Characteristics and Management of PSAAP IV Centers

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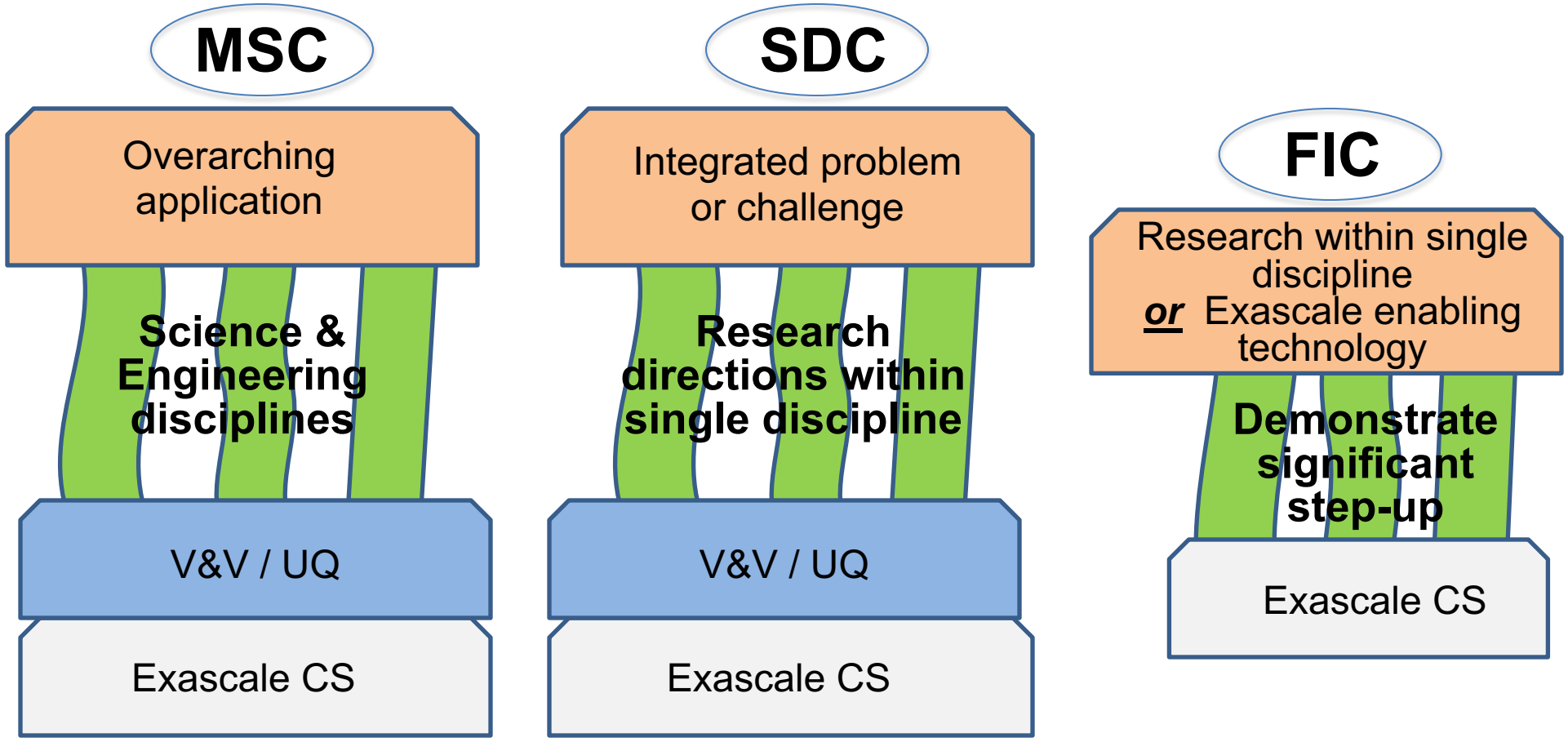
PSAAP IV Pre-proposal Meeting
August 8-9, 2023, Houston, TX
LA-UR-23-28953

