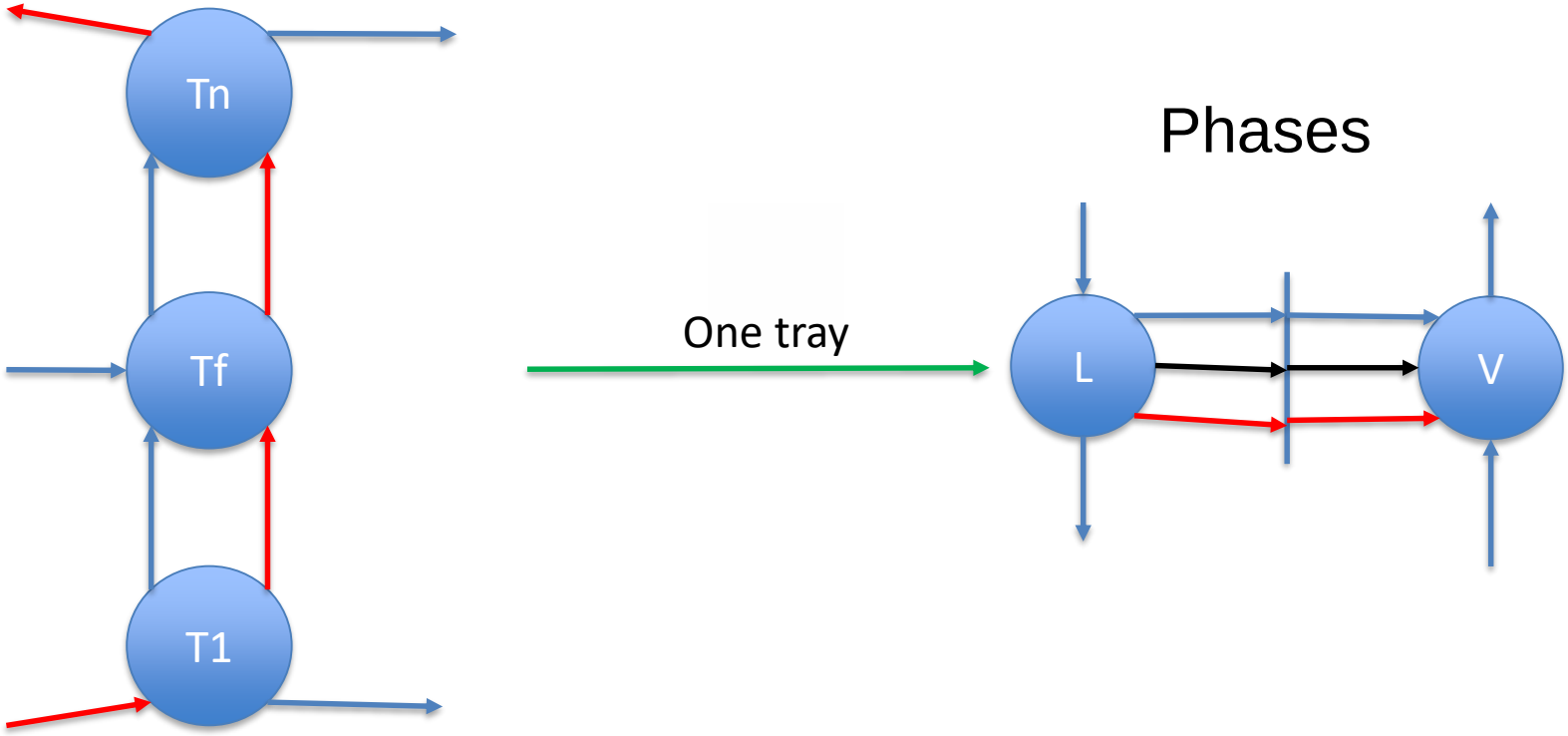
The Unit Model

- Control Volumes



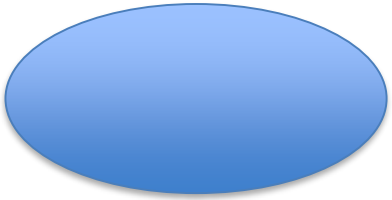
The Distillation Model

- Smaller Control Volumes



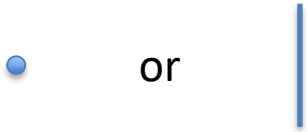
Lumped

Time



Distributed

Time and space



or

Event

Just happens

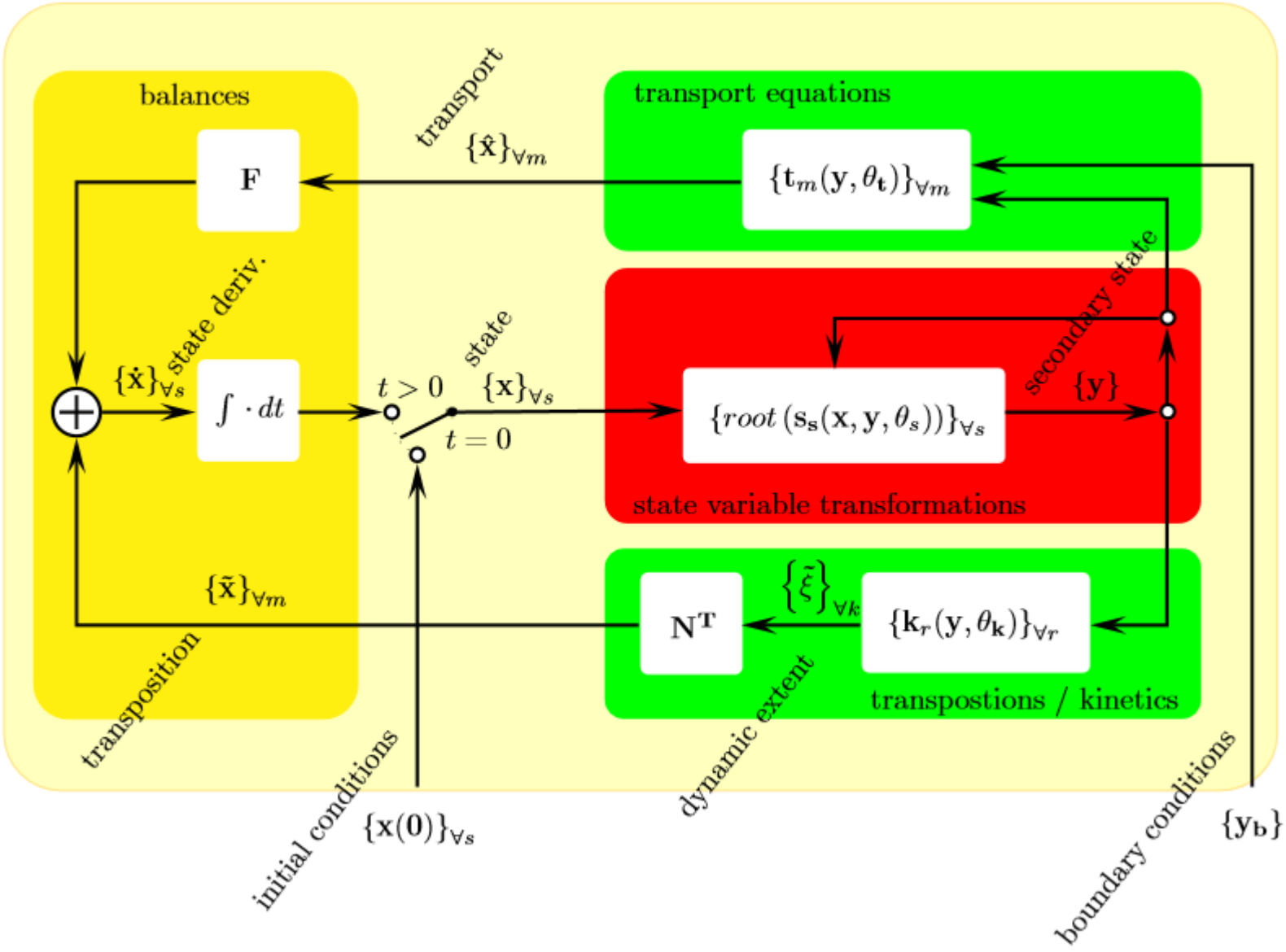
Half Node

Constant

Transport

The Original Ontology: **Mathematics**

- Important concepts:
  - State
    - Token → State
  - Closure
    - State + EOS → Secondary states
  - Transport
    - Secondary state + Mechanism → Transport equation
  - Transposition
    - Secondary state → Kinetics → Dynamic extent + rx → Transposition
  - Balance and differential state
    - Transport + Network + Transposition → Diff. state
  - Signal
    - Input + set-point → error → dynamics → output
  - Connection
    - Measured input → Normalized measured input
    - Output → Manipulation



