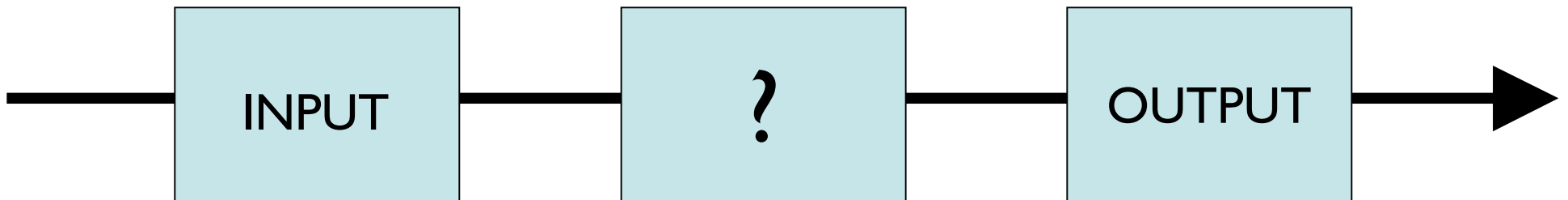




Computer Modeling of Aqueous Chemical Environments

CEE 373, 2 Units



Course Approach

- Loosely structured
- Stress a high degree of cross-functionality
- Think outside the box
- Aim to improve the state of the subject
- Opportunities to contribute
- Knowledge Framework
- Key Component of Skill Set
- Demonstrable Expertise

Objectives

- Build appreciation for the workings of existing models
- Provide experience in constructing program components
- Teach skills necessary for accurate data interpretation

Format

- Experience a software development effort from beginning to end
- Discussion of concepts and applications
- Focus group on available products

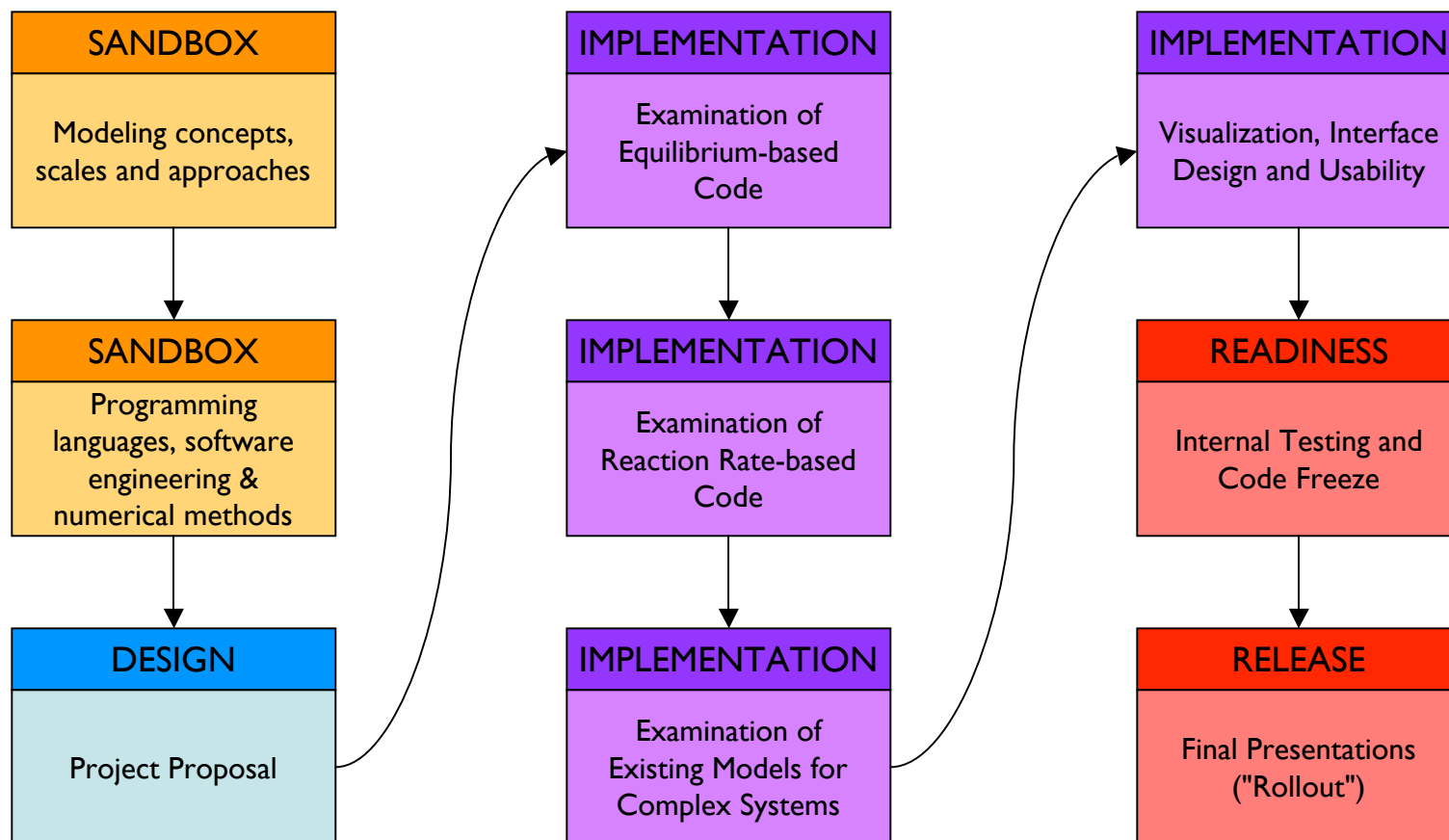
A Software Development Effort

- Sandbox: brainstorming, gathering of new ideas, creativity cycle.
- Design: conceptual development, functional requirements, market requirements.
- Implementation: multiple stages of engineering
- Release: freezing, readiness, and hoping for the best

Focus Group

- Examination of existing products
- Feedback on pros and cons
- Evaluation of new ideas borne of feedback

Roadmap



Term Project Elements

- Innovative
- Independent vs Team Project
- Ground-up vs Add-on
- Use State-of-the-Art Tools
- Full Product Development Process
- Usable

Term Project Elements

- Proposal: Concept and Scope Development
- Proposal: Positioning and Justification
- Proposal: Functional Requirements
- Proposal: Engineering Plan
- Implementation: Prototype, Candidates, Freeze
- Readiness: Testing and Bug Reporting
- Release: Packaging (support documentation)

Term Project Ideas

- Predicting mineral precipitation
- Importance of activity coefficient calculations
- Design of a Help System
- A Test Plan Design and Execution
- Speciation model for ion pairs
- Building a UI
- Closed vs Open System Modeling
- Enhancement with visualization tools
- Proof of Concept: Software for the PDA platform
- Platform-independent coding