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NEAMS Waste IPSC

- Verification & Validation Plan
- Frameworks & Infrastructures Gap Analysis

NEAMS PI Meeting

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Outline

Verification & Validation Plan

- Key Concepts
- VV-UQ Practices
- VV-UQ Evidence Information Management (EVIM)

Frameworks & Infrastructures Gap Analysis

- Enabling Infrastructure
- Analysis Workflow Framework

Path Forward

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Verification & Validation (V&V) Plan for Modeling & Simulation (M&S) Capabilities

Team:

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Reviewers:

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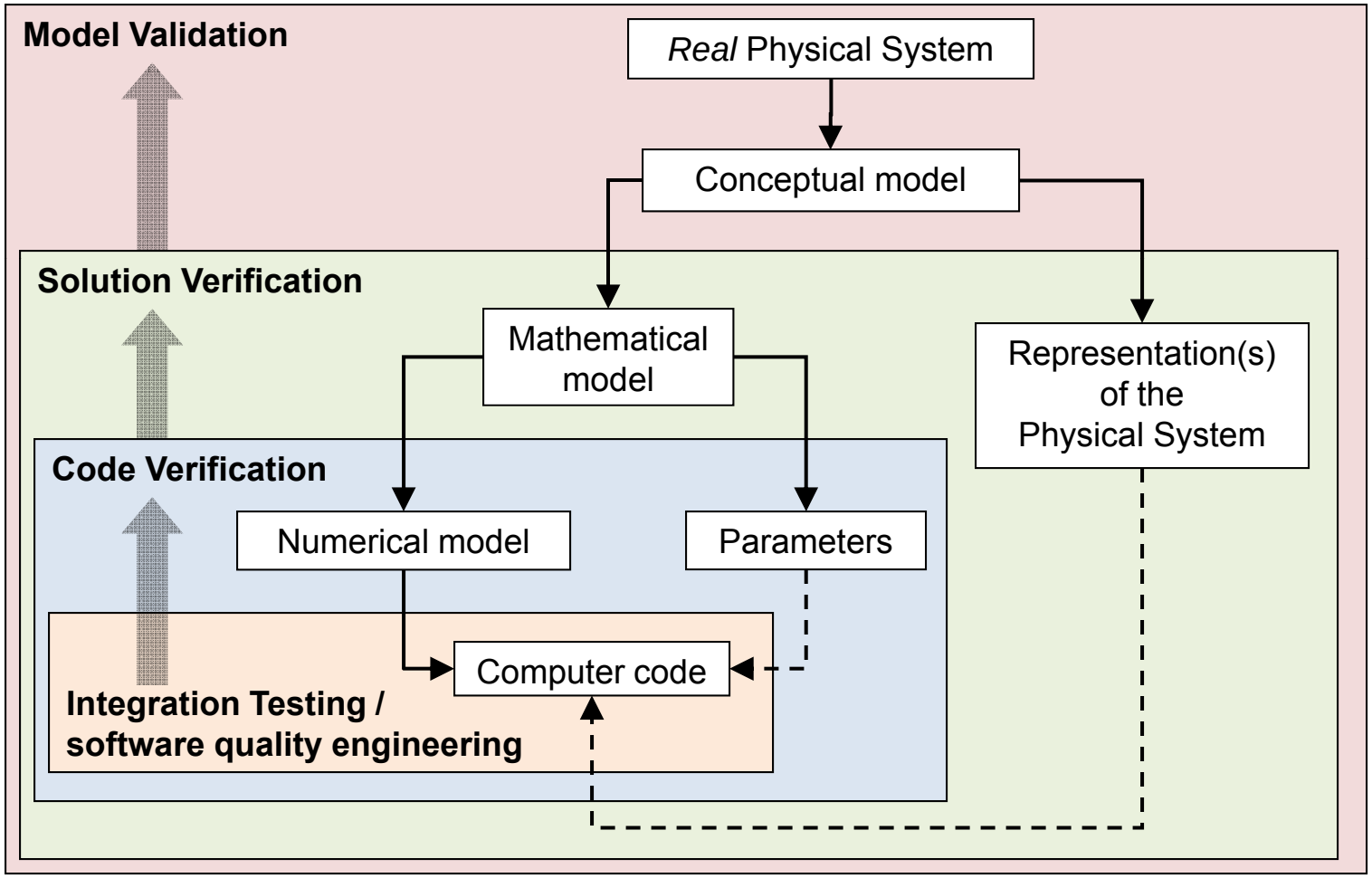
V&V Plan Key Concepts: Confidence in M&S Capabilities