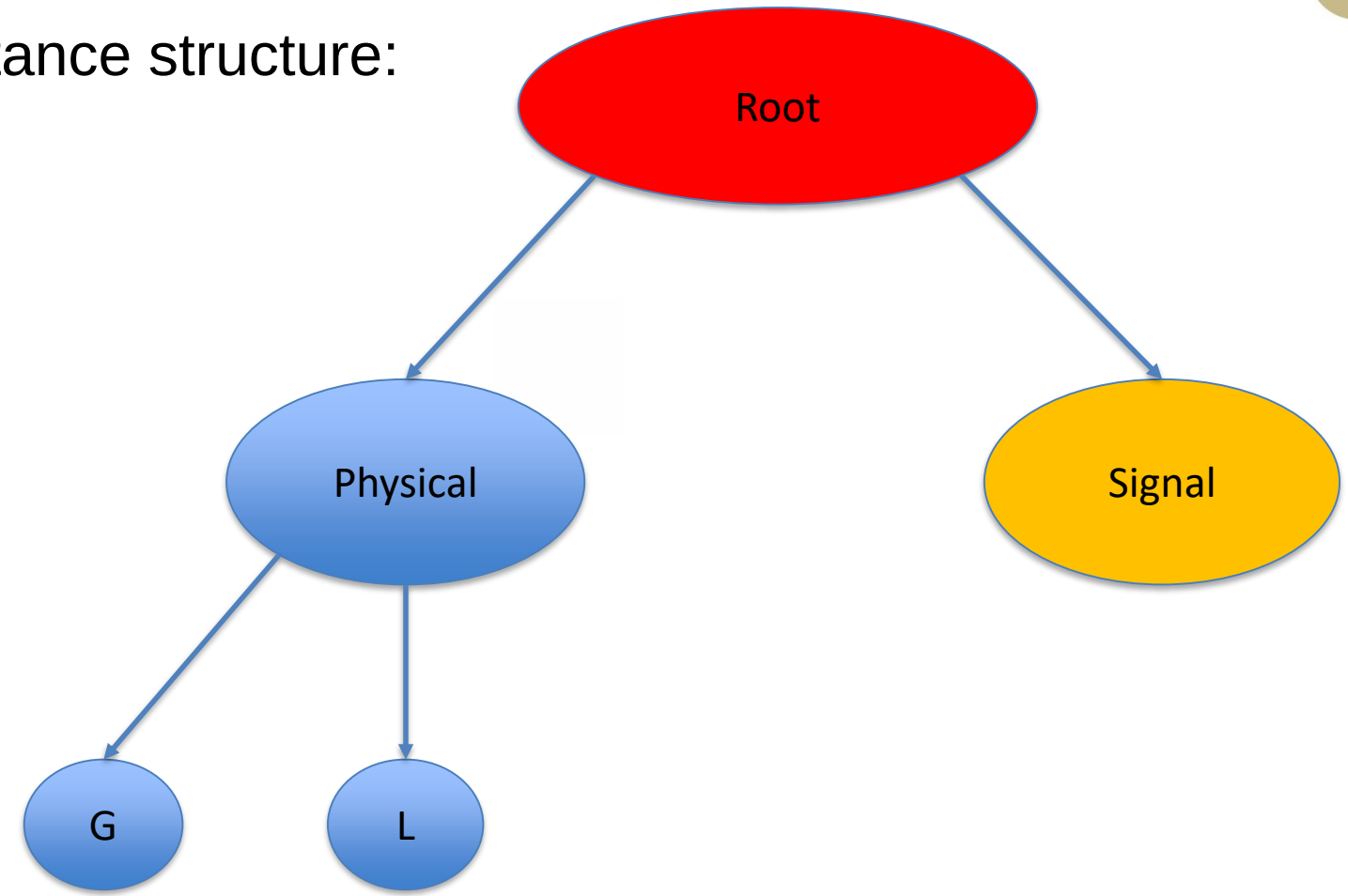
Source: H. A. Preisig, 2016. The ABC of Modelling, Lecture Notes TKP4106 4135. version 2.0, Norwegian University of Science and Technology (NTNU).

