Pros and cons of physics-based and data-driven modeling in industry

Bart Rijksen & Tom Verbrugge

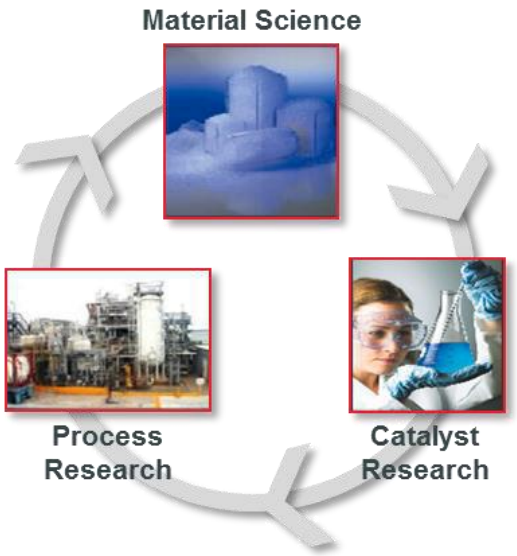
EMMC INTERNATIONAL WORKSHOP 2019
Vienna, Austria

Value of Modeling at Dow

- Speed up the discovery process
  - Design of new materials, formulations, and processes
- Quickly screen various ideas and focus on the most promising ones
  - Save money and time to explore the better ones
- Alert collaborators to possible modes of failure that might not show up in experiments
  - For example, possibility that material would develop fatigue after several years in high temperatures
- Explore regions of stability
  - “wide” vs. “narrow” process window
- Analyze experimental data and develop correlations that could later be justified with fundamental theories (OR NOT!)
  - Design the next generation of experiments
- All in all, work in close collaboration with experimentalists, market researchers, engineers, and often customers, to help answer their questions

Market-driven Innovation Model

An average of 40 new products are launched globally each quarter – driven by innovations in packaging



