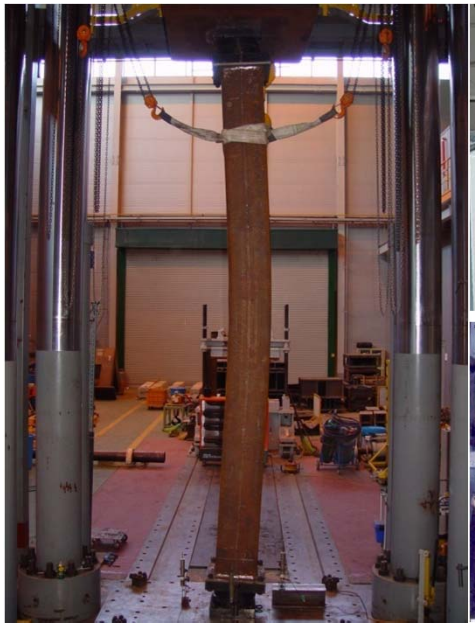
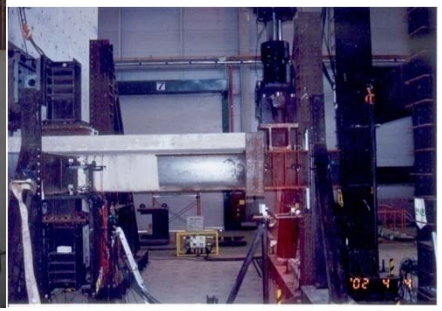
Science and Engineering: Theory / Experiment / Simulation

