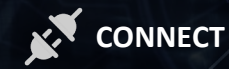


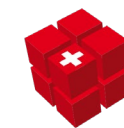


Fall Series 2021  
Modeling & Simulation  
16 Nov 2021



# Computational design and discovery of new processing routes for advanced manufacturing

Dr. Vladyslav Turlo  
Empa

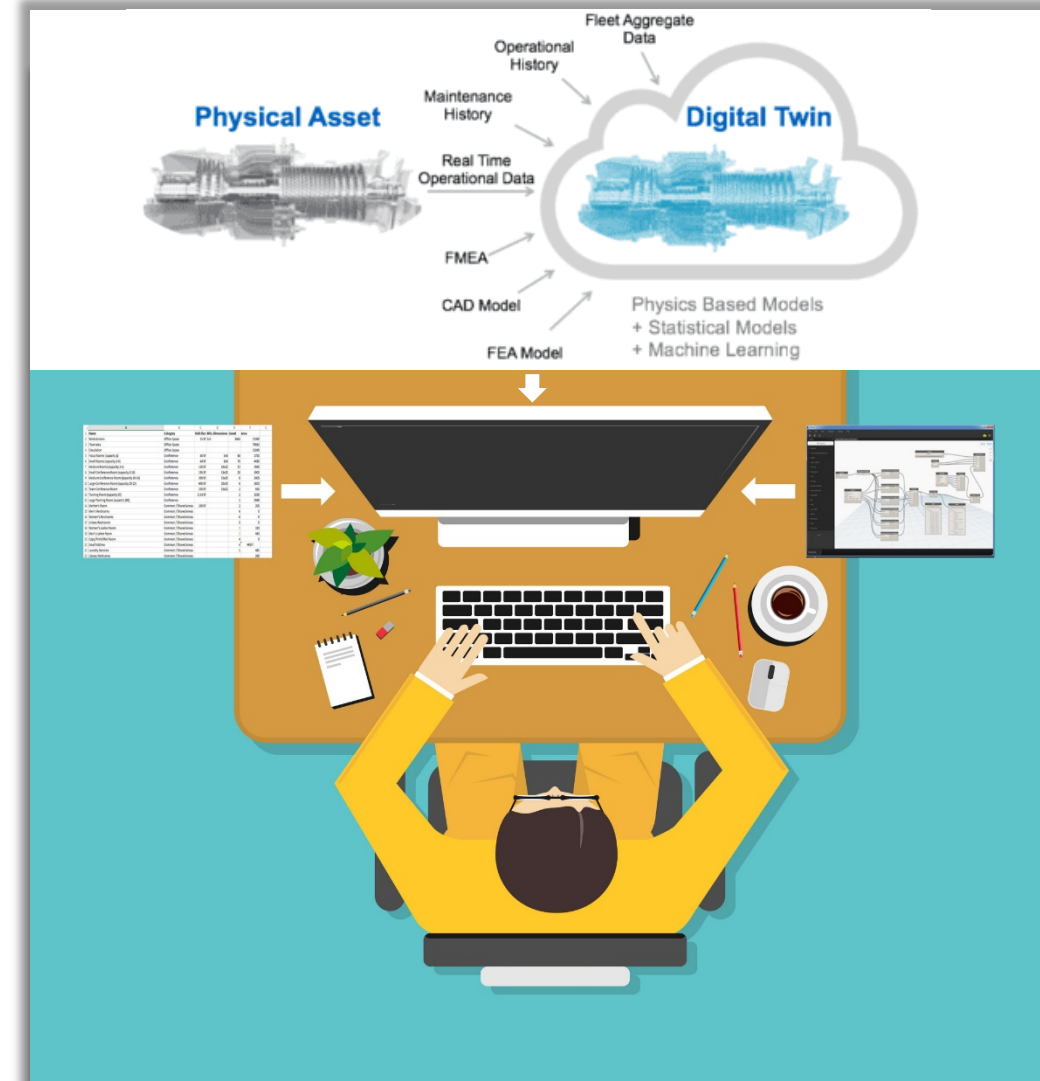


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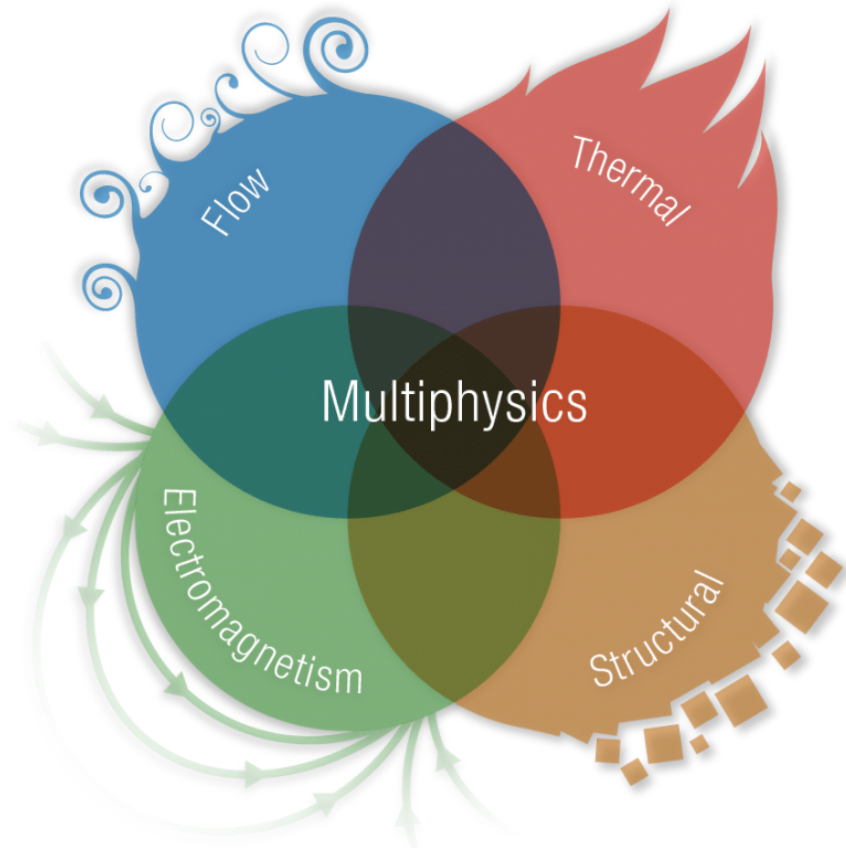
# Motivation «Digitalization»

- **What if you can design new processing routes in front of your computer?**
- **Saving your time and resources**, while dealing with the high complexity
- **Performing ONLY meaningful experiments** that
  - Bring new knowledge
  - Lead to scientific discoveries
  - Drive the innovation

