



Chemical Biochemical and Environmental Engineering



Lean for Scientists and Engineers

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Lean for Scientists and Engineers 2024

- I. Logic and proofs for scientists and engineers
 - Introduction to theorem proving
 - 2. Writing proofs in Lean
 - Formalizing derivations in science and engineering
- 2. Functional programming in Lean 4
 - I. Functional vs. imperative programming
 - 2. Numerical vs. symbolic mathematics
 - 3. Writing executable programs in Lean
- 3. Provably-correct programs for scientific computing

Schedule (tentative)

Logic and proofs for scientists and engineers Functional programming in Lean 4 Provably-correct programs for scientific computing

- July 9, 2024 Introduction to Lean and proofs
- July 10, 2024 Equalities and inequalities
- July 16, 2024 Proofs with structure
- July 17, 2024 Proofs with structure II
- July 23, 2024 Proofs about functions; types
- July 24, 2024 Calculus-based-proofs
- July 30-31, 2024 Prof. Josephson traveling
- August 6, 2024 Functions, definitions, structures, recursion
- August 8, 2024 Polymorphic functions for floats and reals, compiling Lean to C
- August 13, 2024 Input / output, lists, arrays, and indexing
- August 14, 2024 Lists, arrays, indexing, and matrices
- August 20, 2024 LeanMD & BET Analysis in Lean
- August 21, 2024 SciLean tutorial, by Tomáš Skřivan

Content inspired by: Mechanics of Proof, by Heather Macbeth Functional Programming in Lean, by David Christiansen



Guest instructor: Tomáš Skřivan

Schedule for today

- I. Survey for attendees
- 2. Recap Lecture 2
 - I. Revisit syntax vs. semantics
- 3. Proofs with intermediate steps
- 4. Proofs using lemmas from Mathlib
- 5. Junk values, and why 1/0 = 0
- 6. Logical operators
- 7. Proofs with AND and OR

Survey for attendees

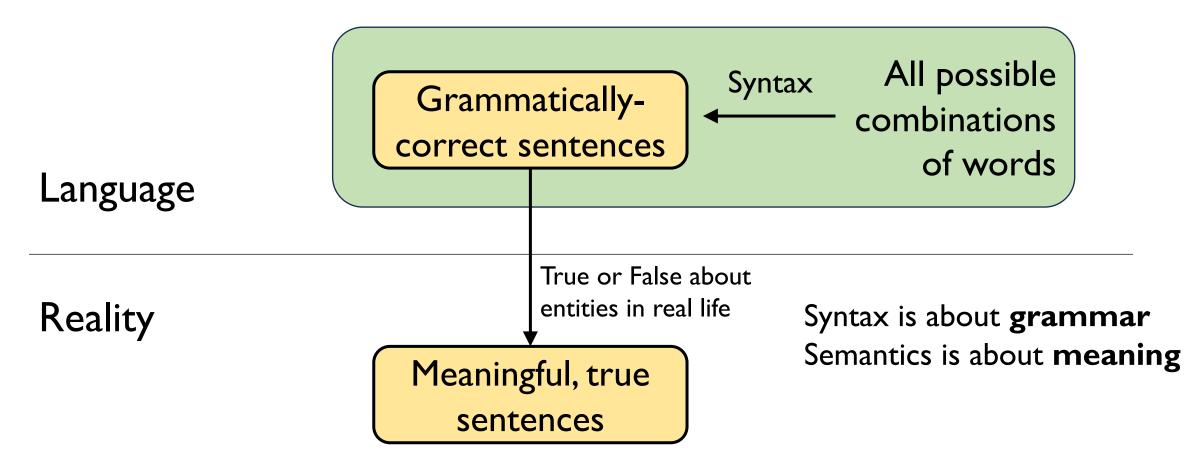
https://forms.gle/pg5JGpTgD1aSCshY6

Poll questions:

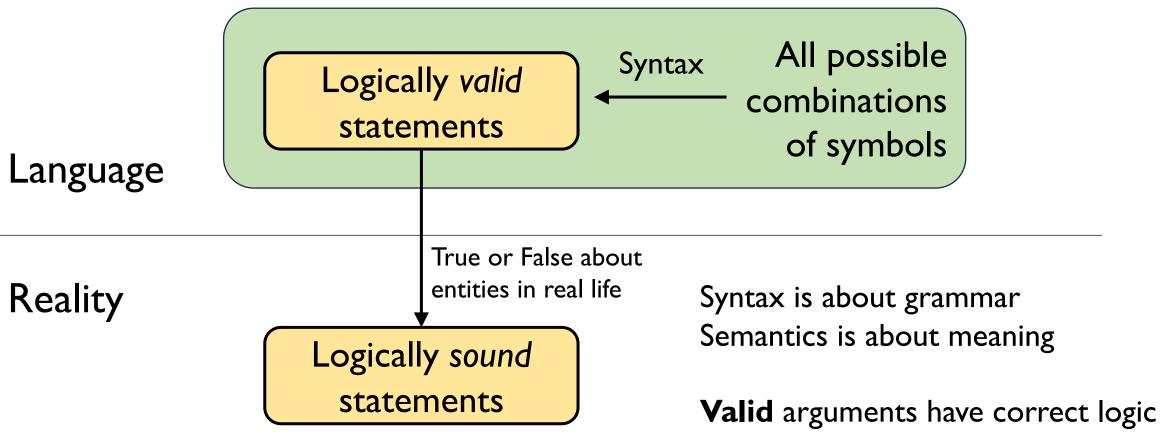
How many hours did you spend with Lean last week (including time in class / listening to recordings?)

Did you explore more Mechanics of Proof exercises from Chapter 1?