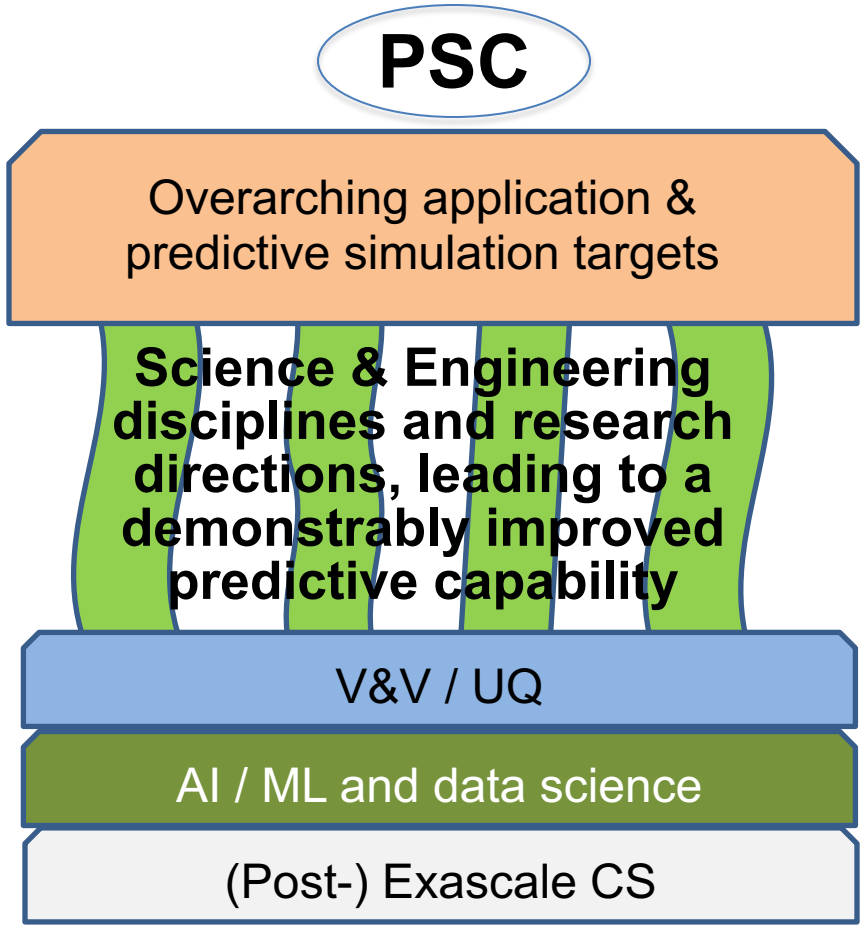
Predictive Science Academic Alliance Program

