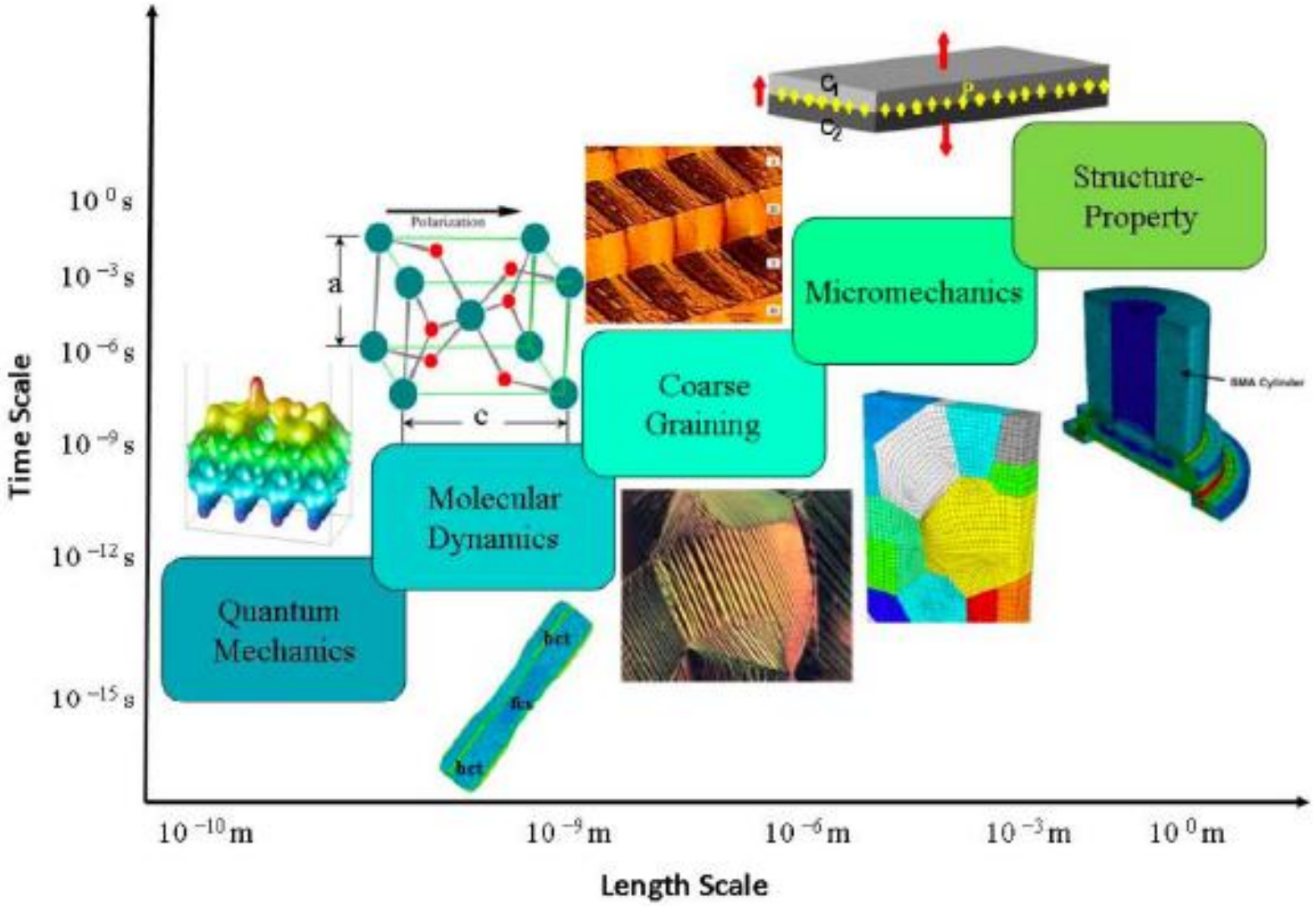