Syntax vs. semantics in natural language

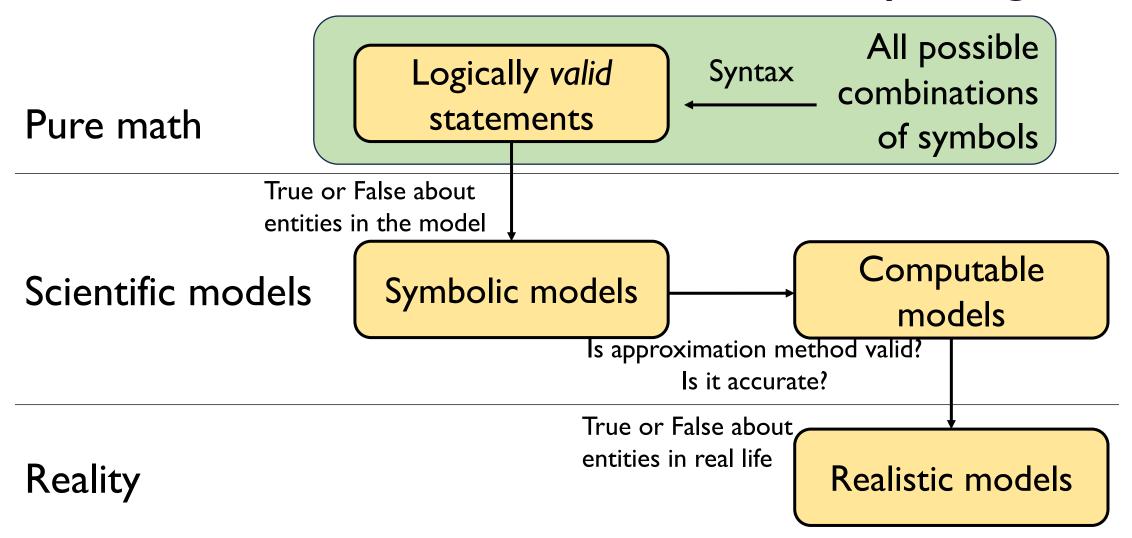


Syntax vs. semantics in logic

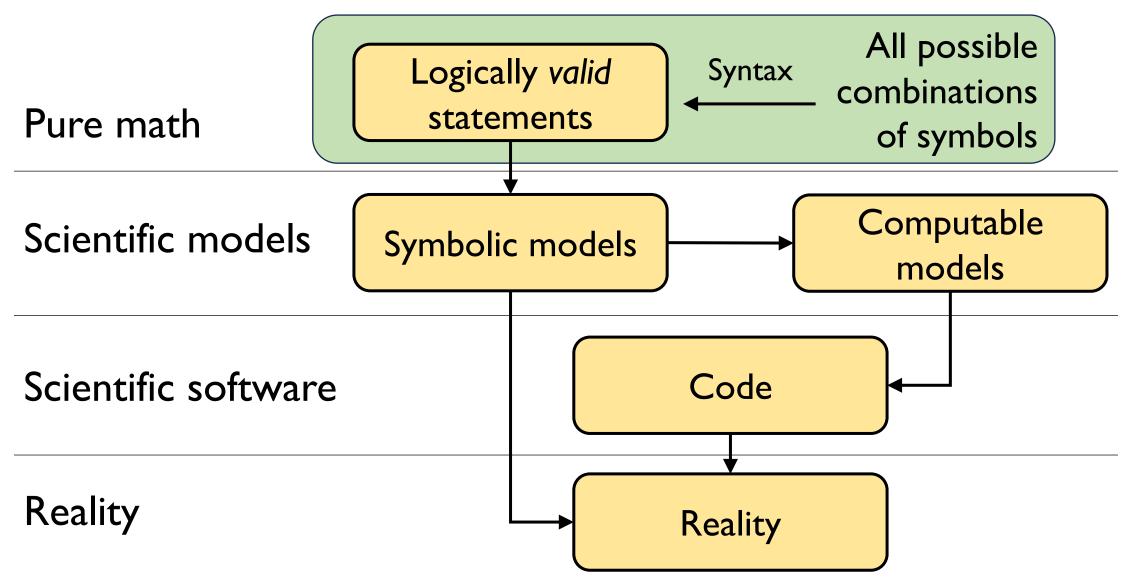


Sound arguments have correct logic also have true premises

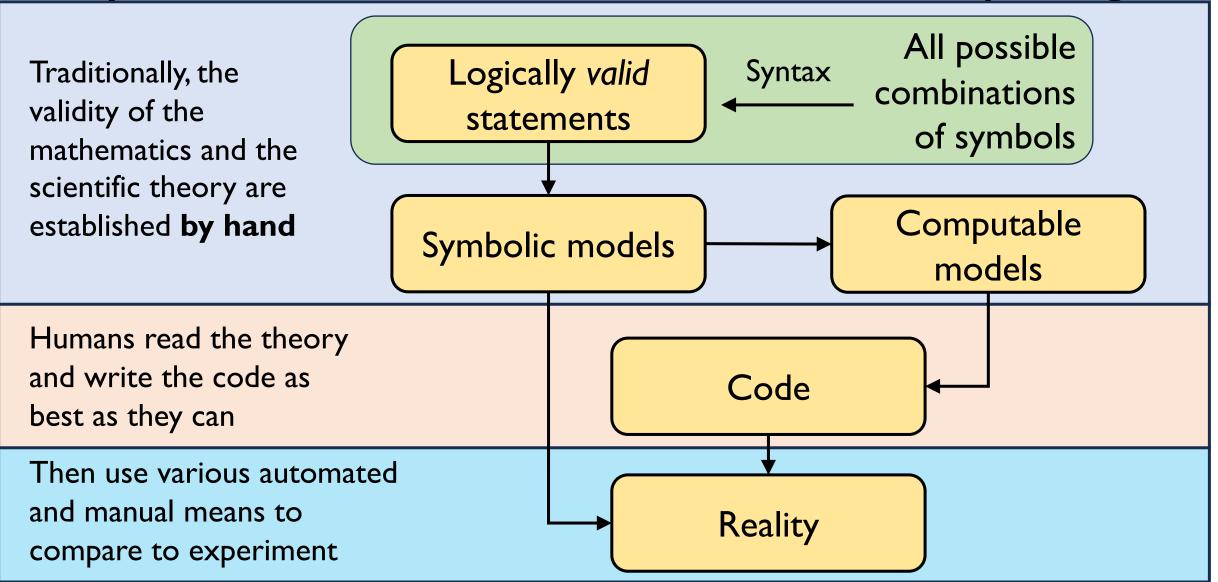
Semantic errors in scientific computing



Syntax and semantics in scientific computing



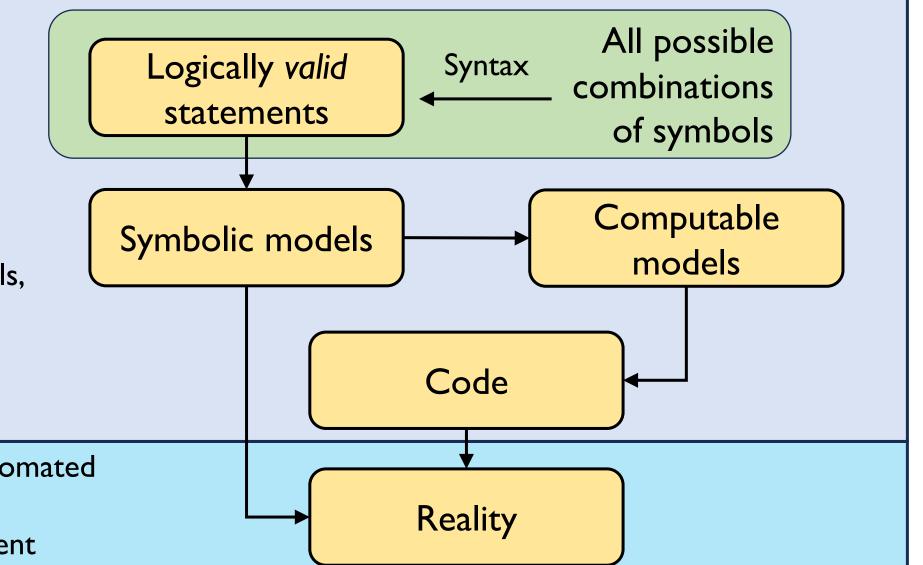
Syntax and semantics in scientific computing