- **Confidence commensurate with risks ← intended use**
  - Challenge problems (low risk)
  - Evaluating and prioritizing development of disposal alternatives'
  - Design of waste forms and engineered environments
  - Analysis to support licensing (high risk)

- **Assessment of Confidence (a.k.a. V&V and UQ assessment)**
  - Cannot afford maximum V&V and UQ for every M&S capability
  - Budget V&V and UQ to meet required <u>level of confidence</u>
  - Proposition: <u>level of confidence</u> ≈ V&V and UQ <u>level of maturity</u>
  - Level of maturity via Predictive Capability Maturity Model (PCMM)
  - Assess <u>level of maturity</u> for every M&S capability (born assessed)
  - Assessment *does not* guarantee high level, only *known* level

V&V Plan Key Concepts: M&S Components ↔ V&V Activities

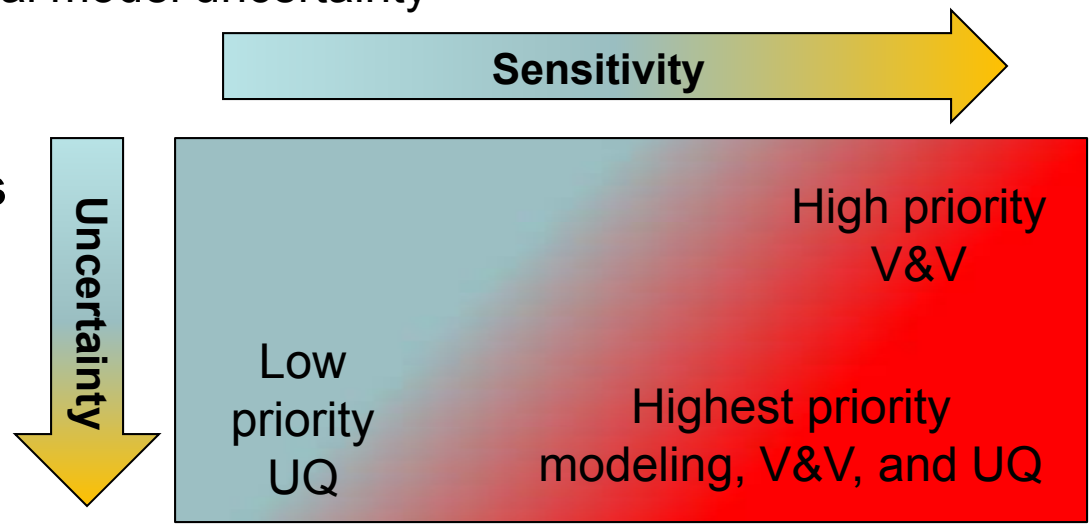


V&V Plan Key Concepts: Uncertainty and Sensitivity

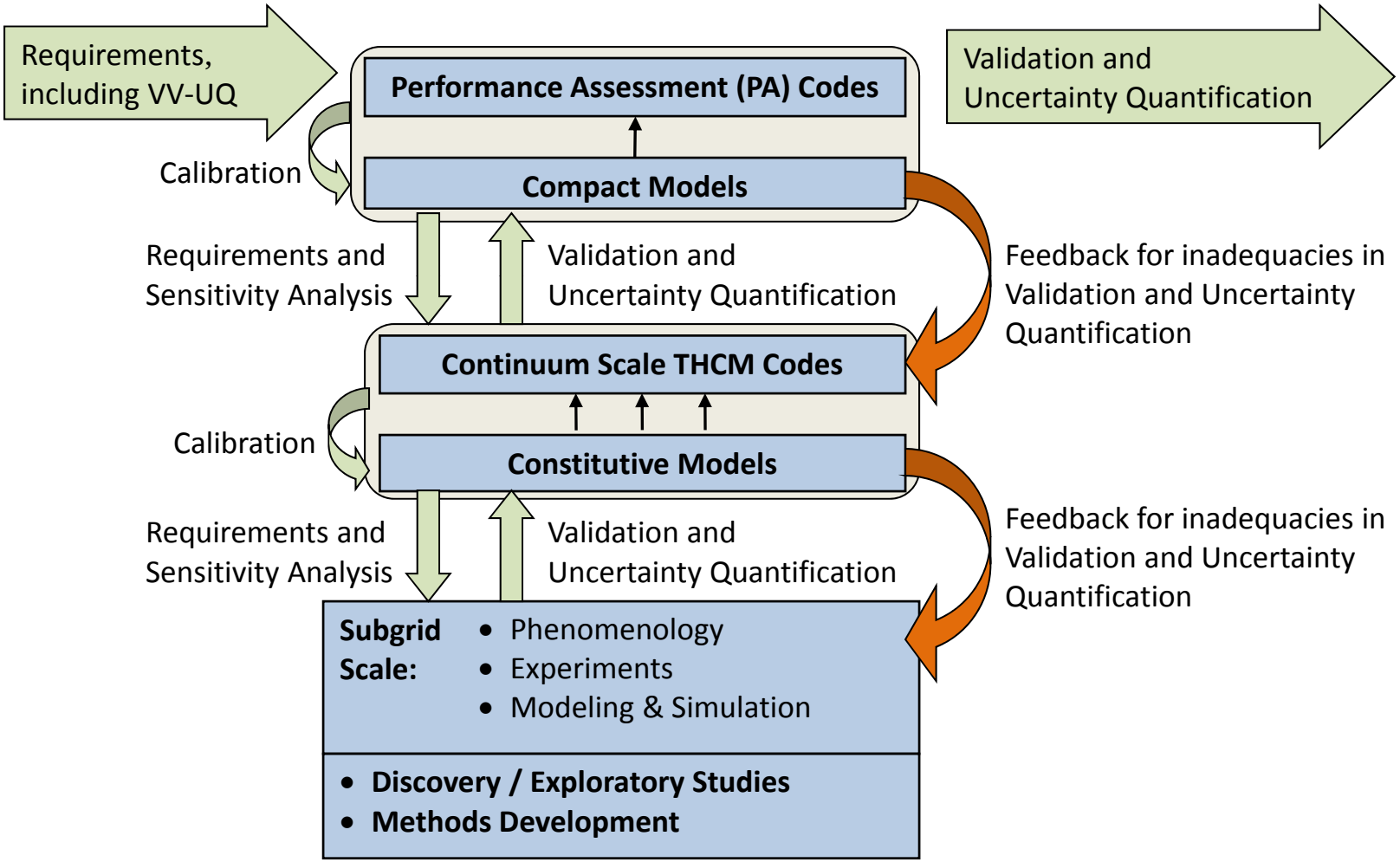
- **Aleatory (stochastic) Uncertainty**
  - Random variability in processes or phenomena (model via parameters)

- **Epistemic (knowledge) Uncertainty**
  - Parameter uncertainty
  - Mathematical model uncertainty
  - Phenomena / conceptual model uncertainty

- **Sensitivity of performance measures to uncertainties**
  - Qualitative analysis
  - Quantitative analysis