The Original Ontology

- Important concepts:
  - Trinity
    - Root, Physical, and Signal
  - Organized information
    - Structure, Behaviour, and Typing
  - Structure
    - Defines the modelling tools (building blocks)
      - Graph, node, arc, frame, and token
  - Behaviour
    - How the modelling tools are applied (connection to math)
      - Based on network
      - Applied to nodes and arcs.
  - Typing
    - How the modelling tools can be specialized
      - New type of graph (node, arc) = new behaviour
  - Inheritance and communication

The Original Ontology

- Inheritance structure:



The Root Ontology

- Shared between physical and signal

```
[structure]  # building blocks
   graph = ['*node', '*arc']    # fixed not to be changed
   frame = ['.time']

[behaviour]  # link to mathematical description
  node = ['state', 'diffstate','constant','network']

[typing]  # specialisation of building block
  graph = ['physical', 'control']
  node  = ['dynamic_0D','event', 'constant']
  arc   = ['bi-directional', 'uni-directional' ]
```

The Physical Ontology

- Shared between gas and liquid

```
[structure]
   frame = ['r_x','r_y','r_z']
   token = ['.mass','.energy','.entropy']

[behaviour]
  node = ['closure', 'transposition']
  arc = ['transport']

[typing]
   graph = ['gas', 'liquid']
   mechanism = {'mass' : ['v','d'], 'energy': ['c','w','r']}
   mass = ['*!species']
```

The Signal Ontology

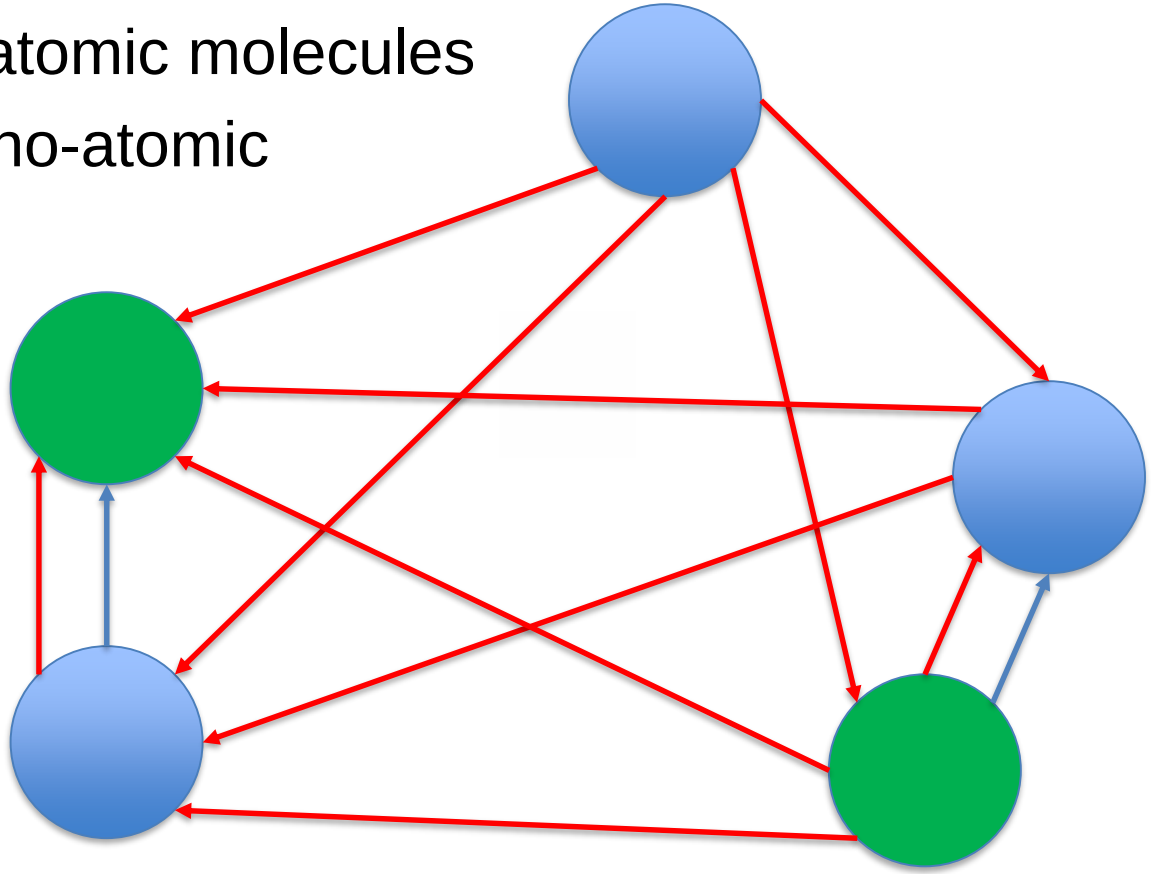
```
1 [structure]
2    token = ['signal']
3
4 [behaviour]
5
6
7 [typing]
8   signal = ['*input', '*output']
9
```