Physical Phenomena

Cost, Safety

Experimental Model





Issue-1

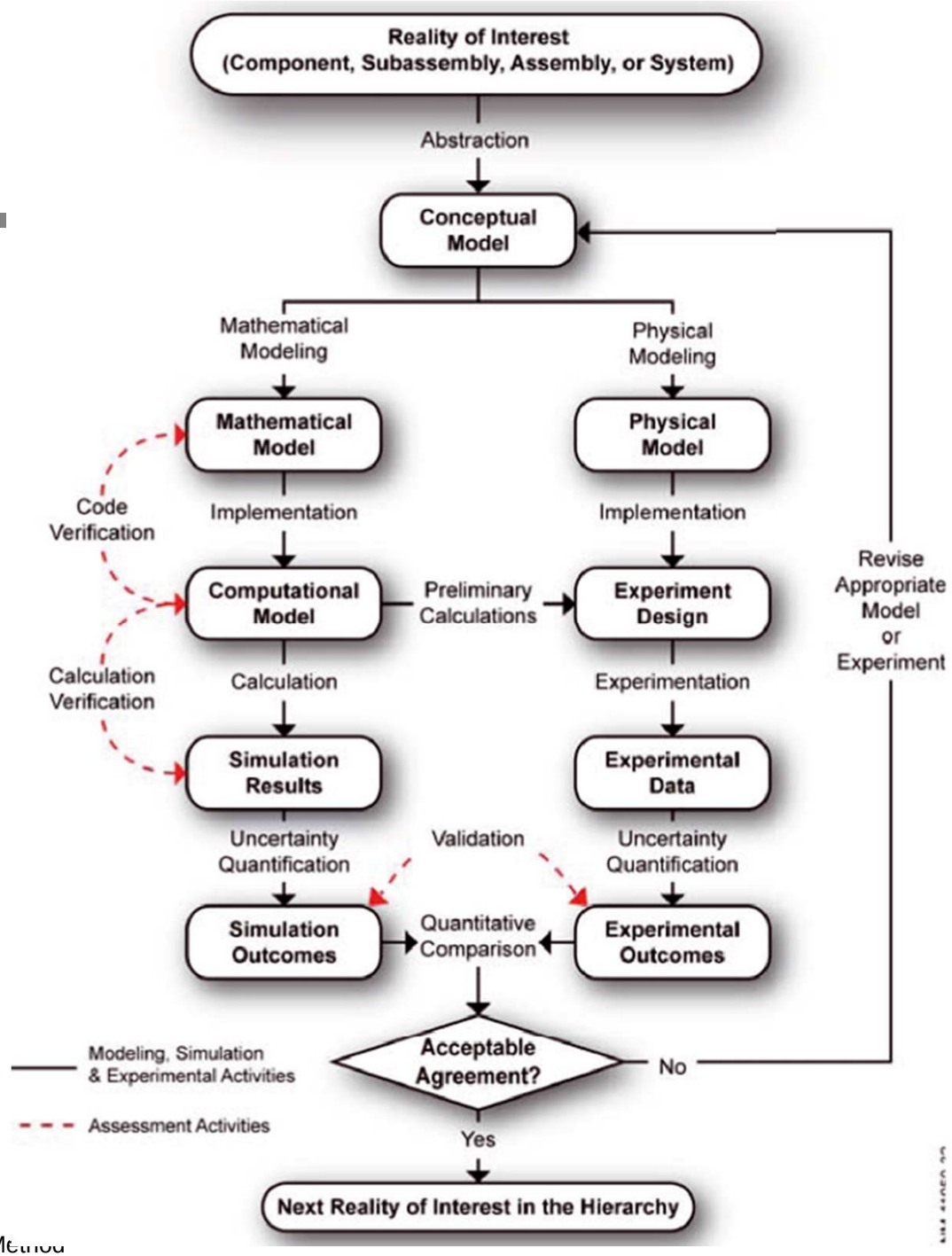
Modeling

Mathematical Model

Theory

Issue-2 V&V

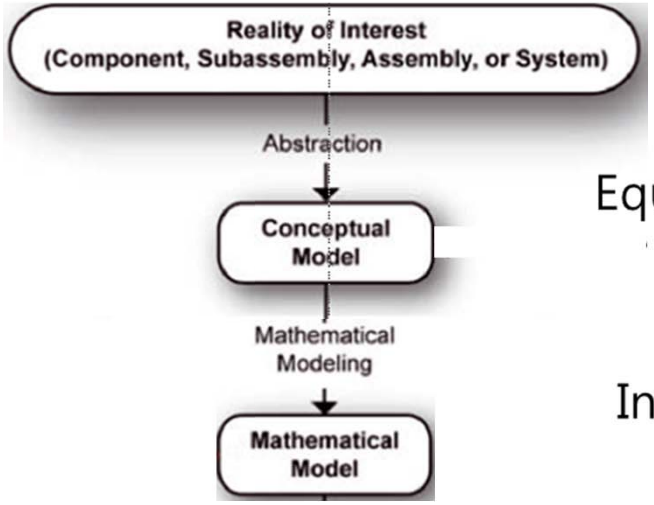
Numerical Analysis


Reality of Interest
(Component, Subassembly, Assembly, or System)
Abstraction
Conceptual Model
Mathematical Modeling
Physical Modeling
Mathematical Model
Physical Model
Code Verification
Implementation
Implementation
Computational Model
Preliminary Calculations
Experiment Design
Revise Appropriate Model or Experiment
Calculation Verification
Calculation
Experimentation
Simulation Results
Experimental Data
Uncertainty Quantification
Validation
Uncertainty Quantification
Simulation Outcomes
Quantitative Comparison
Experimental Outcomes
Acceptable Agreement?
No
Modeling, Simulation & Experimental Activities
Assessment Activities
Yes
Next Reality of Interest in the Hierarchy

Engineering Simulation

- Three types of models
  - Conceptual
  - Mathematical
  - Computational
- Verification: domain of mathematics
  - Process of determining that a computational model accurately represents the underlying mathematical model and its solution
- Validation: domain of physics
  - Process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model

Multi-physics Phenomena



Equilibrium Equation • Constitutive Equation

Solid

Interaction

Coupled Problem

MultiPhase Problem

Fluid

Mass Transfer

Continuity Equation
Equations of Motion

Transport Equation

Electrom agnetics

Maxwell Equation

Mathematical Modeling

- Are there any basic principles to follow when a differential equation is set up?
  - No general answer
- Modeling: art
  - Problem types, simplifying assumptions
  - Chemical engineering: conservation principles
  - Electromagnetic field theory: Maxwell's equations
  - Control theory: block diagram
- Classification
  - Differential equations considered as nature laws
  - Constitutive differential equations
  - Conservative differential equations

