Rebooting Materials Design and Discovery

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6th European Conference on Computational Mechanics (ECCM 6)

7th European Conference on Computational Fluid Dynamics (ECFD 7)

European Materials Modeling Council: Training for Translators I (MS147A)

Outline

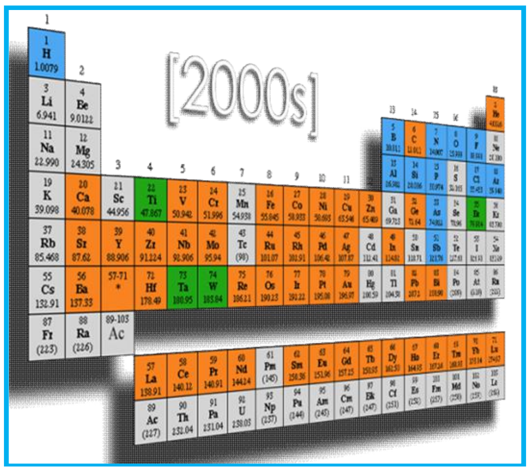
- Materials modeling: *theory* vs. *reality*
- Practice of Materials Modeling
  - Discovery vs. Design
  - Challenges in Semiconductors
  - Vision, strategy, & planning
- Materials Modeling Software Design
- Summary

Materials Modeling *in Theory*

- Materials design and discovery (atomic scale) impacts broadening:
  - Drug discovery (gold standard)
  - Semiconductors (early adopter) ← Large corporation
  - Nanotechnology (nanoparticles) ← Small defense contractor
  - Manufacturing (structural alloys)
  - Batteries/Energy Industry (high growth in last 5+ years)
  - Chemistry (steady chemical and polymer R&D)
  - Materials Genome/NOMAD/Materials Project/SUNCAT /TRI/Citrine (NIST/DOE/DOD/NSF/public/private)

Focus of this talk

Ex: Intel Materials Modeling Range



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Industrial impacts of materials modeling are still in an early stage

/TRI/Citrine (NIST/DOE/DOD/NSF/public/private)

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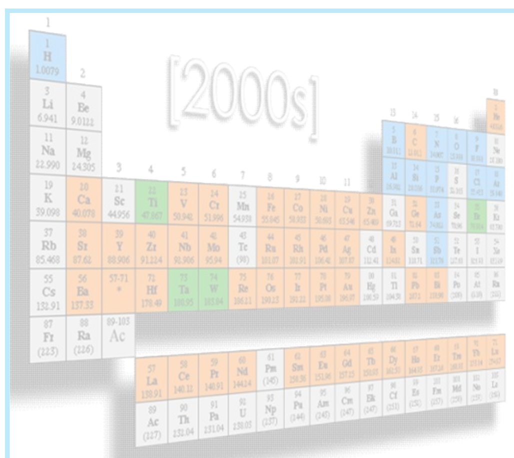
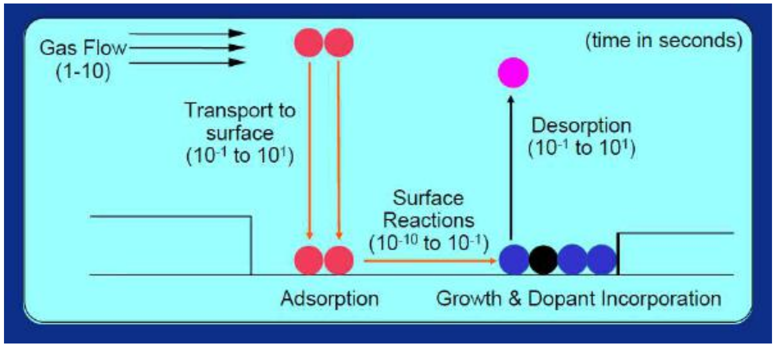


Materials Modeling *in Reality*

- Materials translators are effectively consultants
  - Significant customer learning curve/training required *(risk)*
- Efficacy/impacts limited by accessible distance/time scales and accuracy (*translation risk: over-promised)*