The New Ontology: **Model**

- Important concepts:
  - Newtonian Mechanics:
    - Atoms as point particles
      - Mass, position, velocity, acceleration(force)
      - Newtons 1st. And 2nd. Laws of motion
    - Forces between atoms
      - Newtons 3rd. Law of motion
      - Derived from potential functions
  - Molecular Dynamics:
    - Potentials
      - Derived from position of atoms
      - Inter- and intramolecular bonds
  - Representation:
    - Nodes and arcs

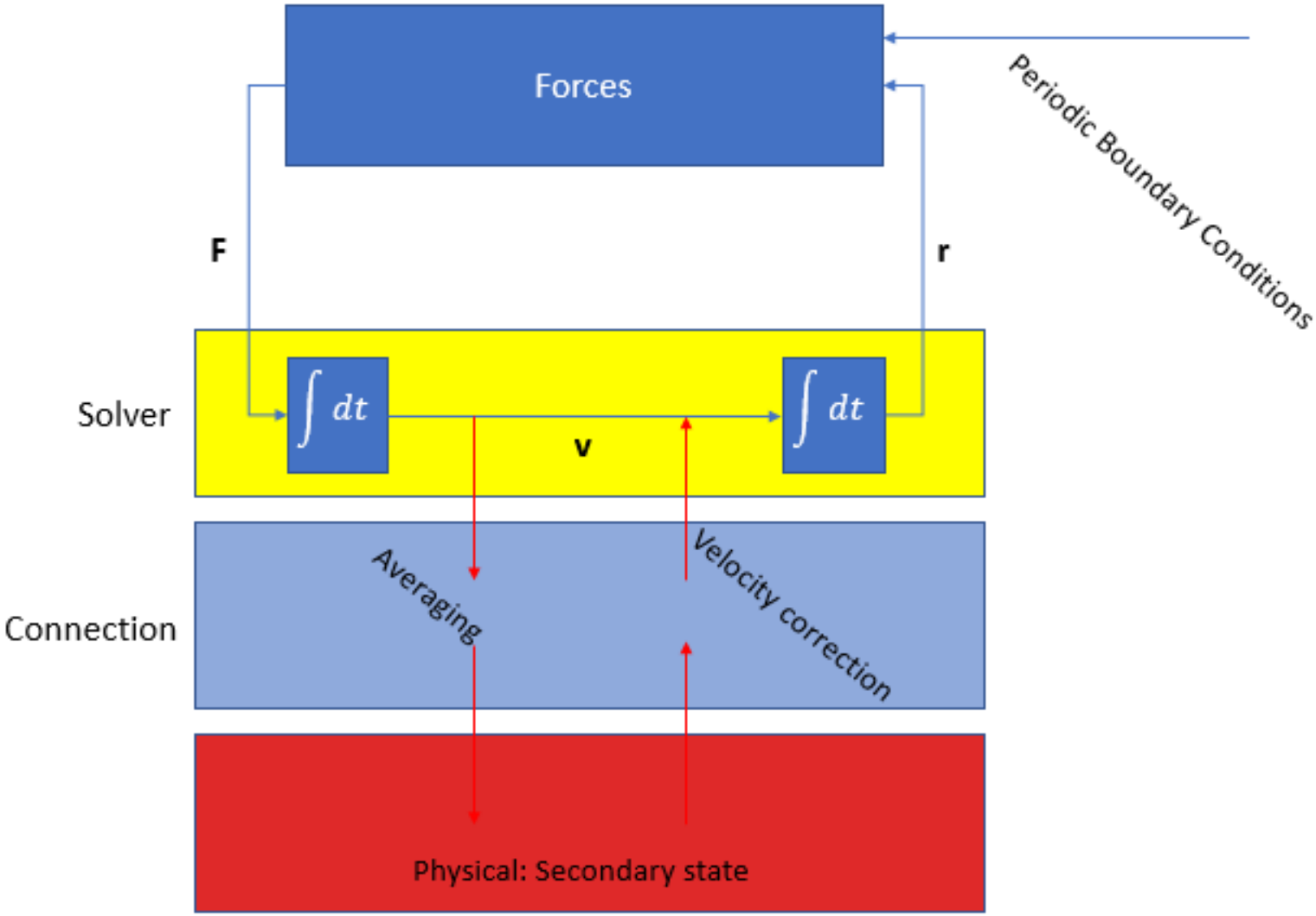
New Example: **Molecular Model**

- 2 x Di-atomic molecules
- 1 x Mono-atomic



The New Ontology: **Mathematics**

- Important concepts:
  - State
    - Frame → State
  - Force
    - State + periodic BC + constriction → Potentials → Forces
  - Diff. state
    - Forces + Mass (+ Network) → Diff. state → state = Diff. state → State
  - Connection
    - State → Averaging → Physical secondary state
    - Physical secondary state → Correction/thermostat/barostat → State