pack STUDIOS
COLLABORATE • INNOVATE • ACCELERATE


Converter

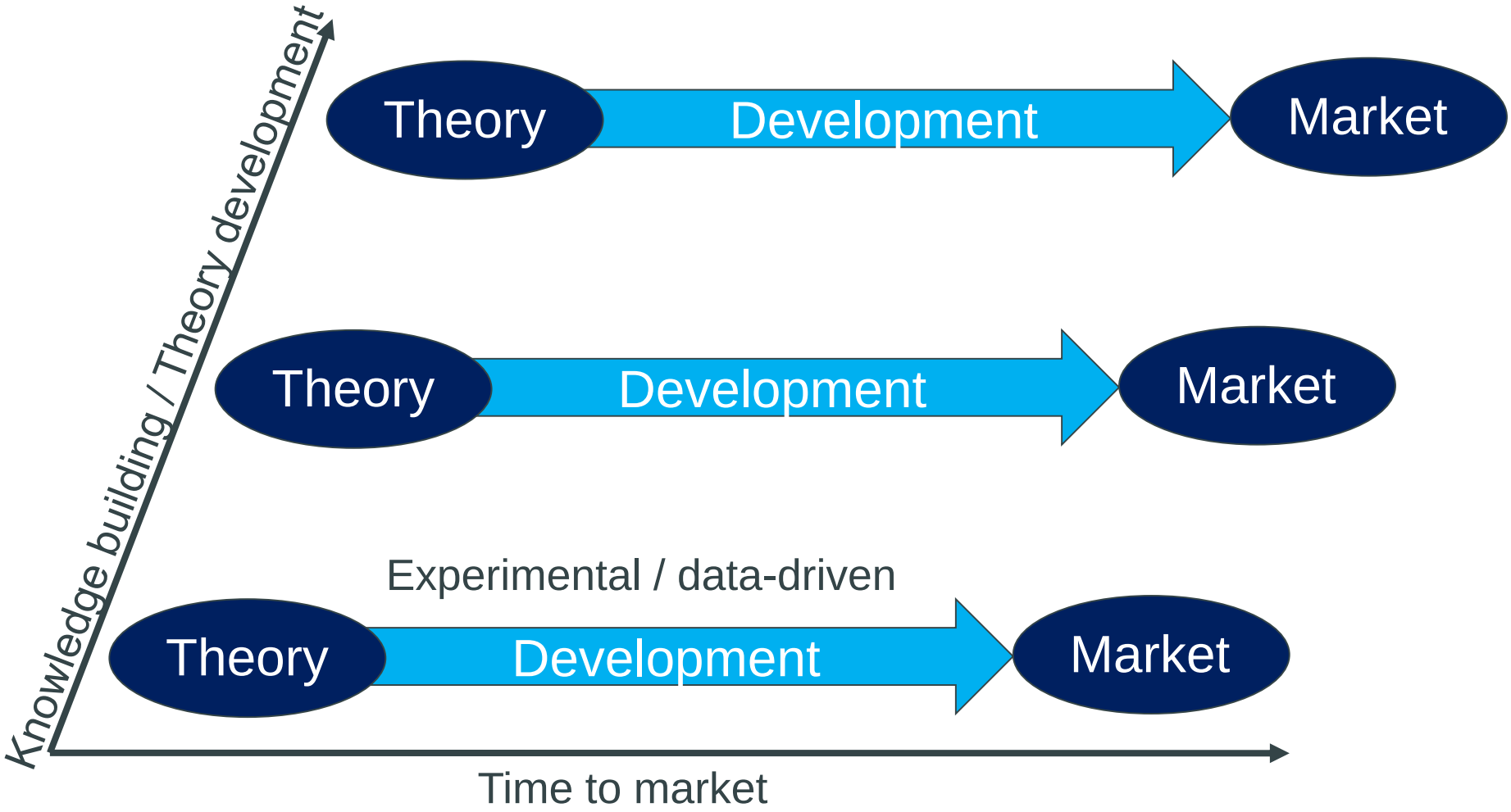

Supplier/Equipment Manufacturer


Brand Owner


Retailer

Research → **Development** → **Commercialization**

Materials Modeling in an Industrial Setting



Modeling in Materials Research

Past -> now

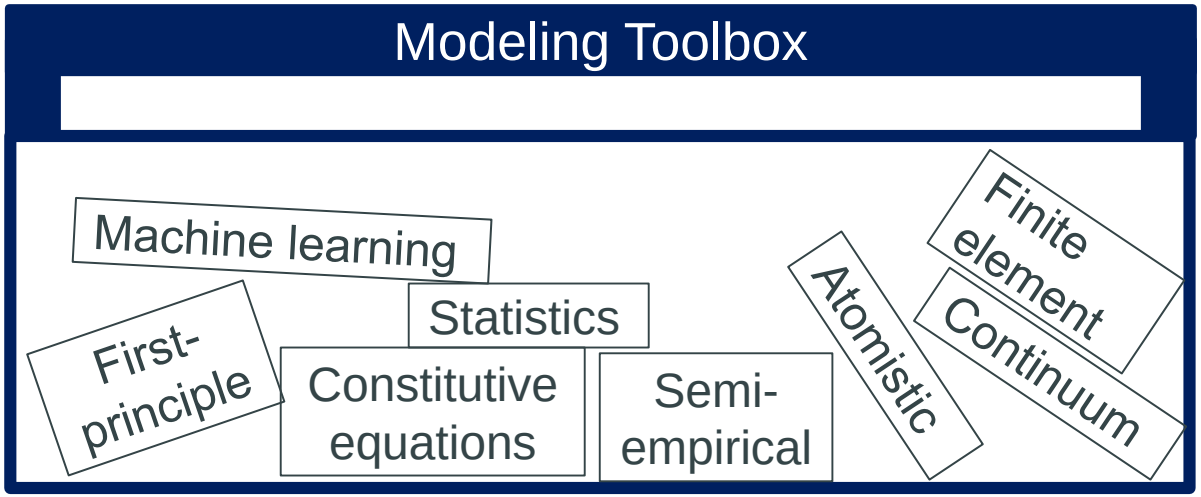
- First run experiments, then use modeling to help explain