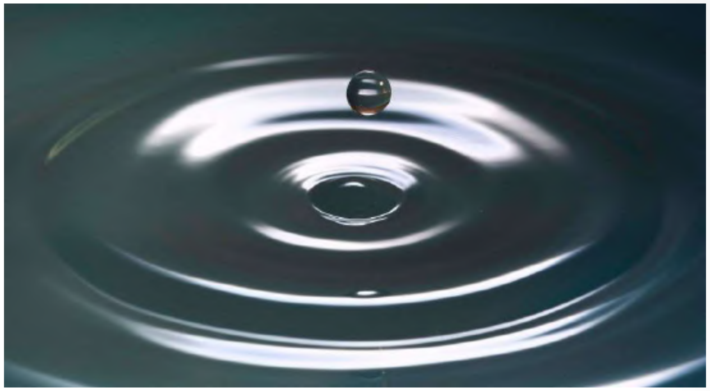
Ex: Range of time and length scales required for Atomic Layer Deposition modeling



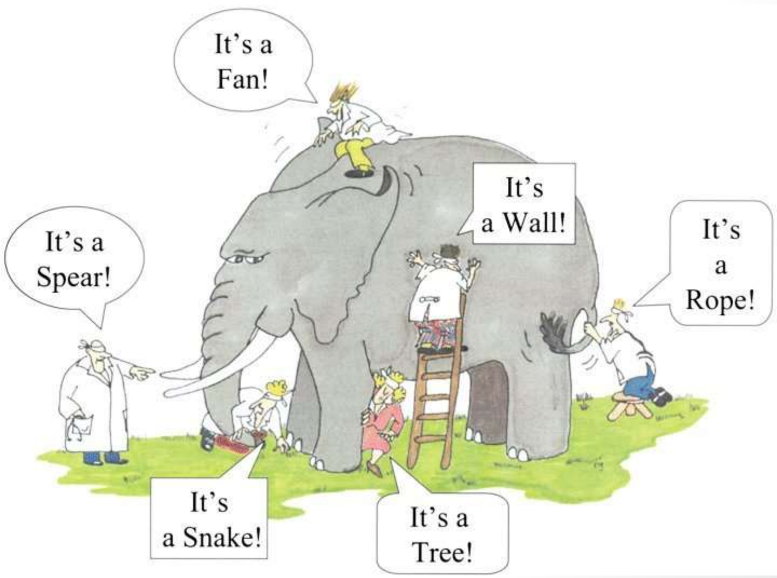
- No silver bullet:
  - Totality of modeling + recommendations + integration with experimentalists is critical
- Impacts to-date lag more mature CFD, FEA, & EDA
  - Hypothesis: Due to failures in both materials modeling translators **practice** and **software**

Materials Modeling in Practice: *A Diversion*

- Is it a "particle" or a "wave"?
  - Neither – reality more complicated
  - "Particle" and "wave" - simplified models (sweep under-the-rug the complexity of reality)

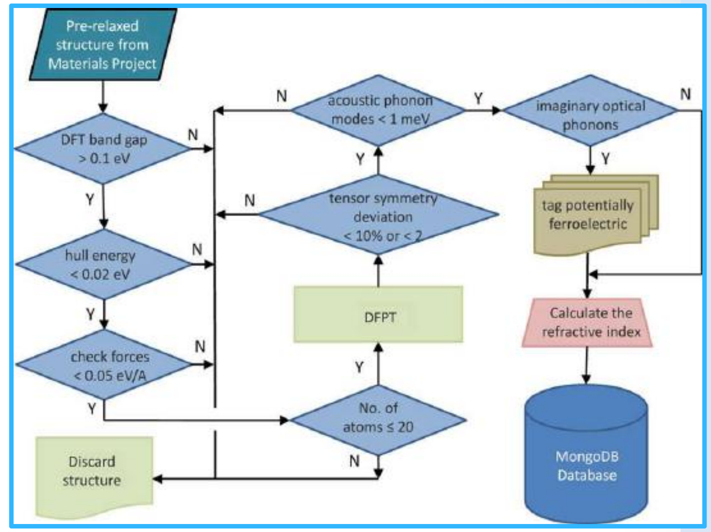


- Translators/scientists often mistake their models for reality
  - <u>Recommendation:</u> spend more time living in reality than the world of your models