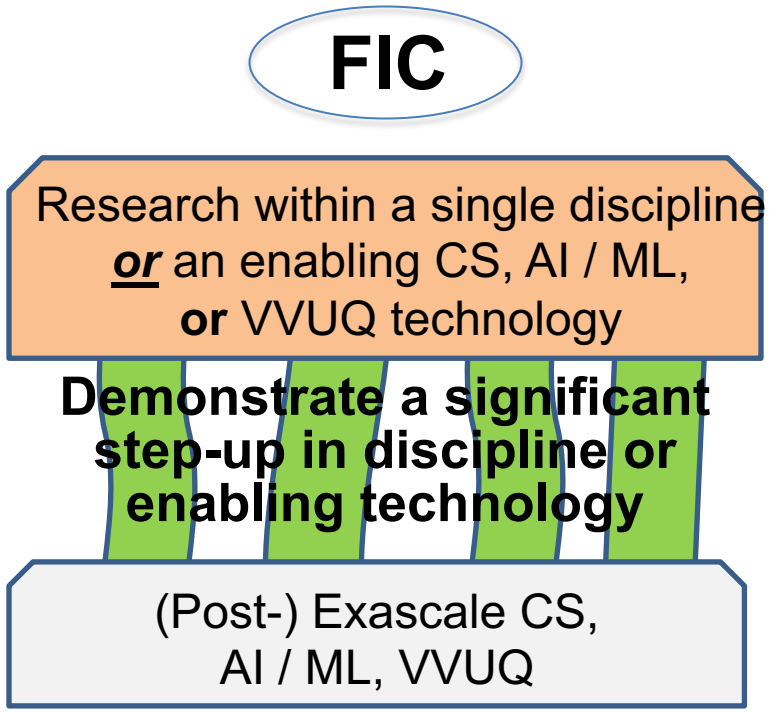
- **Predictive Science:** application of verified & validated computational simulations to predict properties and dynamics of complex systems
- **Primary PSAAP Goal:** establish validated, large-scale, multi-disciplinary, simulation-based *Predictive Science* as major academic, applied research program
- **PSAAP Engages U.S. Academic Community** in making significant predictive modeling & simulation technology advances
- **PSAAP's *Cooperative* Agreements with Universities** involve educating, training, recruiting, and working with top researchers in key disciplines required by stockpile stewardship

Multidisciplinary Simulation Centers – *MSC*
Single Discipline Centers – *SDC*
Focused Investigatory Centers – *FIC*



Predictive Simulation Centers – *PSC*
Focused Investigatory Centers – *FIC*





Tri-Lab Sponsor (TST) & Review (RT) Teams

- **Separate tri-Lab TST and RT for each Center**
  - **Two members from each Lab for MSCs and SDCs (one per Lab for FICs)**
- **TST Serves as technical interface between Centers and Labs**
  - **Works toward ensuring the Center success**
  - **Meets with Centers at least once annually (Spring)**
    - Not a formal review – an informal cooperative exchange
- **Annual Review (Fall) organized / conducted by AST & RTs**

PSAAP Focus on Four Major Integrated Areas

- **Discipline-focused research to further predictive science enabled by effective (post-) exascale computing;**
- **Developing and demonstrating technologies and methodologies supporting effective (post-) Exascale computing in S&E applications;**
- **Utilizing and advancing state-of-the-art AI / ML and data science technologies for predictive simulations;**
- **Predictive Science based on verification and validation, and uncertainty quantification (V&V/UQ) for large-scale simulations.**

Examples of integrated problem/challenge

- **Material science**
  - **Atomistic methods**
  - **Single-crystal response**
  - **Bulk material properties**

  } Integrated problem: computation of bulk response

- **Warm dense matter (WDM)**
  - **Inter-atomic correlations**
  - **Complex atomic excitations**

  } integrated problem: computation of WDM properties

- **Turbulence**
  - **Shock / Acceleration driven turbulence**
  - **Coarse grained simulations**

  } Integrated problem: late-time responses in multiple-shocked material-interface systems

These are examples, not intended as prescriptive!

Evolution towards Predictive Simulation Centers (PSCs) and FICs …

Multidisciplinary Simulation Center

- **Integrated Centers in ASAP, PSAAP I, PSAAP II , PSAAP III**
- S&E based simulation modeling paradigms for Center's *Questions of Interest*

Single-Discipline Center

- **This type of Center was introduced for PSAAP II**
- Produce cutting-edge S&E progress, enabled by exascale CS, supported by pervasive V&V/UQ

Focused Investigative Center (FIC)

- **Introduced for PSAAP III**
- Demonstrate compelling and significant (step-up) scientific advance in single discipline or enabling exascale technology.