Nature Laws

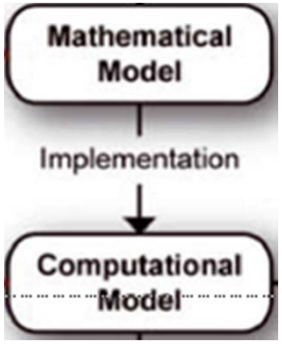
- Mathematical relation that cannot be derived from physical facts
  - Observations
  - No experiment has been designed that contradicts the law
- Examples
  - Newton's law for the motion of a particle
  - Maxwell's laws for the electromagnetic field
  - Schrödinger's equation in quantum mechanics

$$m\frac{d^2\mathbf{r}}{dt^2} = \mathbf{F}$$

Constitutive Equations

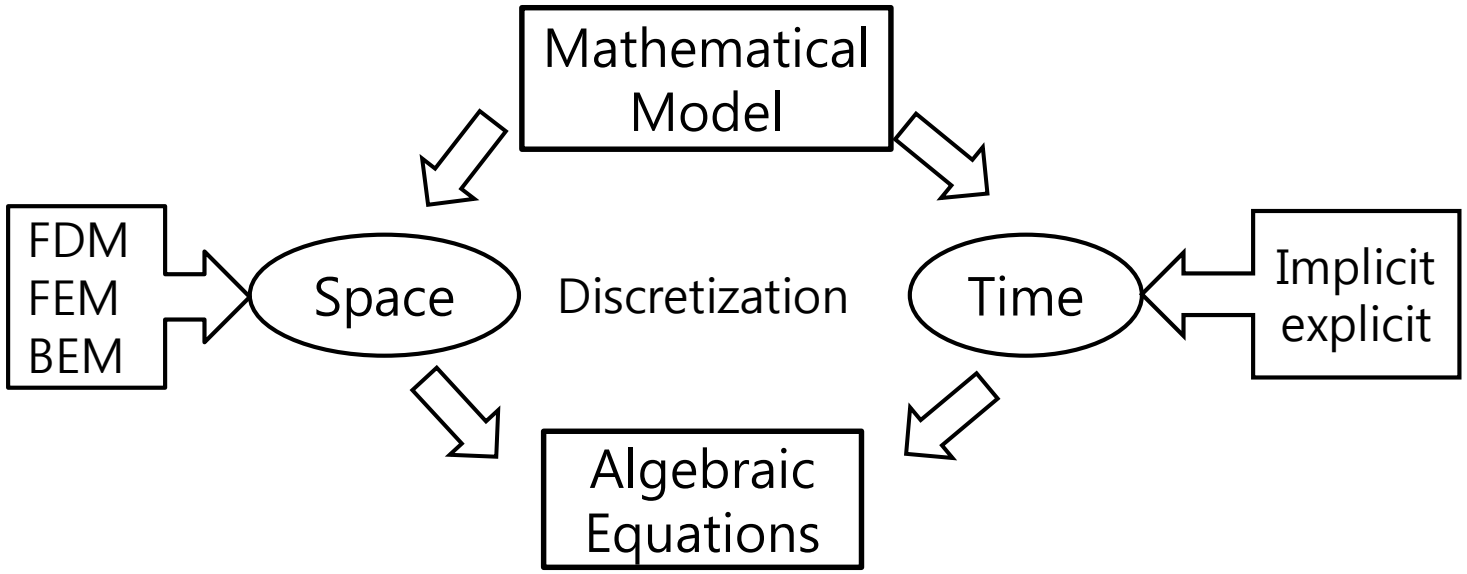
- Mathematical model of the physical properties of a gas, fluid, or solid: empirical nature
  - Observations of a phenomenon
  - Measurements of an experiment
- Examples
  - Equations in heat transfer problems
  - Equations in mass diffusion problems
  - Equations in mechanical moment diffusion problems
  - Equations in elastic solid mechanics problems
  - Equations in chemical reaction engineering problems
  - Equations in electrical engineering problems