Now more shifting towards:

- Use models when designing experiments, run experiments, use modeling to help understand the results

For modeling → use the tools (and specialists) at hand:

- Cost
- Time
- Availabilitiy



High-level Pros and Cons

Data-driven

- ✓ Directly related to experiment
- ✓ Relatively fast (project base)
- ✓ Optimize within design
- ✓ Theory not essential

- Scalability
- Only valid in specified region
- Long term development

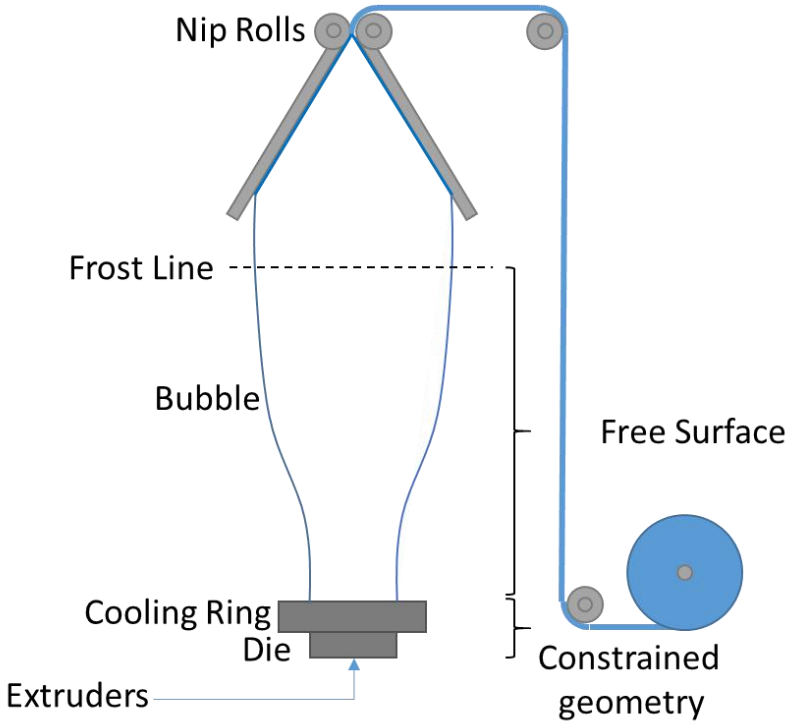
Physics-based

- ✓ Directly from theory
- ✓ Scalable
- ✓ Long term development
- ✓ Robust