Syntax and semantics in scientific computing

Can we represent all of this in Lean, and validate the construction of the math, scientific models, and software, in one system?

Then use various automated and manual means to compare to experiment



Proofs using intermediate steps

- Sometimes, it's helpful to prove a little thing that helps you prove the main thing
- At scale, this is how Mathlib works, as an interconnected web of proofs
- Can also internally define a statement and prove it
- https://github.com/ATOMSLab/LeanChem icalTheories/blob/kepler'sLaw/src/physics/ kepler'sLaw



Should you use have or add a hypothesis?

Using have

New hypothesis

Should you use have or add a hypothesis?

Using have

New hypothesis

We've changed the theorem statement.h2 is "unused"We don't know if hb is true!If hb contradicts any other hypotheses, we're in real trouble

Principle of logical explosion

- You MUST NOT assume a set of premises with a contradiction
- "Principle of explosion"
- <u>https://en.wikipedia.org/wiki/Principle_of_explosion</u>
- Also known as "proving false"
- You can prove anything, which isn't actually helpful
- Lean has tactic "slim_check" that can sometimes detect this by searching for counterexamples
 - Examples here: https://github.com/leanprovercommunity/mathlib4/blob/master/test/slim_check.lean

Proofs using existing theorems

• apply tactic directly updates the goal using a theorem

- Some tactics are aware of a bunch of theorems already
- Other tactics can be "told about" theorems to make them smarter

How to find tactics

- Keep learning them one by one!
- Indexes for Mechanics of Proof, Mathematics in Lean
- Consult lists of useful tactics
 - <u>https://github.com/madvorak/lean4-tactics</u>
 - https://github.com/Colin166/Lean4/blob/main/UsefulTactics
- If you have a tactic in hand, mouseover in VS Code to see documentation and example(s)

How to find theorems

- Keep practicing!
- Search Mathlib documentation
 - <u>https://leanprover-community.github.io/mathlib4_docs/</u>
 - Using the search bar, make a guess about what the theorem would be named, and start checking things that look promising
- Moogle
 - https://www.moogle.ai
 - Describe theorem (or definition) in natural language, the scroll through options
- Consult lists of useful theorems
 - <u>https://github.com/Colin166/Lean4/blob/main/UsefulLemmas.lean</u>
- If you have a theorem in hand, mouseover in VS Code to see documentation and example(s)

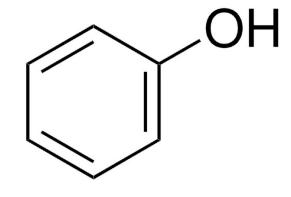
Glossary of logical symbols

\wedge - and

- V or
- ⊐ not
- \rightarrow implies
- ↔ if and only if (implies in both directions)
- ∃ exists
- \forall for all

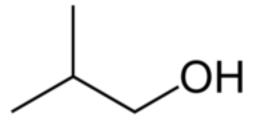
- P: molecule is aromatic
- Q: molecule is an alcohol
- $P \land Q$: molecule is aromatic and an alcohol
- P: true, Q: true then P \land Q: true
- P: false, Q: true then $P \land Q$: false
- P: true, Q: false then $P \land Q$: false
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Phenol

- P: molecule is aromatic
- Q: molecule is an alcohol
- $P \land Q$: molecule is aromatic and an alcohol



isobutanol

- P: true, Q: true then P \land Q: true
- P: false, Q: true then $P \land Q$: false
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Ρ	Q	(P ^ Q)
true	true	true
false	true	false
true	false	false
false	false	false

V:or

- P: contains acrolein
- Q: contains hydrogen cyanide P V Q: acute toxicity
- P: true, Q: true then P \lor Q: true P: false, Q: true – then P \lor Q: true P: true, Q: false – then P \lor Q: true P: false, Q: false – then P \lor Q: false



Р	Q	(P v Q)
true	true	true
false	true	true
true	false	true
false	false	false