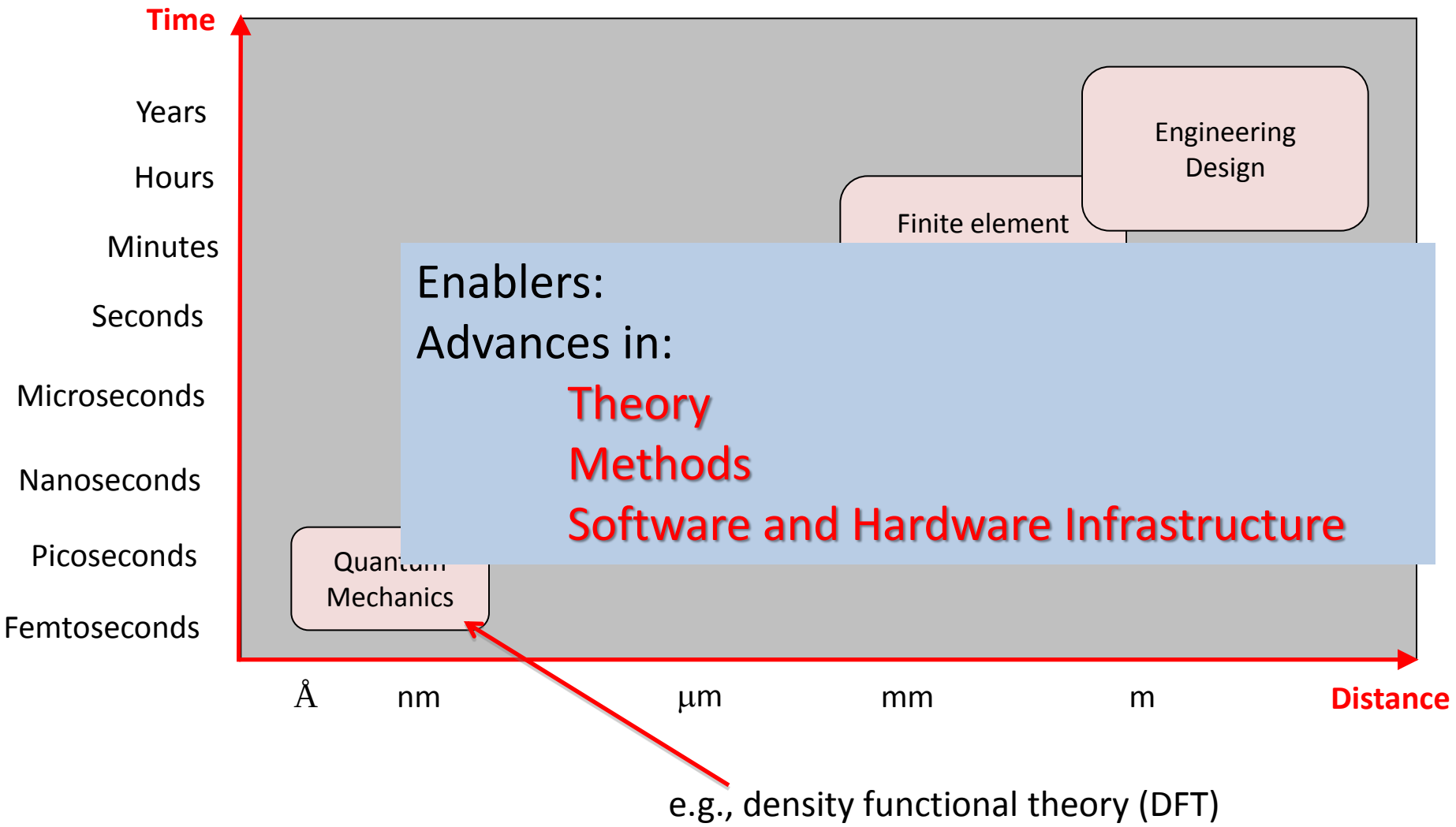
Computational Materials Science