In Practice: Shift From Discovery to Design

- 2 types of typical problems:
  - <u>Screening:</u>
    - *Input:* Materials (A to W) +
      Properties (X, Y, & Z)
    - *Output:* Sub-set of materials (A, H, & J)
      With properties (X, Y, & Z)
  - <u>Optimization:</u>
    - Input: Material (A_0) & Properties (X_0 & Y_0)
      With targets (X_1 & Y_1)
    - Output: Alternate material (B) or re-design (A_1)
      With properties (X_1 & Y_1)

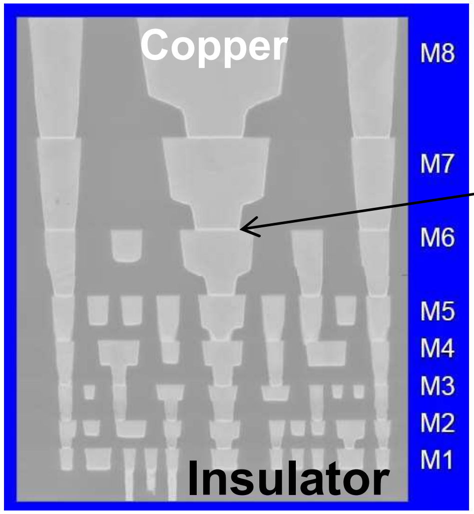


[Nature (Pearson & Prinz)]

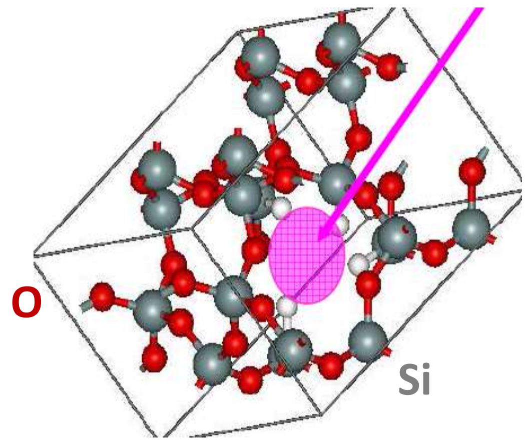
- “Discovered” 1000’s of materials in my career
  - Unable or predict, procure, produce, or productize
- <u>Recommend</u> focusing more efforts on the design of:
  - Slides, experiments, and integration strategy

In Practice: Integration Challenges - Examples

- Semiconductor chips contain numerous material interfaces:
  - Intel's 45nm manufacturing process integrates 9 functional layers
    - Each layer requires 2-5 processing steps and 4 or more materials



- Design of new materials must take into account BOTH:
  - Target material properties (structure-property relationships)
  - Chemistry, mechanical, and thermal interactions with neighboring materials



6/15/2018

Property Vectors: http://propertyvectors.com/

In Practice: Materials Design 2.0 Principles

- Experimentalists have a very hard job
  - Your role: formulate, bounce, and test ideas
  - Your value: reduce experimental iteration ($billion fabrication plants use $million tools)
    - Even identifying why something *didn't* work has value
- Selection criteria variety is critical (co-optimize property vectors)
- Combine as much data as possible (modeling, literature research, characterization data, etc.)
  - Collaboration with disparate background teams critical
- Hierarchical models: study at multiple levels of accuracy and scale if possible
  - Just because you have a hammer, everything isn't a nail

In Practice: Materials Design 2.0 Vision

1. Define problem –
   - Engage with experimentalists
2. Determine property vectors to model
   - Include defects and variations
3. Set expectations
4. Decide on modeling workflow/approach *(all-of-the-above?)*
5. "Support/team-up" not "replace" experimentalists
6. Kick-start/accelerate R&D
   - Demonstrate value

In Practice: Translating Models Into Reality

- One-shot models rarely succeed

Experimentalist (problem definition => modeling request) => HELP!

