Interactive Thermodynamic Database

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PHASES
PSU

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Outline

- The Problem
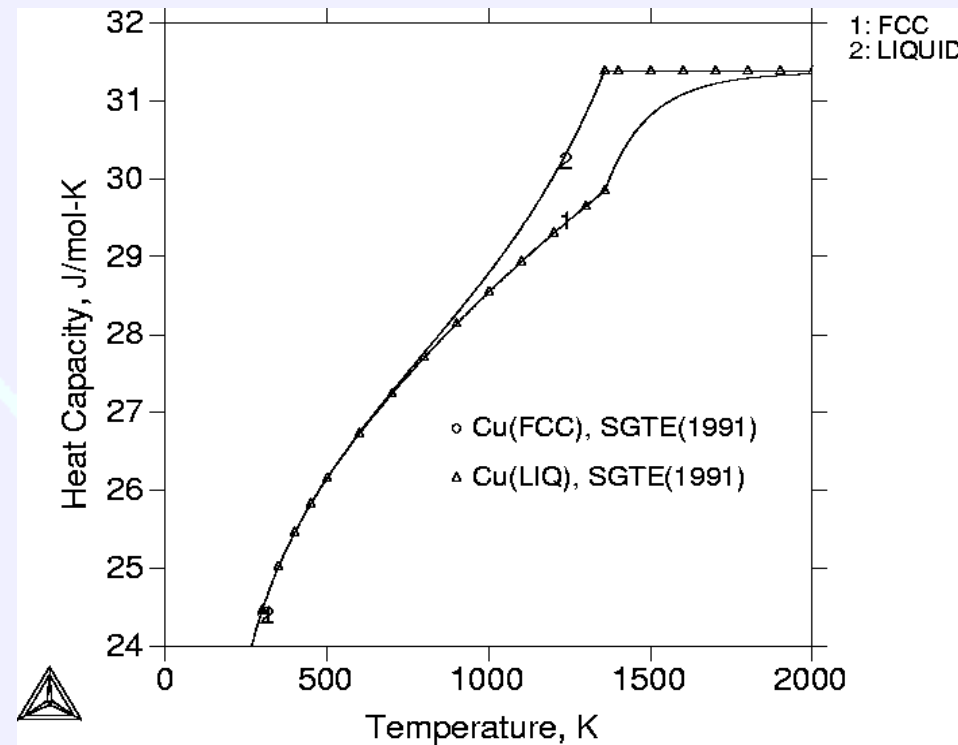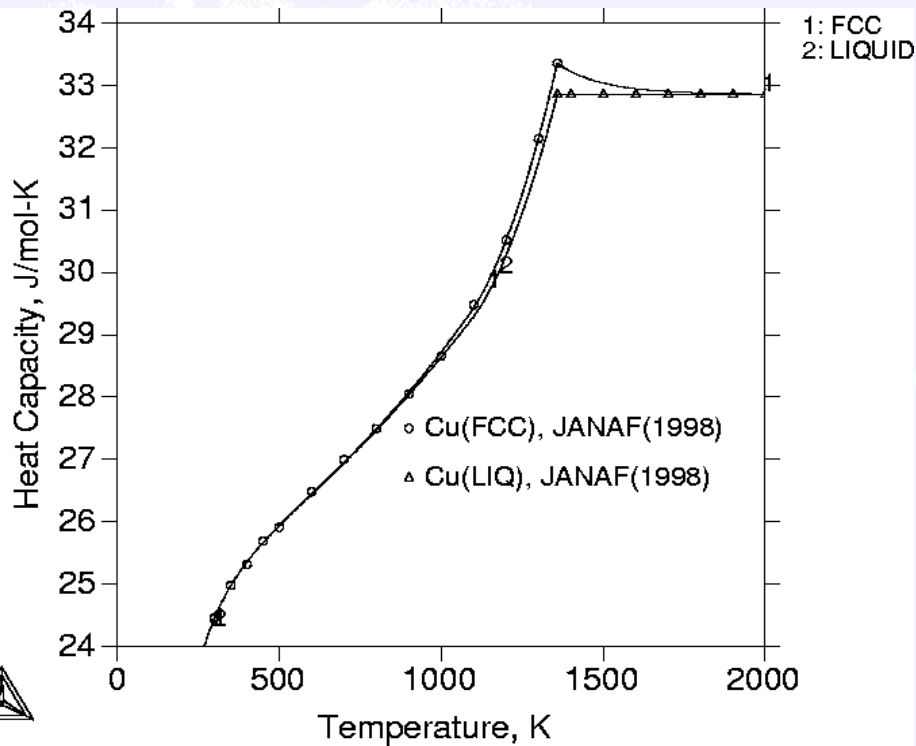
- Proposed Approach