PSAAP IV will support two Center types: Predictive Simulation Centers, and Focused Investigatory Centers

(all are expected to be 5-year awards)

Predictive Simulation Centers: $1.5M – $3.5M/year

- ➢ **Research focus on scalable application simulations (or simulation workflows), targeting large-scale, integrated multidisciplinary or broad single-science/engineering problems**
- \+ **Develop computer science methodologies that will advance (post-) Exascale computing**
- \+ **Utilize and advance state-of-the-art AI / ML and data science technologies**
- \+ **Demonstrate integrated, verified, and validated predictive simulation with uncertainty quantification**
- \+ **Range of award sizes with commensurate expectations:**
  Centers proposing the $3.5M maximum will be expected to make significant advances in all areas (multidisciplinary application, post-exascale CS, AI / ML, and VVUQ).

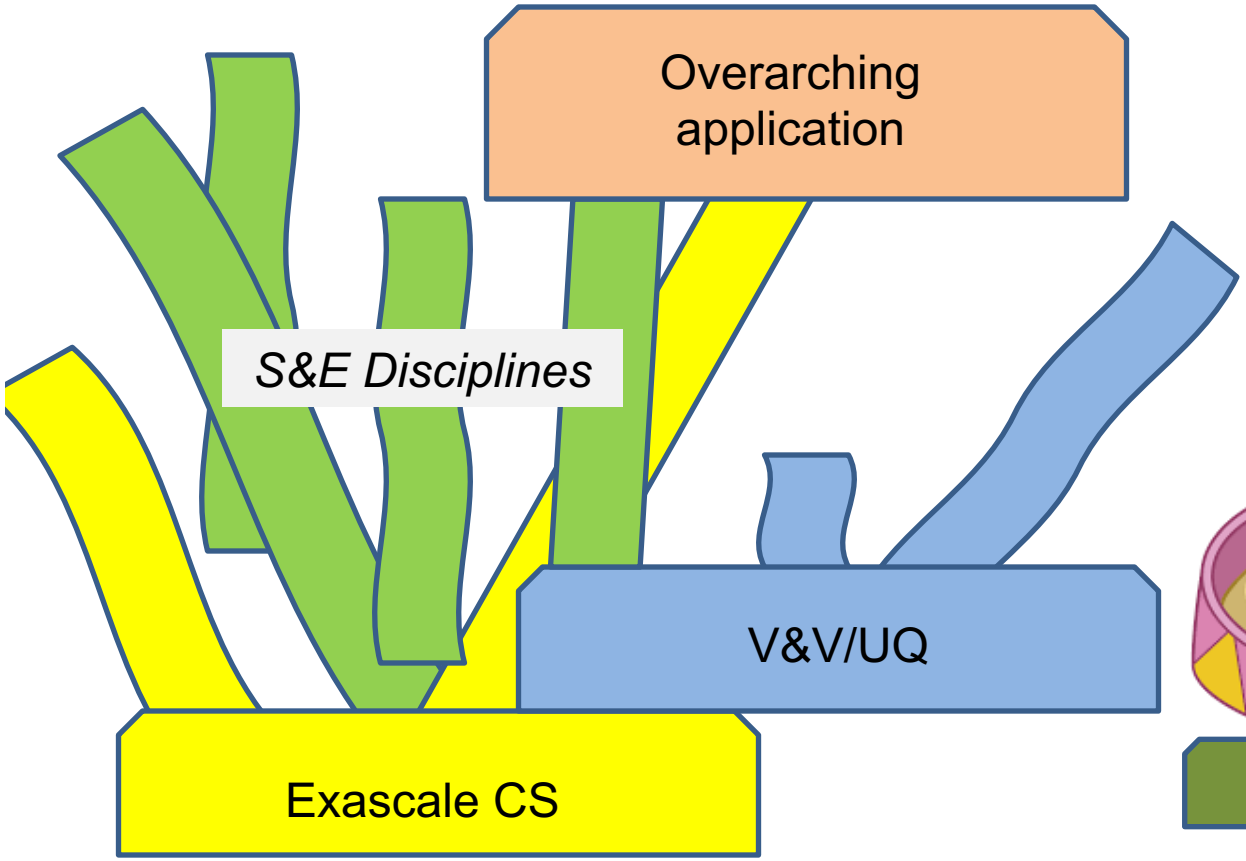
Focused Investigatory Centers (FICs): $0.5M – $1.0M/year