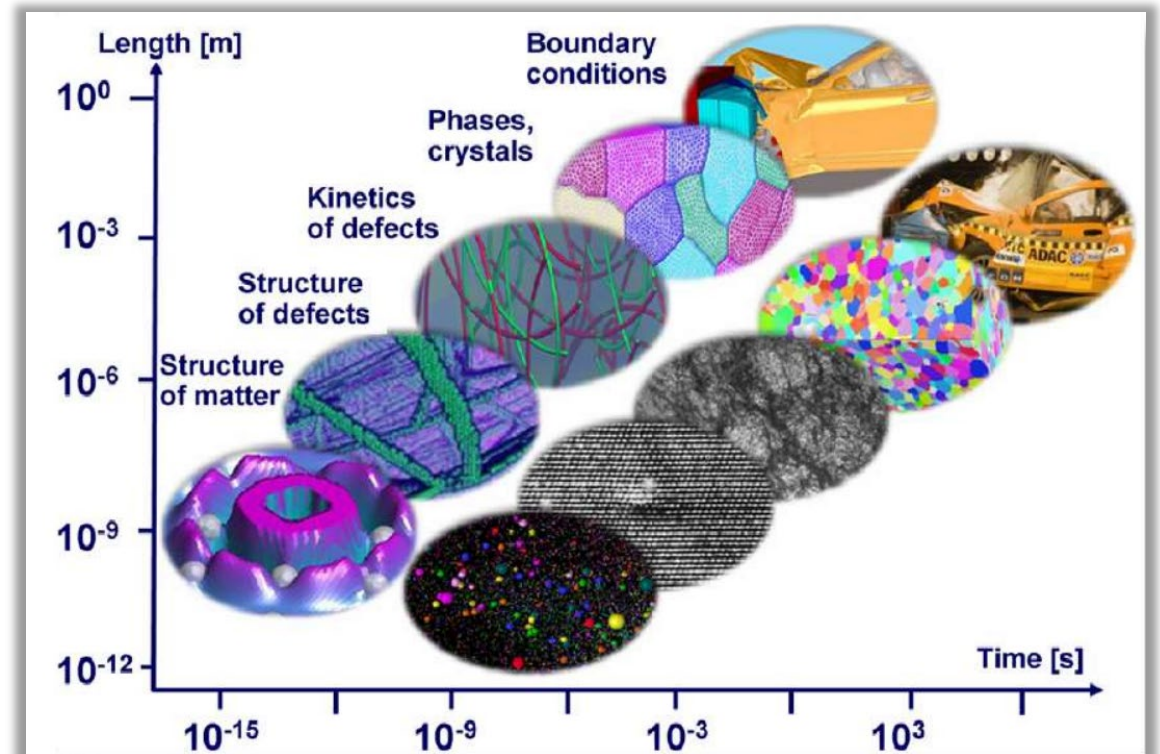


# Understand the nature of your process

- **Single physics vs. multi-physics**

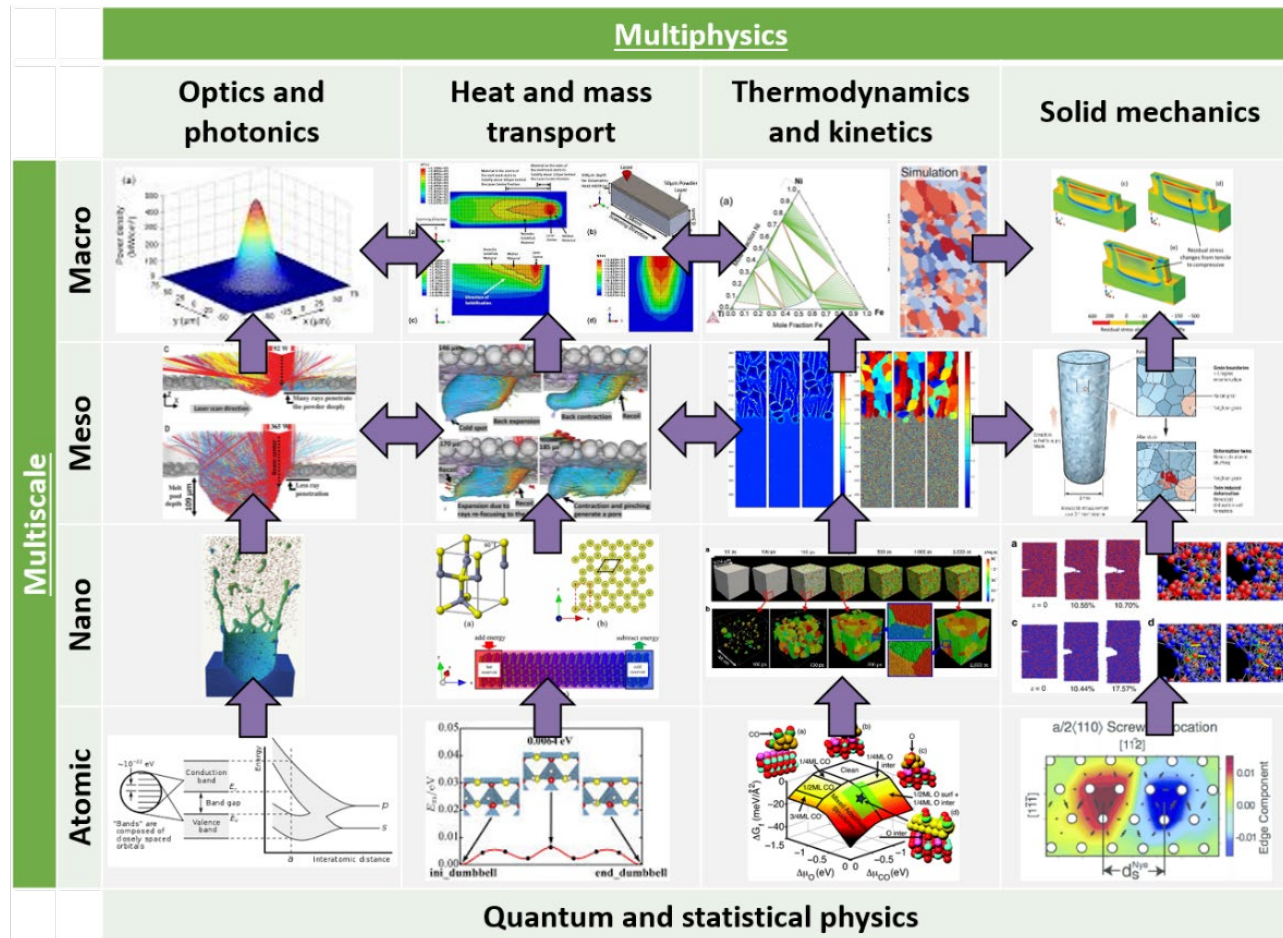