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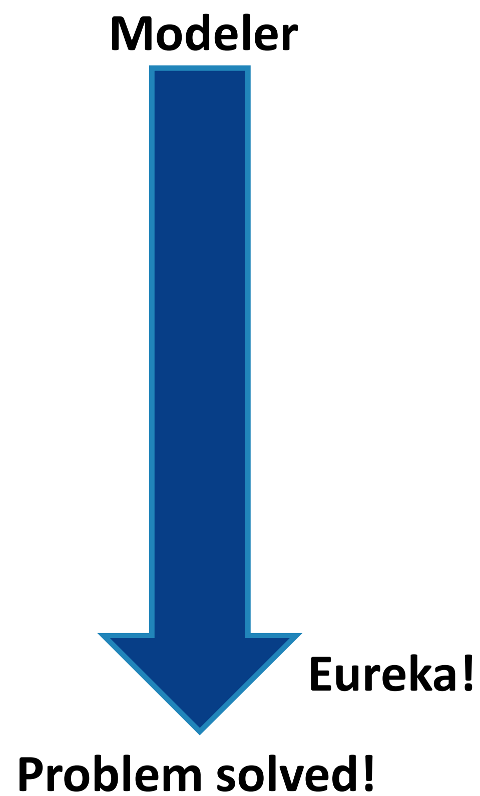

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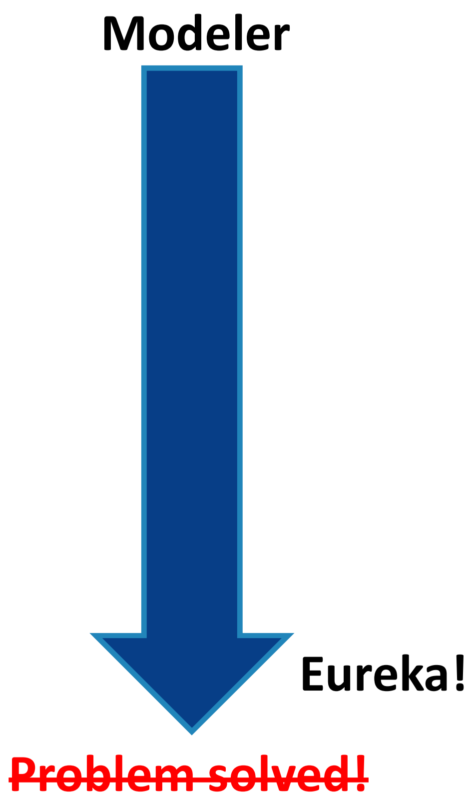

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Modeler (Discovery)

~~Problem solved!~~

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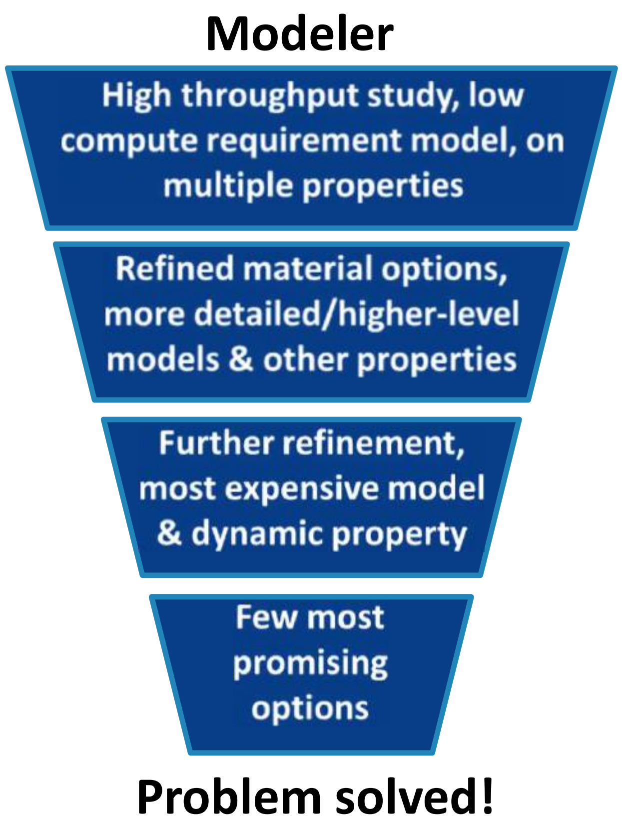