- Slower to develop
- Relation to experiments
- Theory is essential

Understanding Complex Structures Through Physics

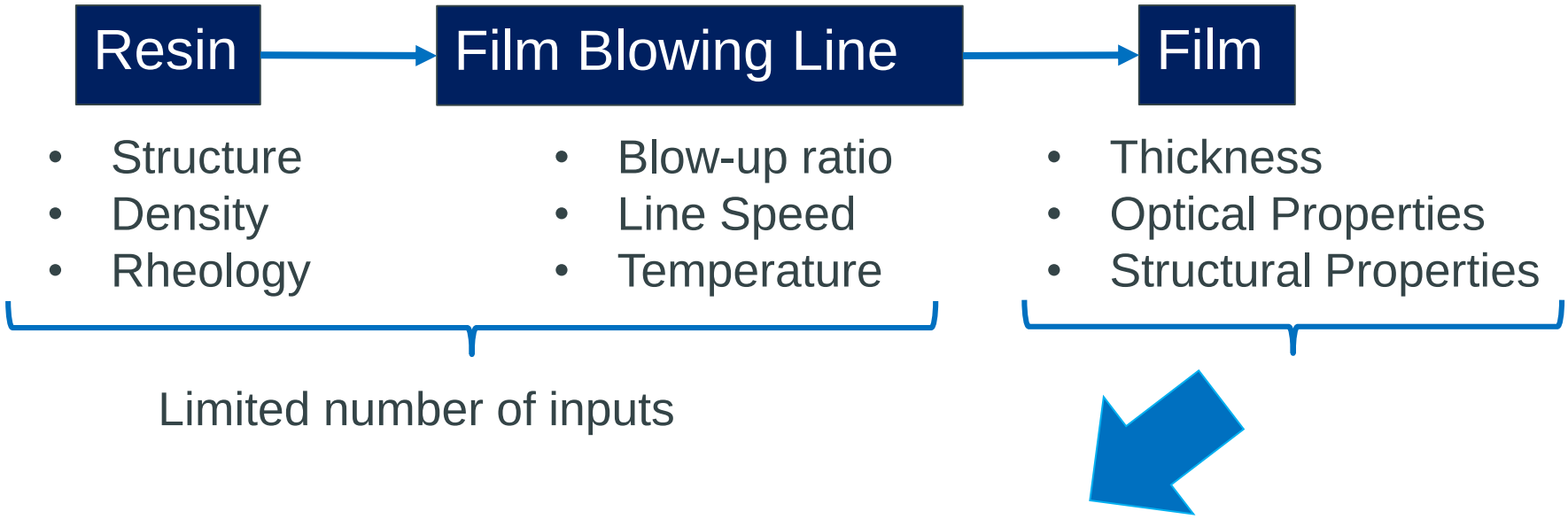
Shape and stress development in cooling air ring and free surface from non-isothermal film blowing simulations



Tatyana Leonova, TU/e
Stef van Eijndhoven, TU/e
Jesús Nieto, Dow Tarragona
Jaap den Doelder, Dow Terneuzen

Understanding Complex Structures Through Physics

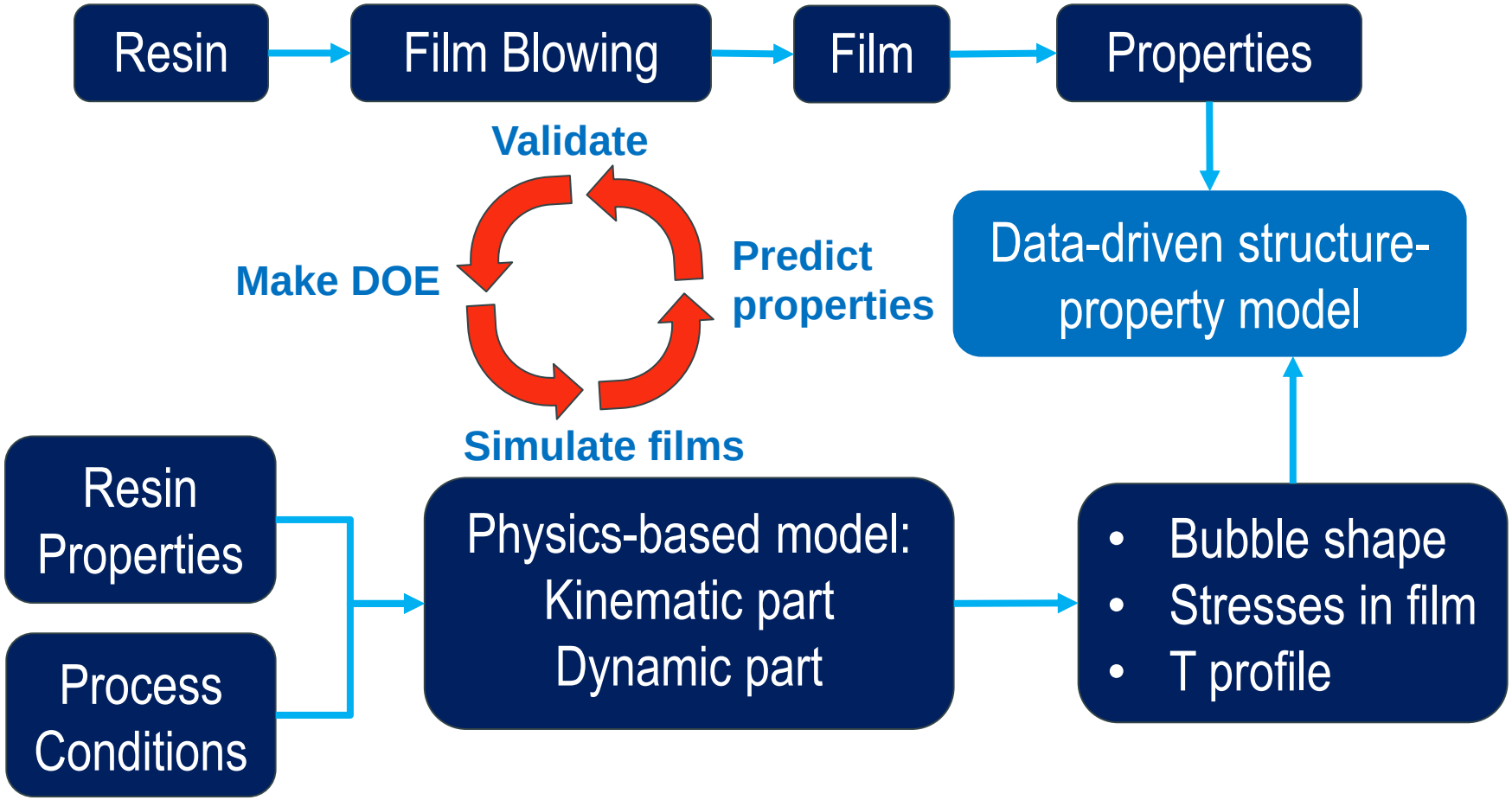
Shape and stress development in cooling air ring and free surface from non-isothermal film blowing simulations