- **Single scale vs. multi-scale**



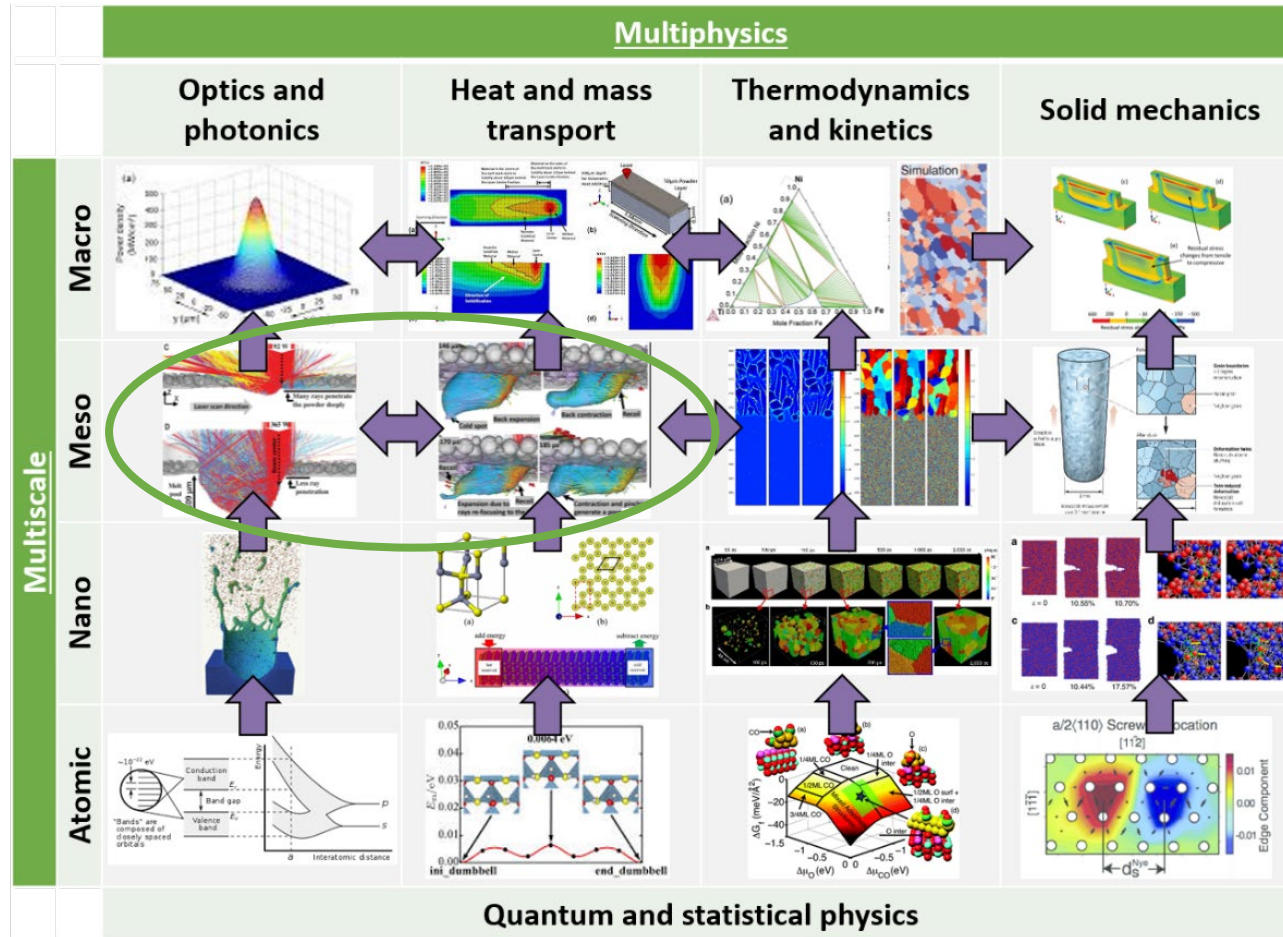


# Example – Laser 3D printing

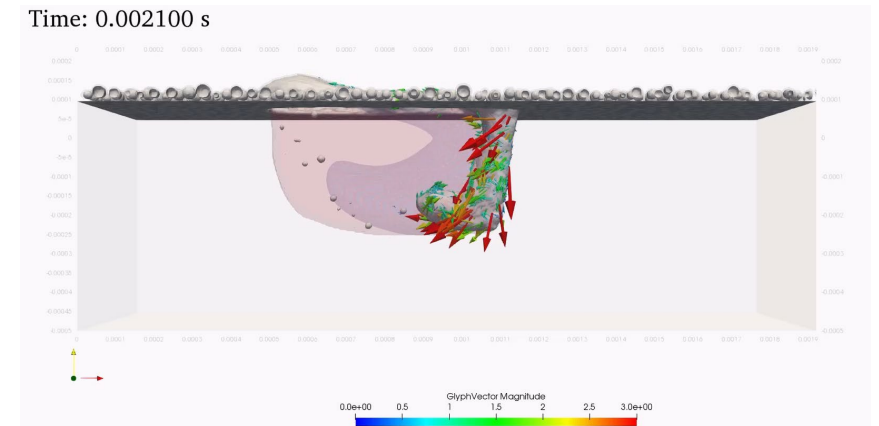