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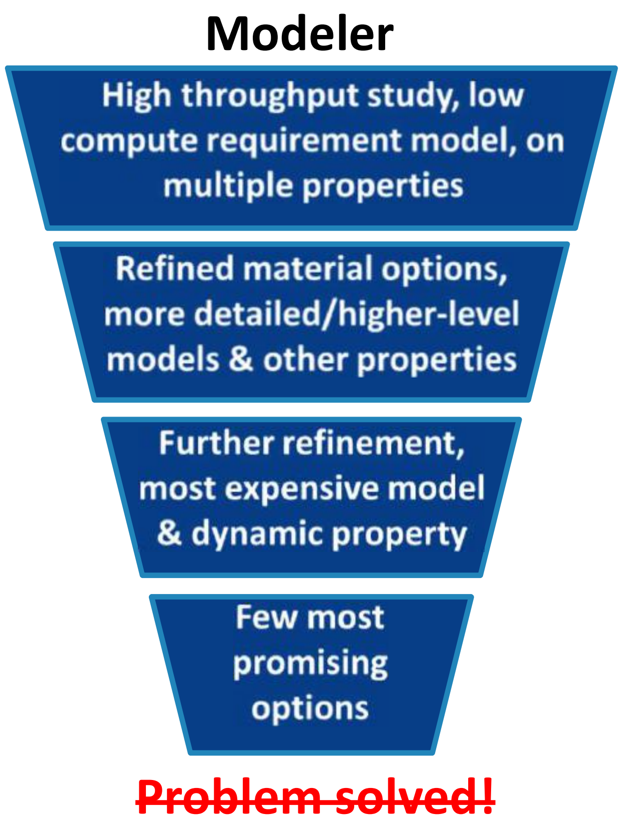

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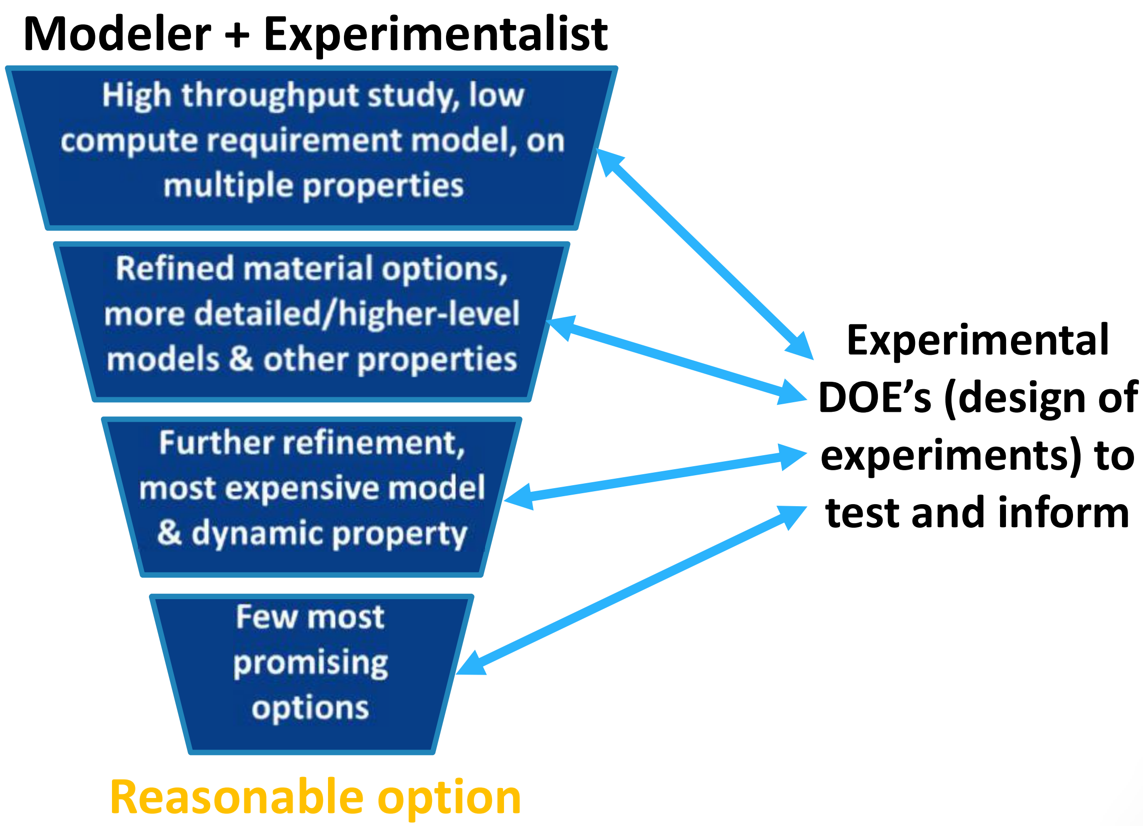