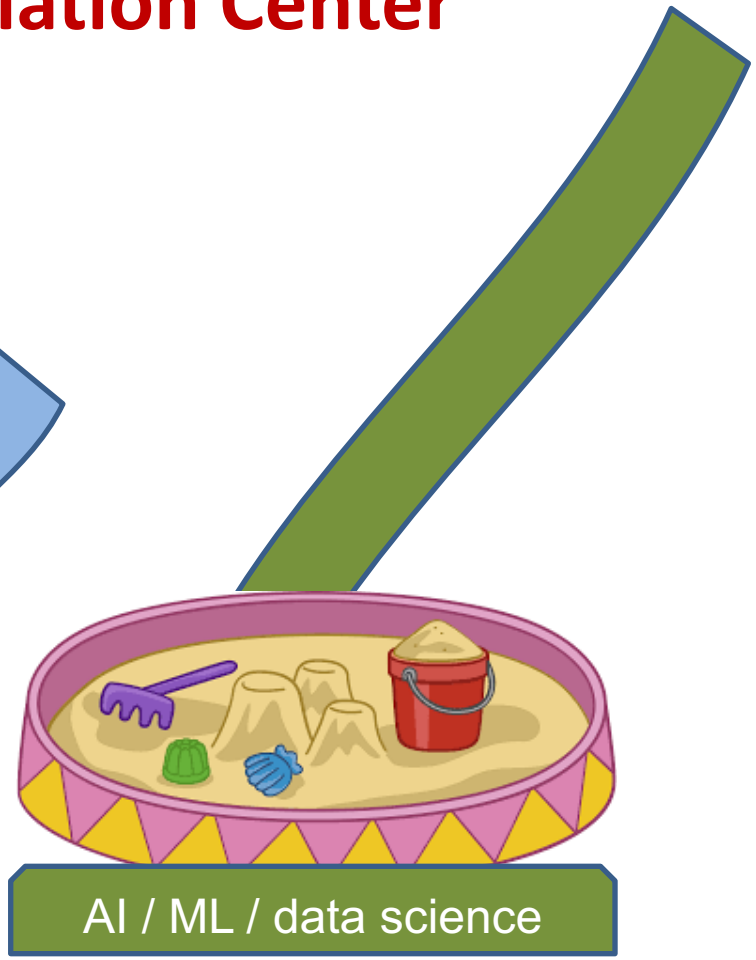
- ➢ **Specific research topic in one or more S&E domains or CS, AI / ML, or VVUQ enabling technologies**
- \+ **Demonstrate significant advance in S&E domain or an enabling technology**

PSCs : Centers Integrating all Research Components

- **Exascale advances *must be* demonstrated for Center's S&E simulations**
- **S&E advances *must be* enabled by exascale-oriented computer science**
- **S&E advances *must be* enabled by AI / ML / data science technologies**
  - **Enhanced predictive capability for either integrated multidisciplinary or broad single S&E problem**
- **V&V/UQ *must be* fully integrated in all aspects of computational science**
  - **V&V/UQ need not be innovative, but must, at minimum, conform to best practices**

A loose collection of independent “stove piped” research projects is NOT acceptable as Predictive Simulation Center





Predictive Science Issues Revisited

Modeling, Observations and Predictive Science *for Questions & Quantities of Interest*

- ***Essentially, all models are wrong, but some are useful – George Box***
- ***Everything should be made as simple as possible, but not simpler – Albert Einstein***