Theme 3:
Fostering Science-based Discovery/Optimization of Novel Multifunctional Materials through Computational Materials Science



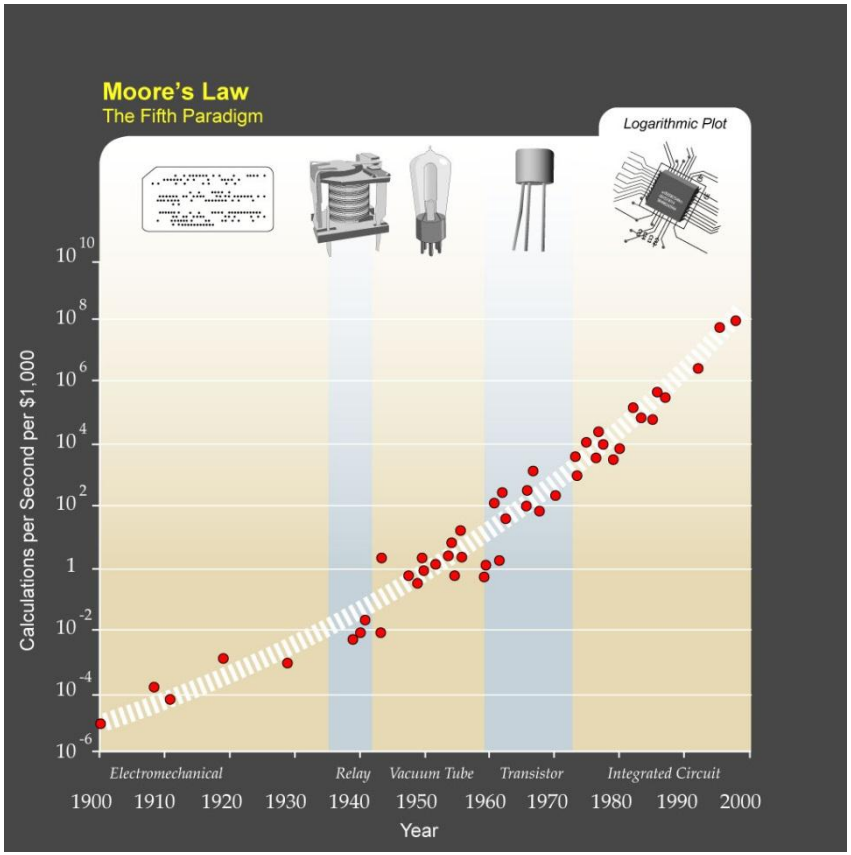
CMS at different "scales"



- If more than one "box" is involved in a computation ➔ multi-scale modeling

Where are we now?

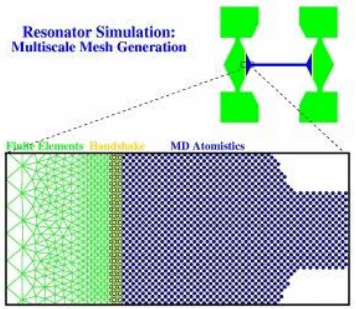
- Theory: Acceptable Level of Maturity
- Methods: Significant advances in past decade
- Infrastructure:
  - Less than a decade ago:
    - Impossible even to think about computer-aided materials design
    - To keep things in perspective:
      - Computing power has increased by two orders of magnitude in 10 years!
      - Will increase by another three in less than ten years
      - Exascale computing



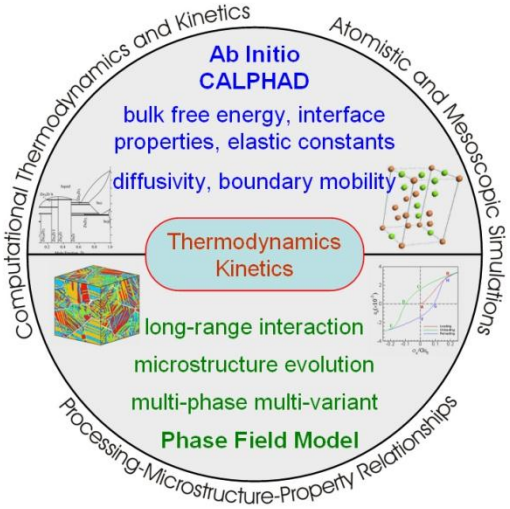
wikipedia

Multi-scale Materials Modeling: Two Paradigms

- Concurrent Modeling:



- Hierarchical Approaches:



Computational Materials Science: How is it used?

- CMS enables:
  - Explain phenomena beyond experimental resolution
  - Discover new unexpected phenomena
  - Predict properties
  - Design new materials
    - Constrains experimental search space

- (General) Challenges:
  - Concurrent or hierarchical modeling?
  - How to exchange information between scales?
  - What to do when phenomena at multiple scales are tightly coupled (parameter-passing not sufficient)
  - How to decide what to ignore?
  - Bottom-up, or top-down?

- (IIMEC) Challenges:
  - How can we use CMS effectively within IIMEC collaboration?
  - Can we take grand challenges from our experimental colleagues?
  - What methods and techniques do we have?
  - What capabilities are yet to be developed?