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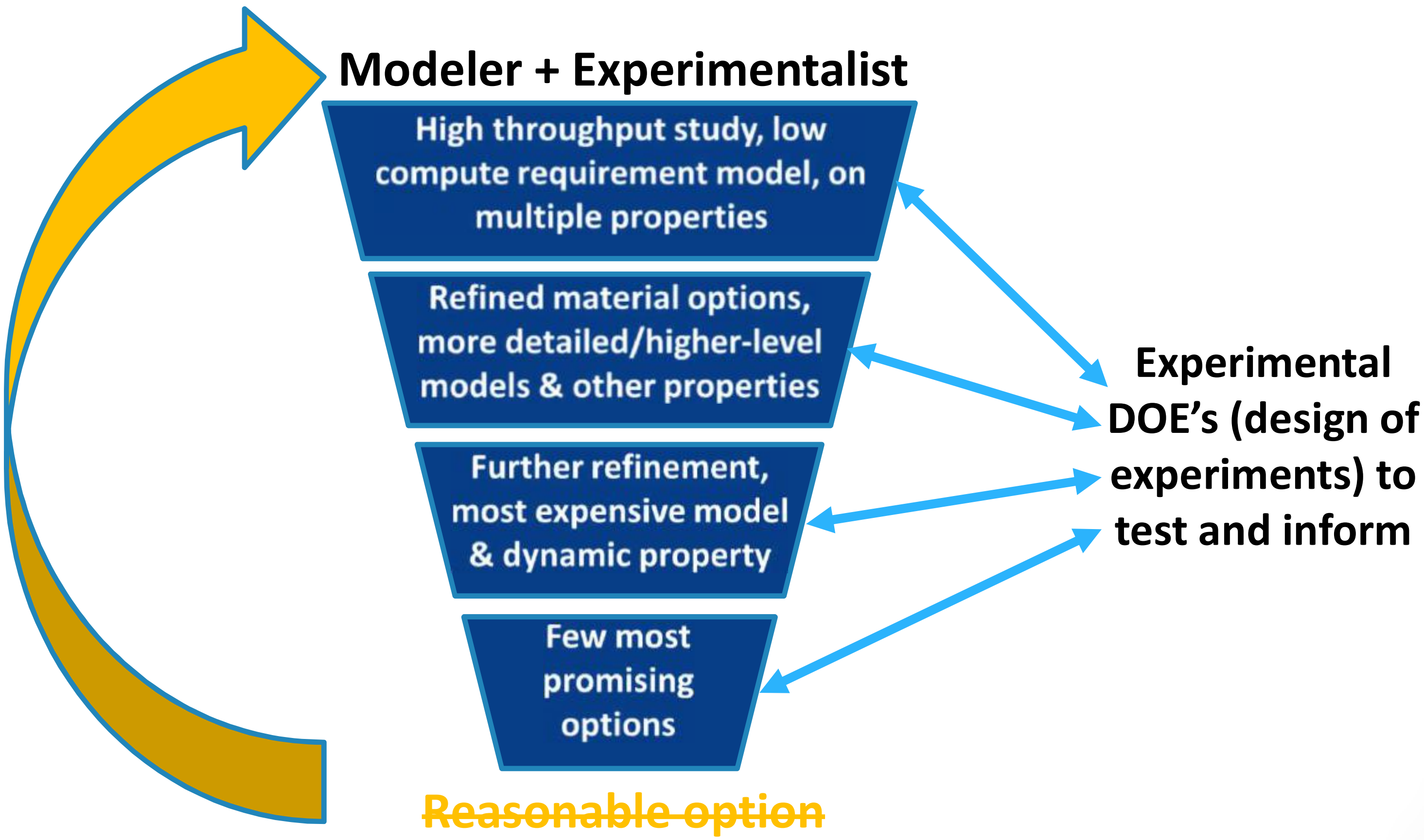