1. Define important physics and scales, and identify relations between them
2. Isolate phenomena of interest
3. Start with a simple model from the literature
4. Stick to one method, software, and scale if possible

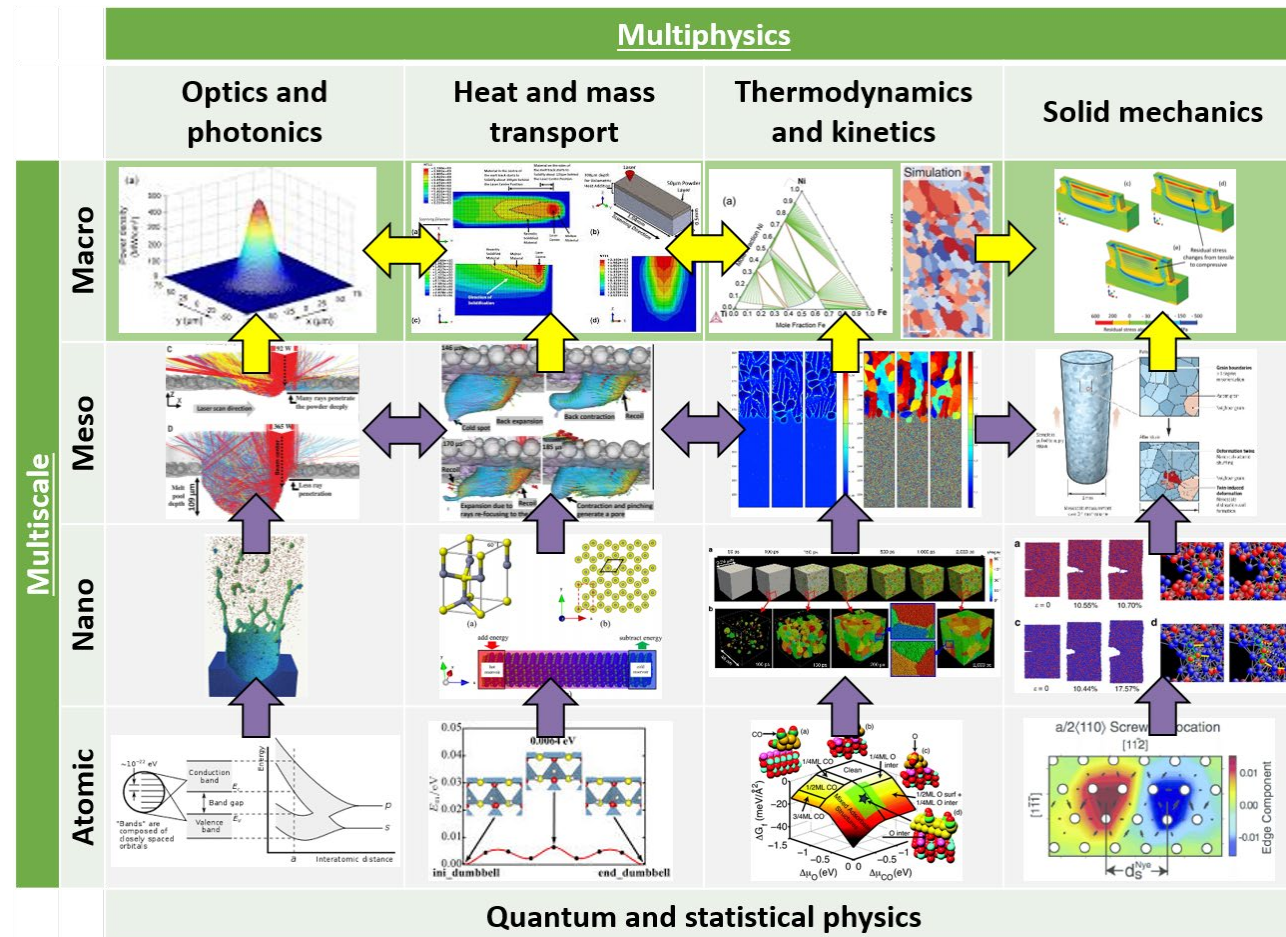
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# Macroscale process modeling