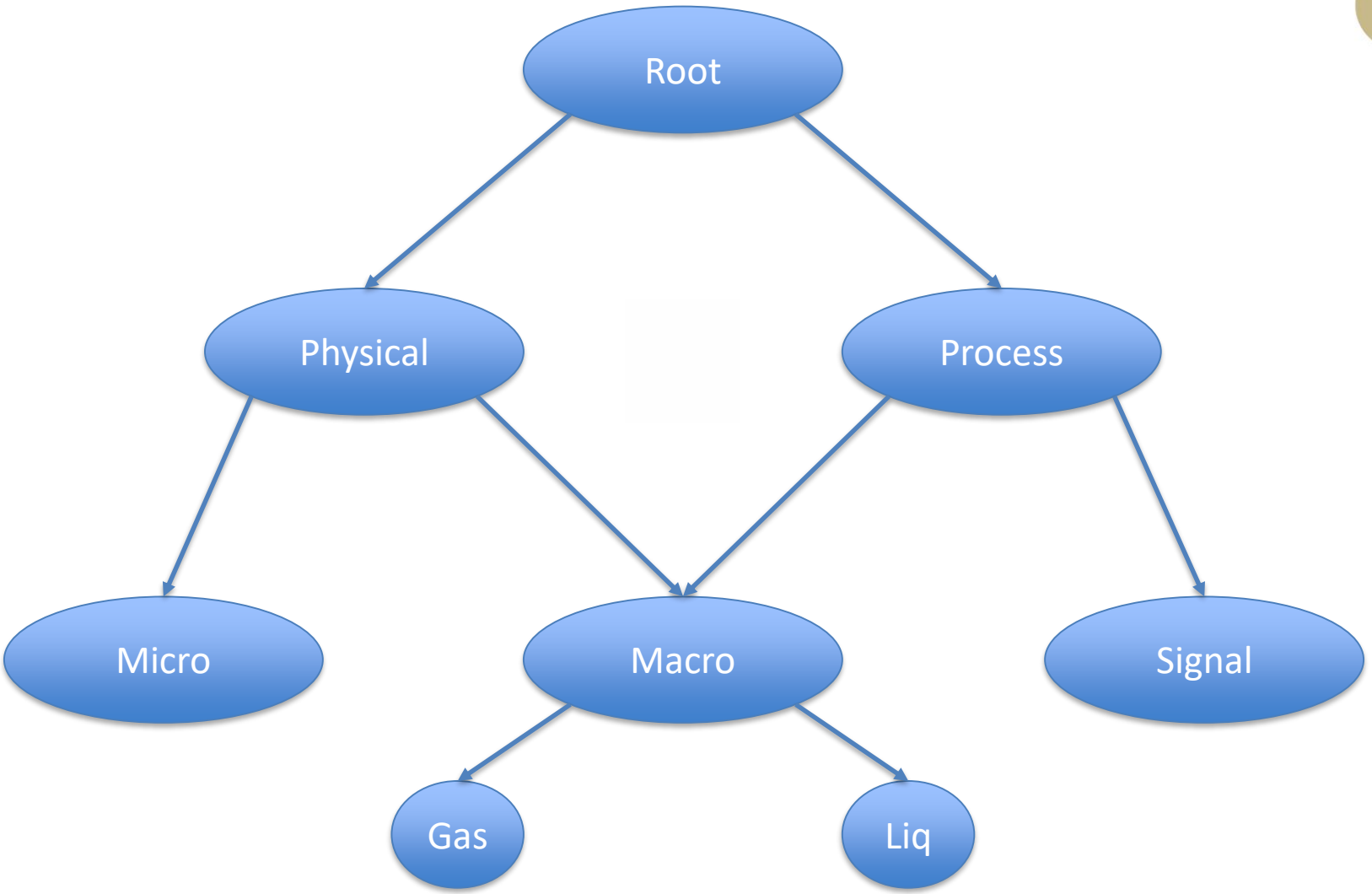

Forces
Periodic Boundary Conditions
F
r
Solver
$\int dt$
v
$\int dt$
Connection
Averaging
Velocity correction
Physical: Secondary state

The New Ontology

- Collection of all information:

```
[structure]
  graph = ['*node', '*arc']
  frame = ['time', 'r_x', 'r_y', 'r_z']
  token = ['momentum', 'energy']

[behaviour]
  node = ['state', 'diff_state', 'constant', 'network']
  arc = ['constant', 'force']

[typing]
  force = ['intra', 'inter']
  node = ['dynamic_0D']
  arc = ['bi-directional']

```

The Extended Ontology



The Extended Root Ontology

Shared Between all

```
[structure]
  graph = ['*node', '*arc']
  frame = ['time']

[behaviour]
  node = ['state', 'diffstate','constant','network']
  arc = ['constant']

[typing]
  graph = ['physical', 'process']
  node  = ['dynamic_0D']

```

The Process Ontology

Shared between Macro-physical and Signal

```
1 [structure]
2
3 [behaviour]
4
5 [typing]
6   graph = ['macro-physical','signal']
7   node = ['event','constant']
8   arc = ['uni-directional']
9
```

The Extended Physical Ontology

Shared between Micro- and Marcro-physical

```
[structure]
  frame = ['r_x', 'r_y', 'r_z']
  token = ['momentum', 'energy']

[behaviour]

[typing]
  graph = ['micro-physical', 'macro-physical']
  arc   = ['bi-directional']
```