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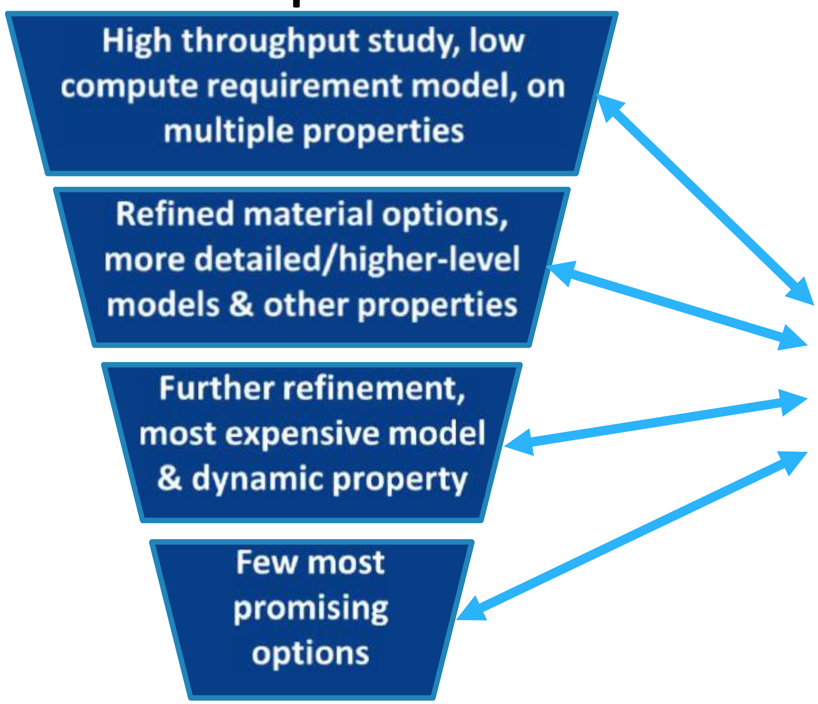
Informed Modeler + Experimentalist – Iteration N



Experimental DOE's (design of experiments) to test and inform

Better option

Reality: hit rate close ~10% is successful *(complications, too expensive, too risky, change in direction)*

In Software: 5% Error Death Spiral

- Experimentalist don’t trust modelers
  - Modelers don’t feel appreciated by experimentalists
  - Usual strategy:
    - Validate and convince
    - Cajole, plead, beg … ☹
- Ph.D.’s trained to be THE world expert
  - Minimize error and maximize depth of insight
  - Develop new functionals/methods to increase accuracy
- Add so-so programming skills
- Recipe for **brilliant software** that is **terrible for productivity and ease of use**

Emulate Software Success Stories

- Schrodinger ($120M drug discovery contract - Sanofi)
  - Heavily parameterized tool for spatial docking of molecules
- Synopsys ($2.8B USD):
  - Drift diffusion plus circuit design
- CFD/FEA Industry (Billons USD):
  - Dependable highly customizable models w/ reliable results
  - Accessible to Bachelor's & Master's level degrees
- All offer:
  - Dependability and reliability
  - Abstraction and implementation of acceptable usage defaults
  - Simplification and automation of workflows (+ accessibility)
- <u>Software developers:</u> focus more on the above and less on 100% accuracy
  - All-of-the-above rarely promise 95% accuracy

Rebooting Materials Design & Discovery: Summary

- Full promise of materials modeling techniques not yet realized – largely a <u>failure in translation</u> that requires a *reboot* of <u>translators</u> behavior:
  - <u>In practice</u>
    - Tight engagement loops with experimentalists
    - Set expectations *(≥95% accuracy likely not possible)*
    - Shift from discovery to design
    - Consider integration with neighboring materials and processing (multiple properties, variations, and complications)
  - <u>In software design</u>
    - Focus on pragmatism with automation and increased engineering judgement

Thanks for your attention!
Any questions?