- Current Status

Problem in Database Development

- Time
  - Takes a long time to train a student
  - Afterwards, it becomes a routine, largely an engineering process
- Static
  - Original data for generating the databases are not archived, a great value loss.
  - Multicomponent system based on lower-order systems.
  - Daunting task in modifying a multi-component database

An Example

- Al-Cu-Mg-Si system
  - If the model parameters of one component are changed, one needs to
    - ➢Modify three binary and three ternary systems.
    - ➢Check the quaternary system.
  - One may not have all the previous original data used in the modeling.
- Multi-component system
  - Even more formidable.

An Example: Cu

The Problem:
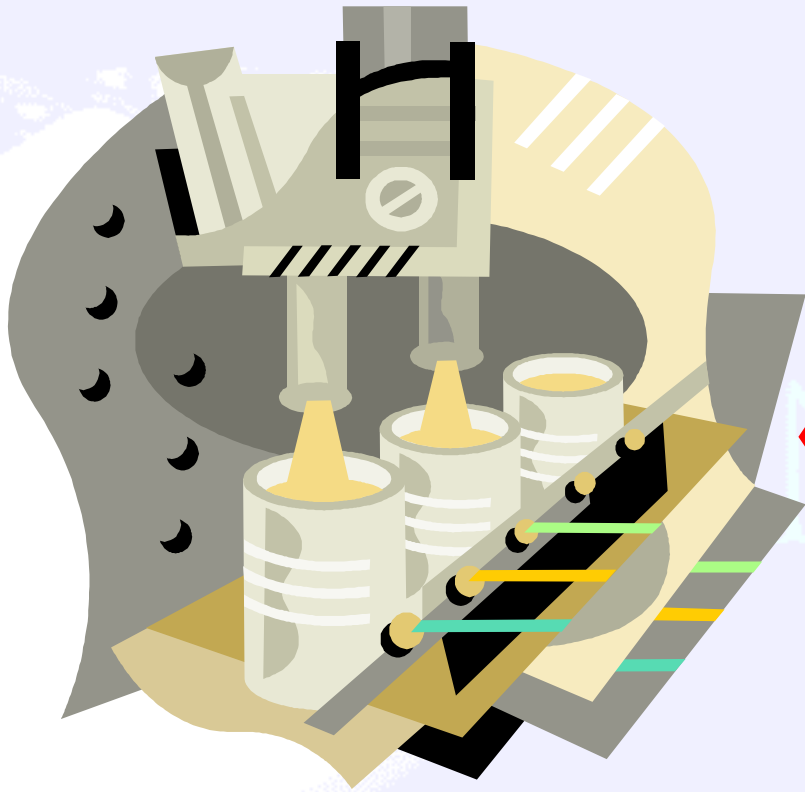## Data Management and Database Improvement

Data A (1970)

Data A' (1980)

Data A'' (…)

Data A''' (2003)

INTERNAL REVENUE

Proposed Approach

Automate the process **Store them efficiently**

NSF ITR Project

Chart of Software Architecture

First principles calculation

Wide-area distributed software architecture grid enabled with Globus; Each step may have MPI based parallelism