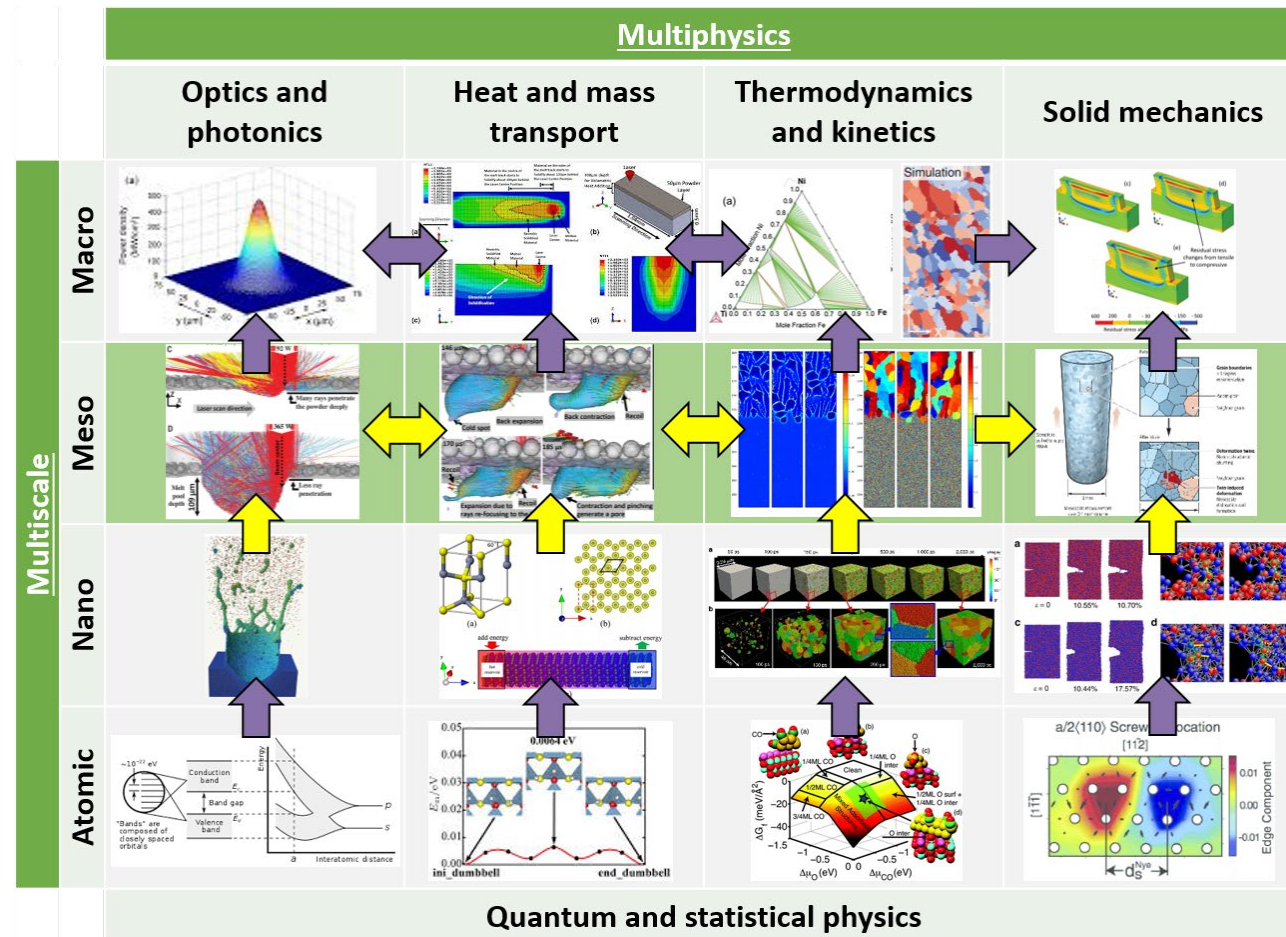
- Enabled by a wide range of commercial software



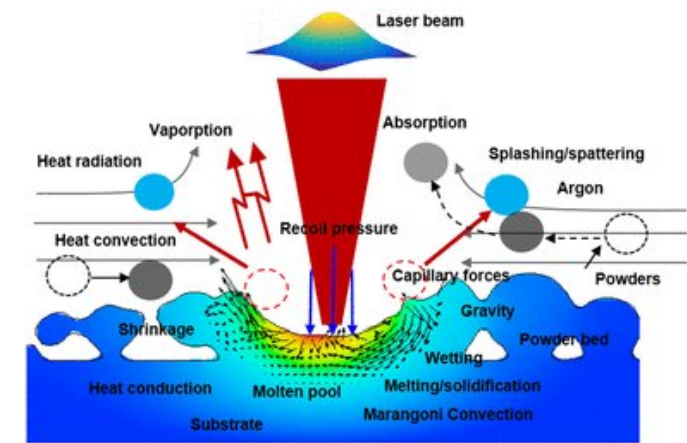
- Apply effective parameters, measured experimentally or obtained from lower scale models