Discretization: Mathematical → Computational

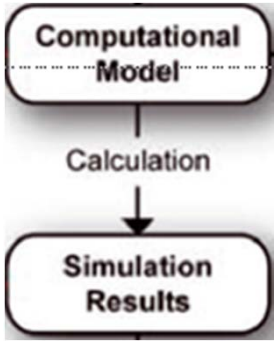


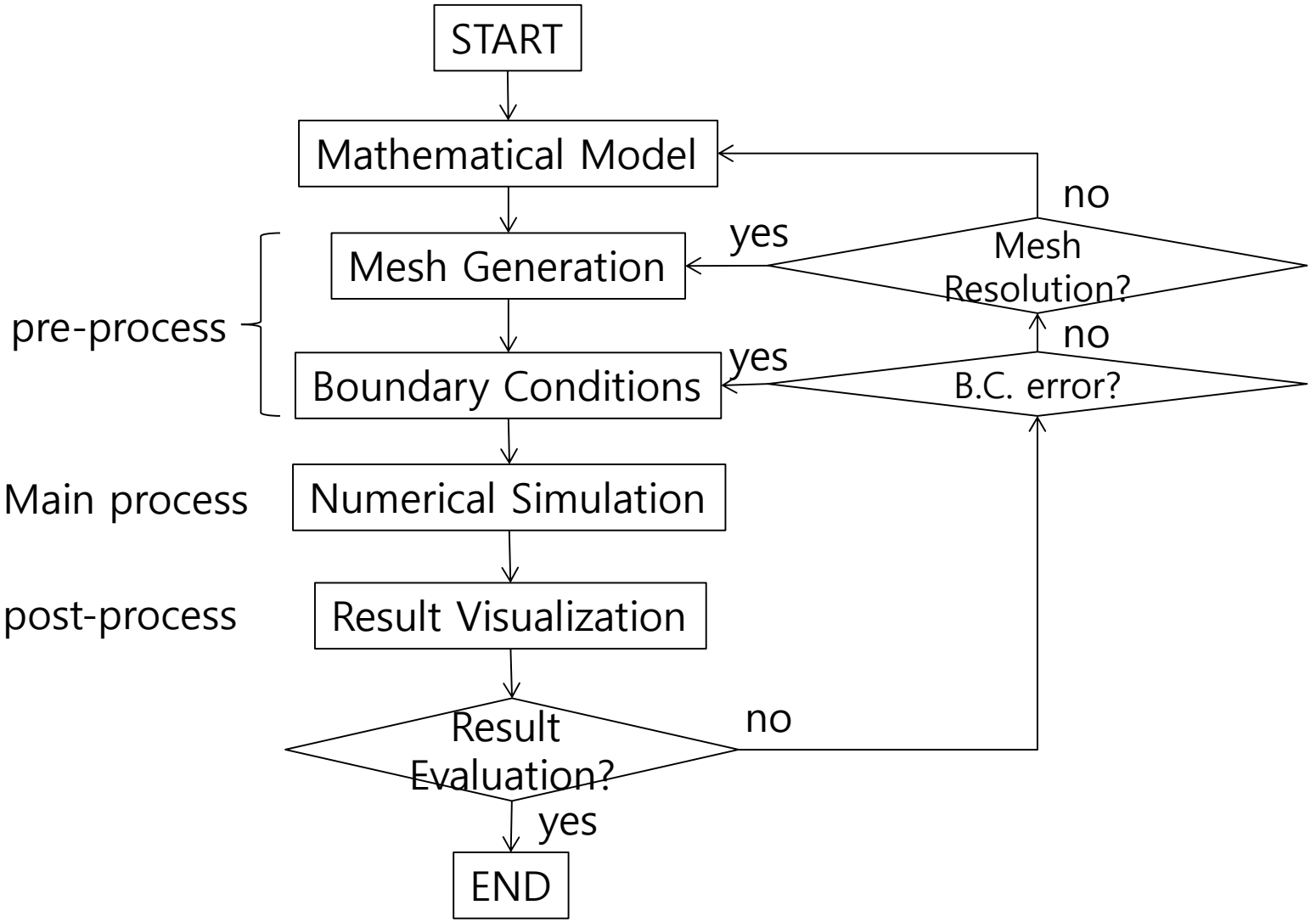
$$\phi(x,t)$$

$$A\frac{\partial^2\phi}{\partial x^2}+B\frac{\partial^2\phi}{\partial x\partial t}+C\frac{\partial^2\phi}{\partial t^2}+D\frac{\partial\phi}{\partial x}+E\frac{\partial\phi}{\partial t}+F\phi+G=0$$



Simulation Process





Verification

- Code verification
  - Mathematical model and solution algorithms are working correctly?
  - Domain of software developers: Software Quality Assurance techniques along with testing of each released version
  - To compare code outputs with analytical solutions
- Calculation verification
  - Discrete solution of the mathematical model is accurate?
  - Domain of user of the software
  - Estimating the errors in the numerical solution due to discretization
  - Mesh-to-mesh comparison: to determine the rate of convergence of the solution

Validation

- Answering the adequacy of the selected models for representing the reality of interest
  - Mechanics (physics) included in the models sufficient to provide reliable answers to the questions posed in the problem statement

- Interaction between mathematics and physics in V&V process
  - Close cooperation among modelers and experimentalist
  - ‘cross-talk’ activity to model the same conceptual model, e.g., fixed-end condition
  - Segregation of the outcomes
- Role of uncertainty quantification (UQ)
  - Different experimental results
  - Distributed numerical and physical parameters

ASME V&V 10-2006 - Guide for Verification and Validation in Computational Solid Mechanics