V&V Plan Key Concepts: Three Scales of Modeling & Simulation



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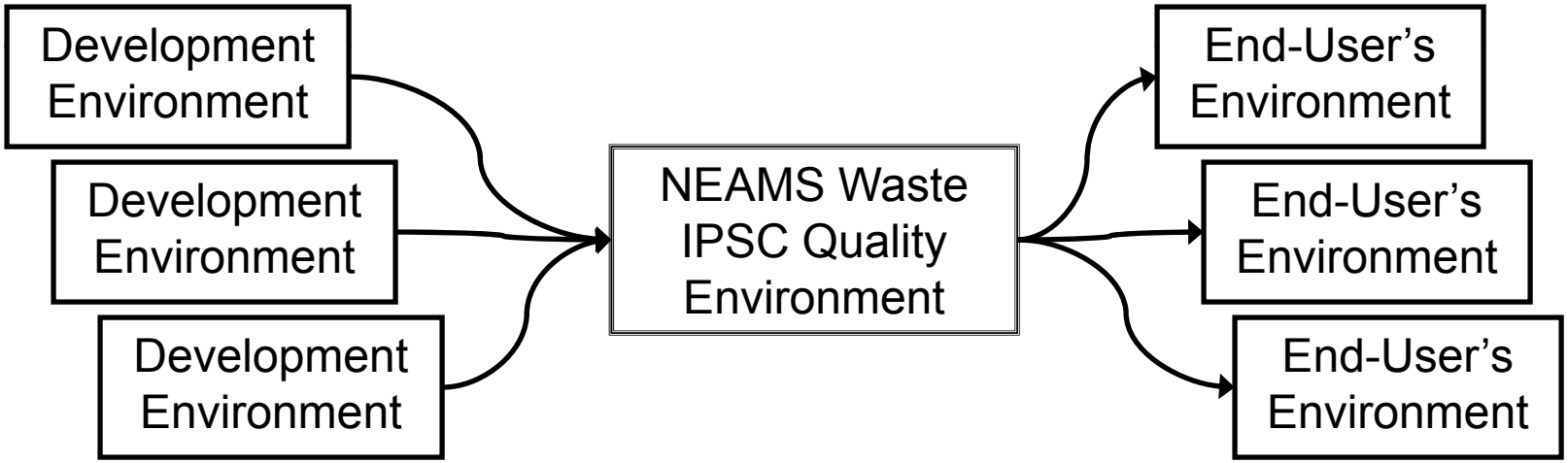
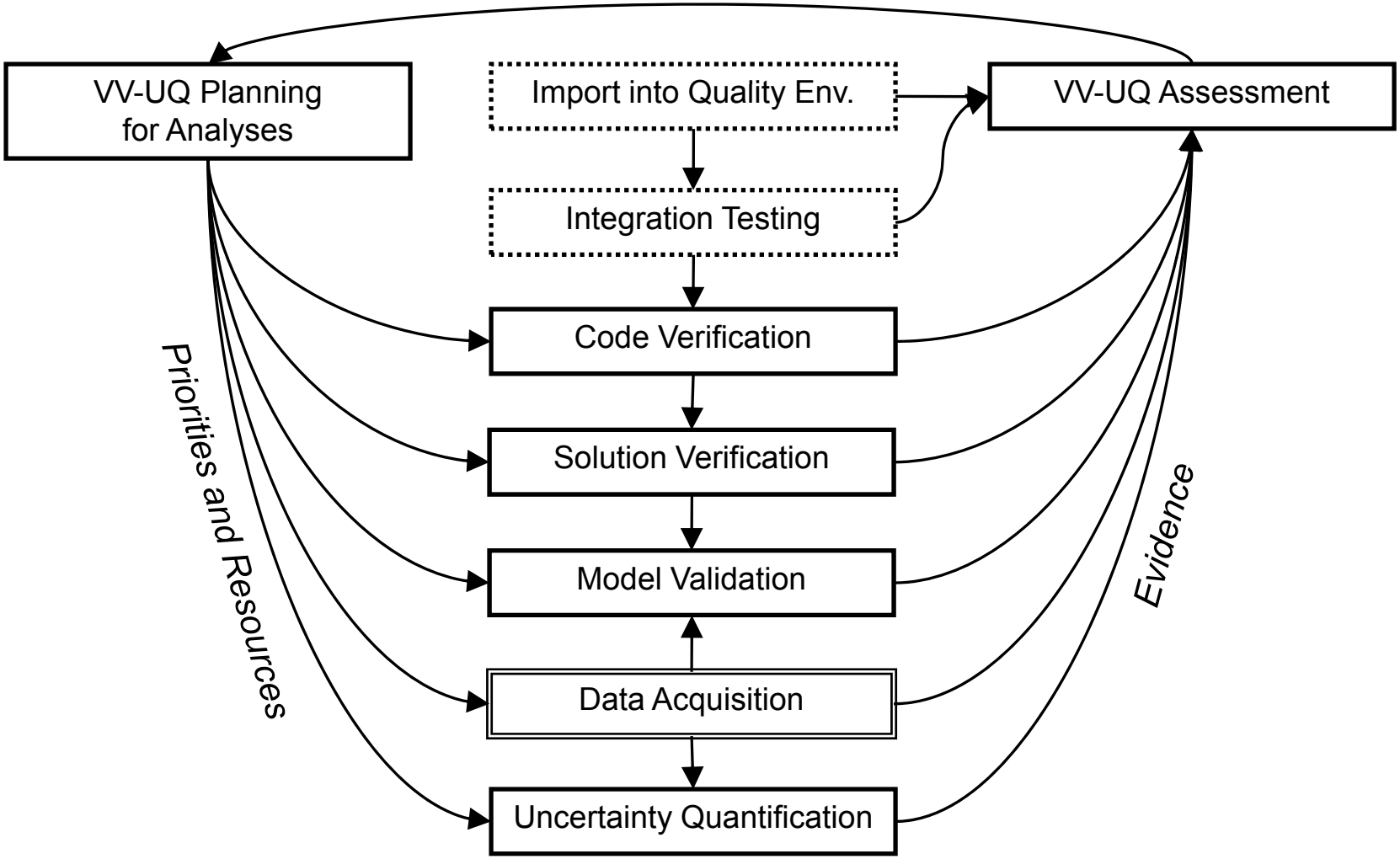
V&V Plan Key Concepts: Evidence Management and Traceability