# Mesoscale process modeling

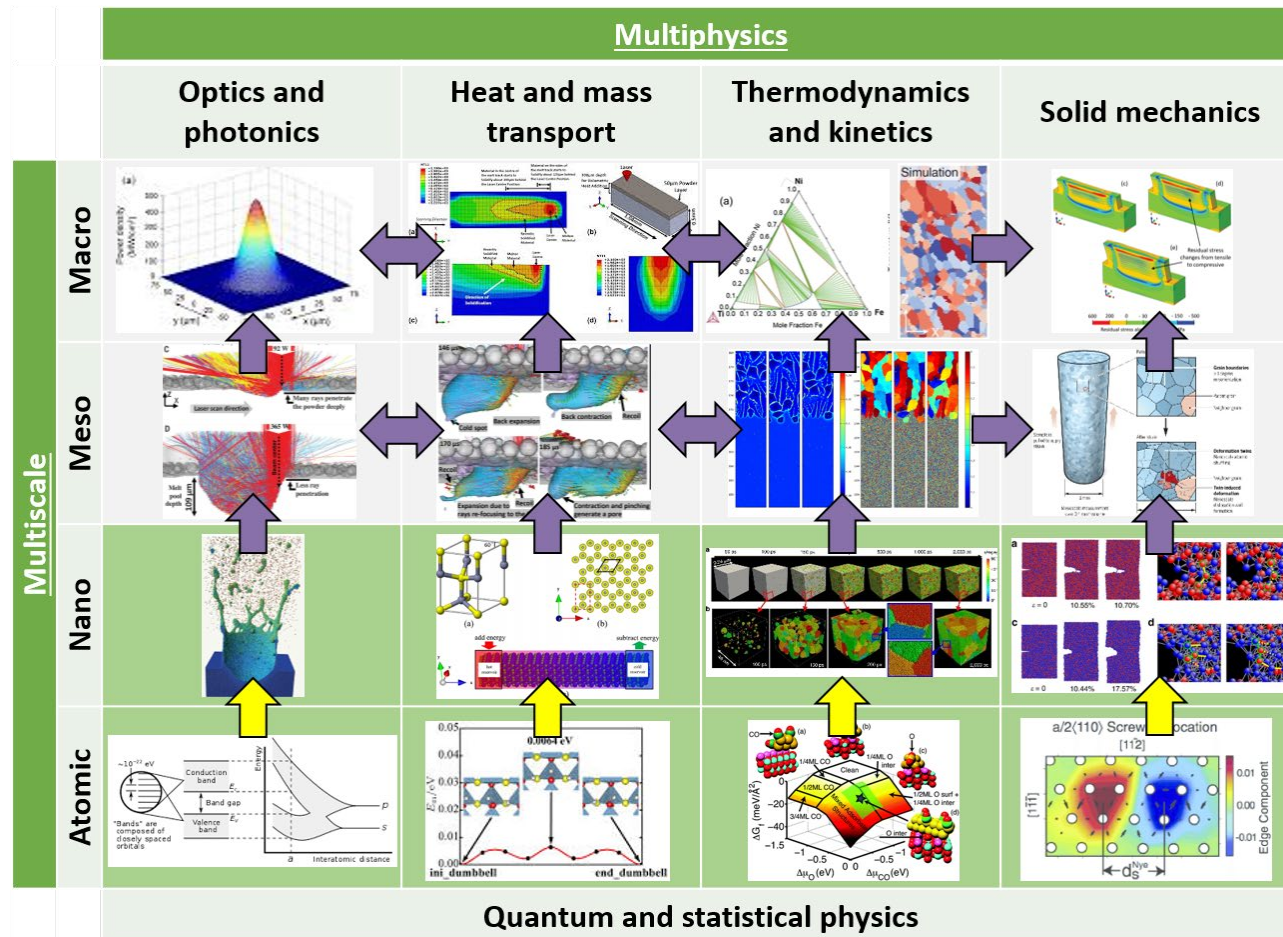


- Explicit and highly complex



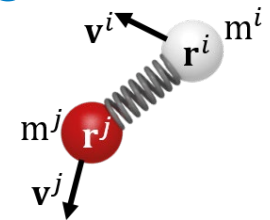
- Contain the largest number of parameters
- Use real material properties

# Atomic-to-nanoscale process modeling



- Multi-physics is realized through interatomic or pseudo potentials

Empirical or  
Semi-empirical or  
First principles (DFT)



- All material properties are defined!