Computational & Laboratory Observations are inherently Intrusive

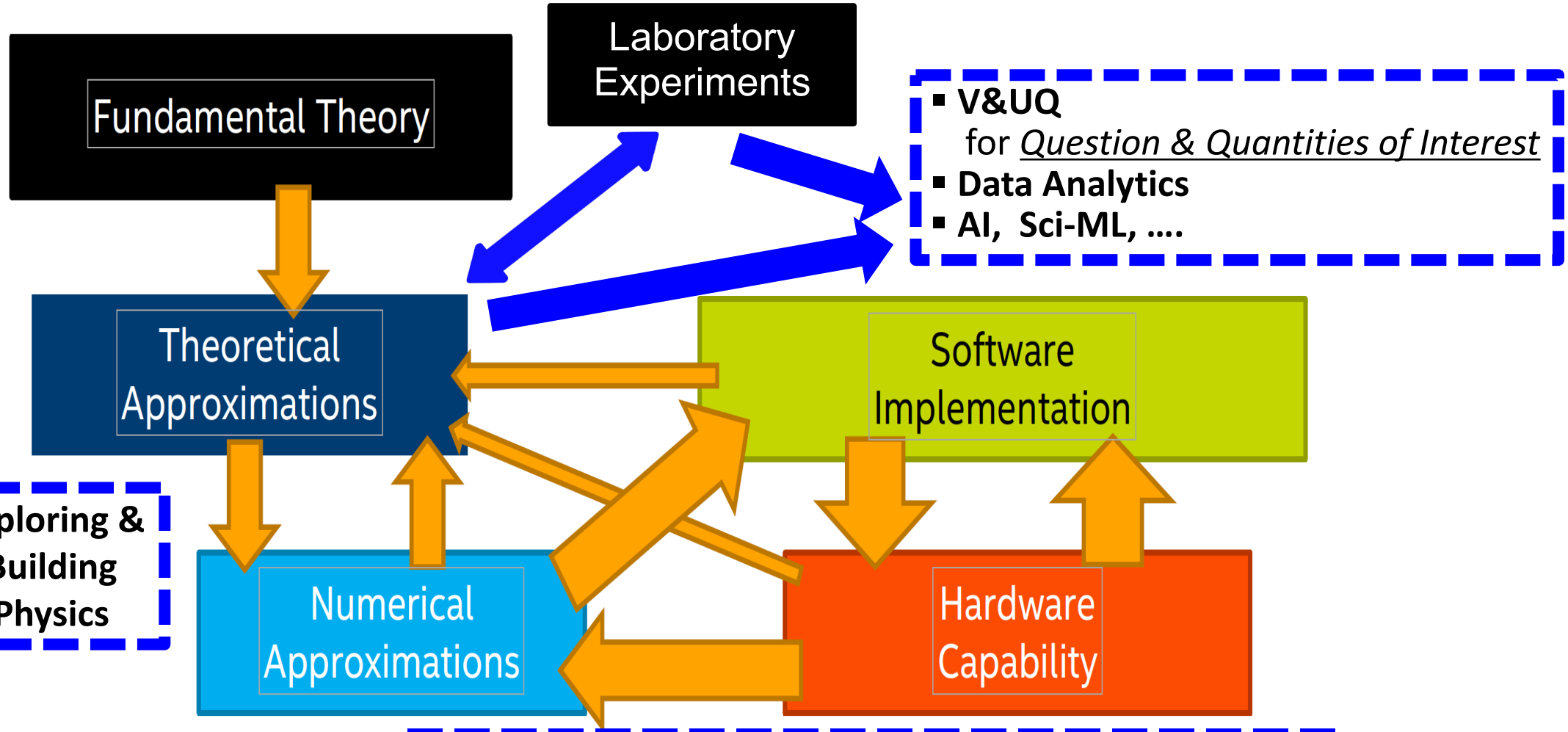
[due to characterization & modeling uncertainties]

while nature controls the physics independently

- ***What we observe is not nature itself, but nature exposed to our method of questioning.***

  Our scientific work in physics consists in asking questions about nature in the language that we possess and trying to get an answer from experiment by the means that are at our disposal ***– Werner Heisenberg***

Predictive Science Constrained by Strongly Interacting, Models, Experiments, Theory, Numerics, Software, and Hardware



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