- **Capture V&V and UQ Evidence**
  - Produced by performing V&V and UQ activities
  - Produced for a given version of a M&S capability
  - Produced from a given set of tests, experimental data, observational data
  - Traceability of results to activity, version, tests, and data
- **Traceability of Composed V&V and UQ Evidence**
  - Imbedding; e.g., material model embedded in mechanics model
  - Code coupling; e.g., fluid + structure in a single code
  - Workflow; e.g., output of one code is input to next code
  - Multi-scale; e.g., PA model abstracted from continuum model
- **Consumption of V&V and UQ Evidence**
  - Queries and reports for assessment and presentation

V&V Plan Key Concepts: Lifecycle Subset Focused on V&V and UQ



V&V Plan Key Concepts: Lifecycle Subset Focused on V&V and UQ



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V&V Plan Practices: Expected Enabling Practices

- **The usual and customary for good software engineering:**
  - Version Control (software, files, etc.)
  - Software Development (good software engineering)
  - Acquisition (software, data, etc.)
  - **Import to Quality Environment**
  - Build and Test
  - Integration
  - Integration Testing
  - Release & Distribution

V&V Plan Practices: Code Verification

- **Verify that Code correctly implements Numerical Model**
  - Precondition: Integration Testing eliminated fundamental coding errors
- **Practices**
  - Documentation, test matrix, test plan, testing tools, run & maintain tests
- **Testing Techniques**
  - Asymptotic convergence for spatial discretizations
  - Analytic solutions (for simple problems)
  - Method of manufactured solutions
  - Benchmark problems
  - …

V&V Plan Practices: Solution Verification

- **Verify that Numerical Model solves Mathematical Model**
  - For required (non-trivial) problems of interest (e.g., validation problems)
  - Precondition: successful Code Verification
  - Estimate errors in the numerical solution of mathematical model