Statistical physics

“macroscopic” properties  
(temperature, pressure, etc.)

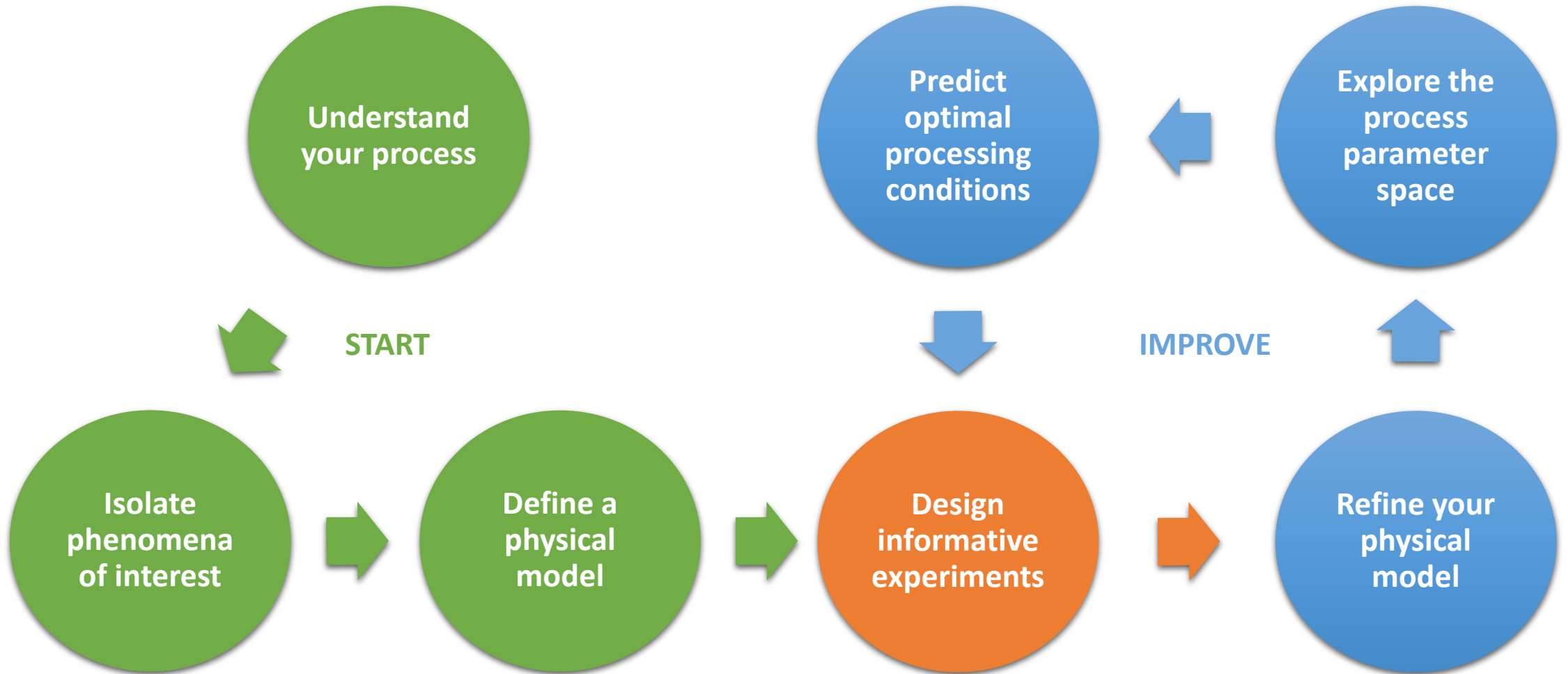


Quantum physics

“microscopic” information  
(atomic positions, charges, forces, etc.)



# Essential synergy with experiment



# Take Home Messages



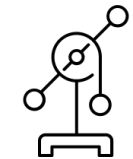
- **Understand the nature of your process**

Identify essential physics and proper scales, and define relations among them



- **Find the right numerical methods and software**

Aim to use only one software per model and do not hesitate to ask for help from developers



- **Start with a simple model**

Try to minimize the number of unknown model parameters



- **Improve the predictive power on your model**

Design proper experiments, aim for maximum information with minimum efforts

# Thank you very much for your attention!

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Materials Science and Technology



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