Prior knowledge/experience:
Some film properties are strongly related to molecular orientation which takes place during the process, and is then frozen as the film cools down!
Whereas resin characteristics are measured in the molten state.

Fundamental Theory in Parallel to Experiments

Use physics-based models to obtain knowledge base
Use data-driven models to connect to experimental results

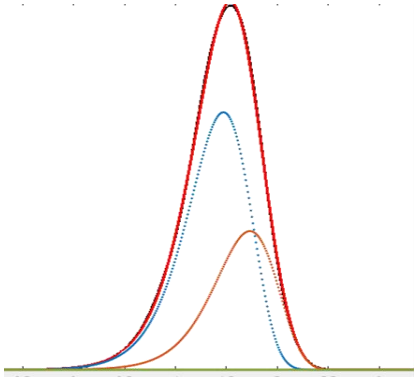


Use Fundamental Theory to Generate New Structures

The Relationship between Low-Density Polyethylene (LDPE) Optics and Molecular Structure

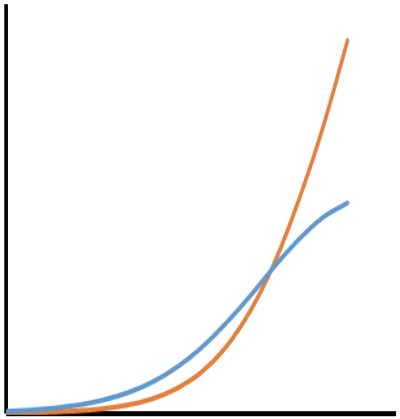
Inputs: Polymer structure

- Molecular Weight Distribution
- Long Chain Branching



Intermediate:

- Constitutive behavior (G', G'')