- **Practices and Techniques**
  - Review inputs and outputs
  - Assess sensitivity of solution to parameters (e.g., equation solver tolerance)
  - Confirm solution is in the asymptotic convergence regime
  - Adapt the discretization to enter the asymptotic convergence regime
  - Compute a posteriori estimate of numerical solution error

V&V Plan Practices: Data Acquisition

- **Acquire experimental or observational measurement data; for**
  - Requirements analysis and conceptual model development
  - Qualitative sensitivity analysis and mathematical model development
  - Model validation
  - Uncertainty quantification

- **Practices**
  - Identify source(s)
  - Acquire data into VV-UQ evidence management system
  - Assess data quality and uncertainties
  - Address gaps in data quality and uncertainties

V&V Plan Practices: Uncertainty Quantification

- ***Quantification* of uncertainties in model parameters**

- **Significant challenges**
  - Different M&S scales have different mathematical models and parameters; upscaling uncertainties from lower scale to higher scale models
  - Aggregating uncertainties from coupled M&S capabilities
  - Costly sampling-based approaches

- **Practices**
  - Calibrate: use measurement data to reduce model parameter uncertainties (an inverse problem)
  - Propagate aleatory uncertainties through models (via sampling)
  - Propagate epistemic uncertainties through models

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V&V Plan Practices: Model Validation

- **Validate that the model sufficiently matches the real world**
  - Simulation results versus experimental & observational measurement data
  - For quantities of interest; a.k.a. performance measures
  - Within the domain of interest; a.k.a. intended use

- **Multiple Scales of M&S**
  - Measurement data ← subgrid scale models
  - Subgrid scale M&S results ← continuum scale models
  - Continuum scale M&S results ← performance assessment scale models

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V&V Plan Practices: V&V and UQ Assessment

- **Define Levels of Maturity for V&V and UQ practices**
  - Proposition: level of maturity ≈ level of confidence
  - Foundation: Predictive Capability Maturity Model (PCMM)
  - Qualitative metrics, and some quantitative metrics when substantiateable
  - Will evolve

- **Assess Level of V&V and UQ Maturity (PCMM)**
  - Maintain assessment data in V&V evidence management system
  - Re-assessment / updates as additional V&V and UQ is performed
  - Identify gaps with respect to required level of maturity (confidence)

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V&V Plan Practices: V&V and UQ Planning

- **Plan V&V and UQ work to achieve required level of confidence**
  - For M&S capabilities to be used in the anticipated analyses

- **Practices**
  - Analyze confidence requirements and gaps for the analyses
  - Develop analyses-specific V&V and UQ plan to address deficiencies

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V&V Plan: Evidence Information Management

- **Electronic Repository of V&V and UQ evidence**
  - V&V and UQ Practice artifacts, metrics, and traceability
  - Access controls, maintenance, configuration management, etc.
  - Maintain information integrity and quality
- **Support V&V and UQ metrics**
  - Extensible as V&V and UQ processes evolve
  - Aggregate metrics derived from coupled M&S capabilities' metrics
  - Metrics for level of confidence (≈ level of maturity)
- **Timely capture and update**
  - Support optional "direct deposit" from a V&V or UQ analysis workflow
- **Search, retrieval, and reports**
  - Traceability for package of evidence for aggregated M&S capabilities

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V&V Plan: Evidence Information Management Dependencies and Interfaces

- **Requirements Management**
  - Evidence that requirements have been met traceable to requirements
  - How well? Metrics derived from PCMM
- **Software Configuration Management**
  - V&V applied to particular version(s) of models
- **Analysis Data Management**
  - V&V practices performed via analyses
- **Model Parameters (e.g., material properties) Management**
  - V&V and UQ of model parameters

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Frameworks & Infrastructures Gap Analysis

Priorities:

1. Enabling Infrastructure for the Quality Environment
2. Analysis Workflow Framework for V&V and UQ of Challenge Problems
3. Code Coupling Framework

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Enabling Infrastructure for the Quality Environment