The Macro-Physical Ontology

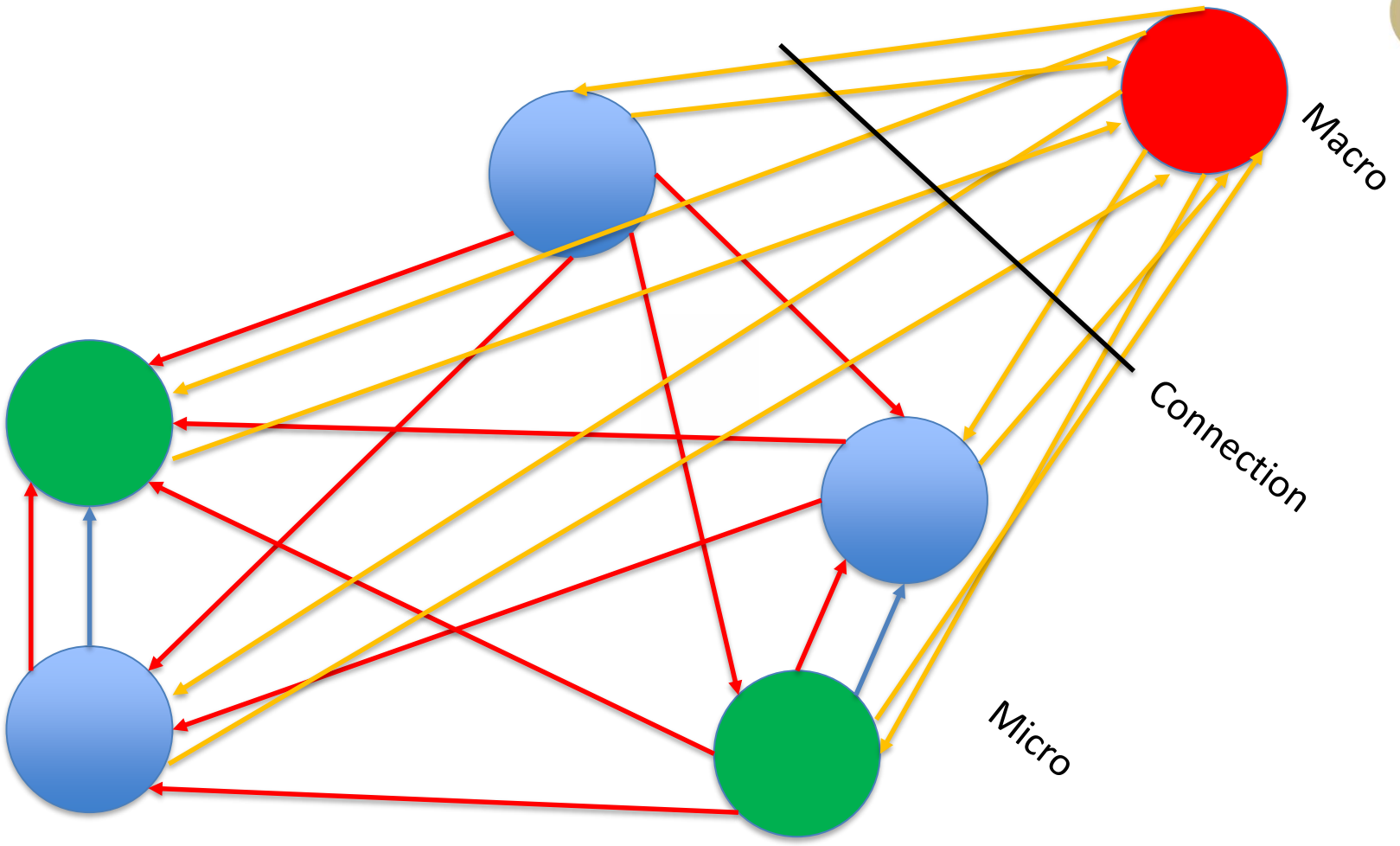
Shared between Gas and Liquid

```
[structure]
  token = ['mass','entropy']

[behaviour]
  node = ['closure', 'transposition']
  arc = ['transport']

[typing]
  graph = ['gas', 'liquid']
  transport = {'mass' : ['v','d'], 'energy': ['c','w','r']}
  mass = ['*!species']
```

The Micro-Physical Ontology

```
1 [structure]
2
3 [behaviour]
4   arc = ['force']
5
6 [typing]
7   force = ['intra-force', 'inter-force']
8
```

Example: **Extended Model**



Possibilities and Problems

- **Pros:**
  + Extend to include Newtonian mechanics
  + Communication between Micro- and Macro-physical
  + Introduces momentum to the physical
- **Cons:**
  - Does not satisfy the criterion of being formal
    - State is dependant on frame not token
      - New interpretation
  - UI-modelling issue: web of arcs
  - Not possible to currently implement
    - Probably need refinement of the ontology