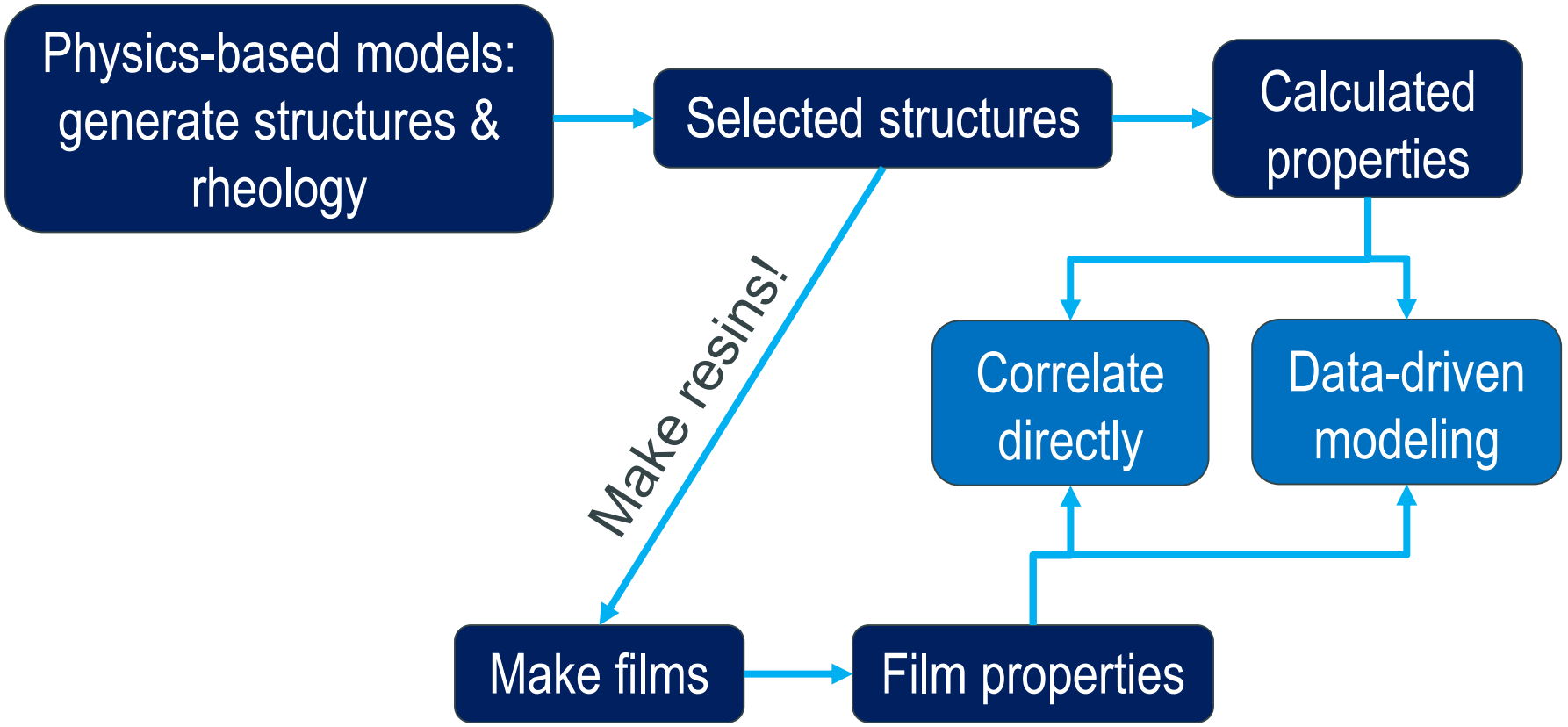


Outputs/Target film properties:

- Haze
- Gloss
- Clarity

Fundamental Modeling in series with Experiments

Fundamental theory as a driver for experiments
Use data-driven modeling to close the loop



Take Away Message

- Theory development is not industries primary goal... but... fundamental understanding is of vital importance!
- Choice of modeling techniques → pragmatic
- Data-driven modeling is easier to relate to reality, and is generally a bit quicker.
- First-principle modeling provides us with a better understanding of the problem at hand.
- The combination of the two, however, is a double win!
  - Theoretical data improves the data-driven modeling.
  - Better connection between theory and experiment.

Thank You

The best way to predict the future is to invent it.

Theodore Hook