- **Support Acquisition, Integration, Test, V&V, Fix, and Deployment of modeling & simulation capabilities**

- **Need: Software Configuration Management**
  - Version control and traceability
  - Build (source to executable) and test harness
  - Issue tracking & change requests
  - Software deployment

- **Need: Requirements Management**
  - FEPS / PIRT and other requirements

- **Need: Project Management**

Enabling Infrastructure for the Quality Environment

- **Candidate Enabling Infrastructure Software**
  - Version control: ‘git’
  - Build & test: ‘cmake’ and ‘ctest’
  - Issue tracking: ‘Trac’
  - Project management: ‘Trac’
  - Requirements management: ‘DOORS’

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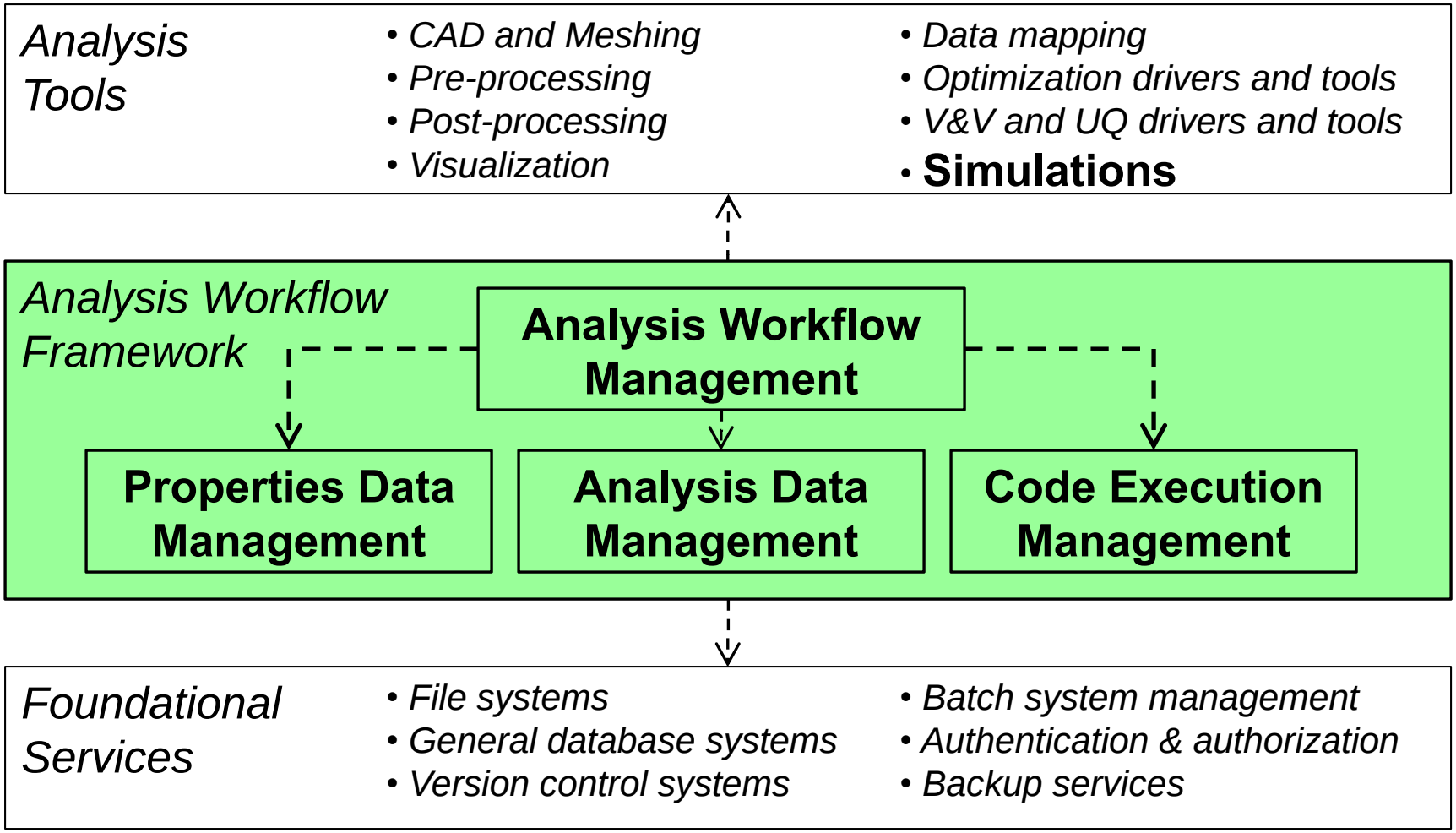
Analysis Workflow Framework



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Analysis Workflow Framework: Strategy

- **Collaborate for knowledge, resources, and shared solutions**
  - Pervasive need:
  - DOE Used Fuel Disposition (UFD)
  - DOE Advanced Simulation Capability for Environment Management (ASCEM)
  - DOE Advanced Simulation and Computing (ASC)
  - Commercial world: "Product Lifecycle Management (PDM)"
    - *Critical to computer aided engineering (CAE)*
    - *Specialty of: Collaborative Product Development Associates, LLC*

- **Steps:**
  - Requirements
  - Gap analysis, evaluation, and acquisition
  - Pilot Project to prototype use of acquired product
    - *Apply to Challenge Problem codes and analyses*

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Analysis Workflow Framework: Candidates

- **Commercial (some leading contenders):**
  - GoldSim: extensively used in Yucca Mountain Project and will be for UFD
  - PHX AnalysisLibrary and ModelCenter (Phoenix Integration)
  - TeamCenter (Siemens)
  - Hyperworks (Altair)
  - Windchill (PTC)
  - SimManager (MSC Software)
  - …
- **Public Domain:**
  - SALOME (Open CASCADE)
  - Kepler (Kepler Project Team)
- **DOE Lab:**
  - DART Workbench (SNL/ASC)
  - ASCEM Platforms and Integrated Toolsets (ASCEM multi-lab team) (GS^3)
  - NiCE at ORNL

Code Coupling Framework

- **Coupling of modeling & simulation capabilities into a single executable simulation code**
  - Desirable: highly modular toolkit with good software engineering
  - A few successful examples

- **Constraints & Strategy**
  - Do not have the resources to develop required capabilities from scratch
  - Choose code(s) that best meet program requirements
  - Leverage and collaborate as much as possible
  - *Accept the code's coupling framework, if the code has one*

- **Customer / supplier, Collaborator, or Developer role?**
  - Potential is determined by resources we can bring to the table

Path Forward: Policies

- **Policy: Maximize acquisition and minimize development**
  - Enabling Infrastructure
    - *Good commercial & non-commercial options*
  - Analysis Workflow Framework
    - *Several commercial possibilities – cost is a concern*
    - *A few non-commercial possibilities – sufficiency is a concern*
  - Code Coupling Framework
    - *Accept what selected codes already use*

- **Policy: Perform V&V and UQ activities as analysis workflows**
  - V&V and UQ workflows produce evidence to be managed
  - Use the same tools that we expect end-users to use

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Path Forward: FY11 Plan

- **Deploy Software Quality Environment**
  - Evaluate, acquire, and configure existing tools for enabling infrastructure
- **Collaborative Pilot Project for Analysis Workflow Framework**
  - Organize collaborative team and identify their pilot project use cases
    - *NEAMS Waste IPSC Challenge Problem*
  - Evaluate, acquire, and configure existing analysis workflow framework
- **Develop and Apply Initial V&V and UQ Processes and Metrics**
  - Implement in the quality environment + analysis workflow framework
    - *Prototype and analyze requirements for evidence management*
  - Apply to FY11 challenge problem code(s) and analyses
  - Evaluate initial V&V and UQ processes and metrics – for improvement
- **Agile approach for M&S Capabilities, Frameworks, and Processes**
  - With pervasive policy to prefer acquisition (re-use) over development