Client 1

CALPHAD data optimization

Design 1, completes using last 2 steps

Pure binary, Ternary system Database
DB 1

Experimental Results Database
DB E

Multicomponent Database
DB 2

Client 2

multicomponent phase field modeling

Microstructure Database
1/2/3 diemnsions
-Elastic constants/phase
DB 3

Design 2, involves all 4 steps

FE analysis of simulated microstructure

Mechanical Response Database
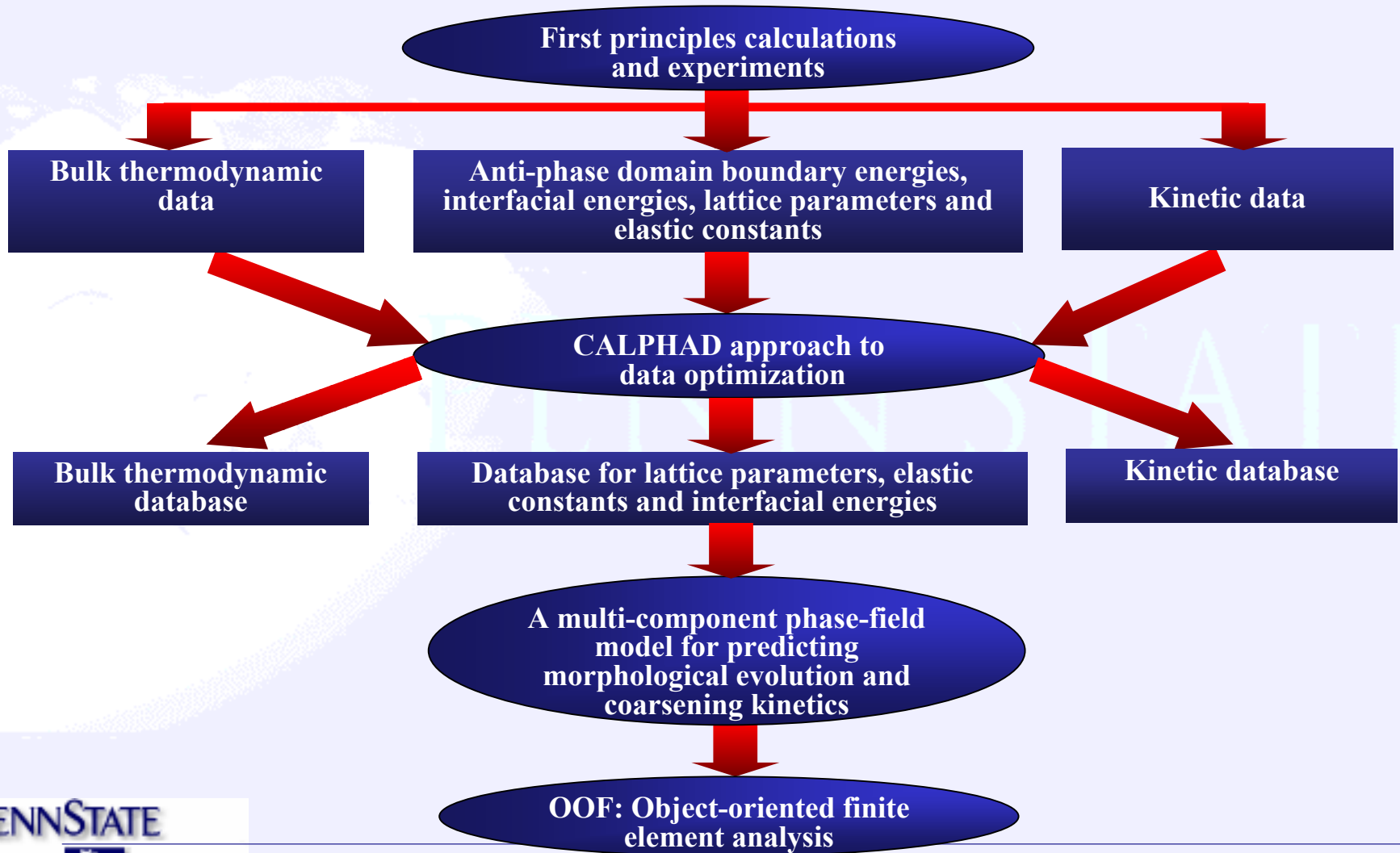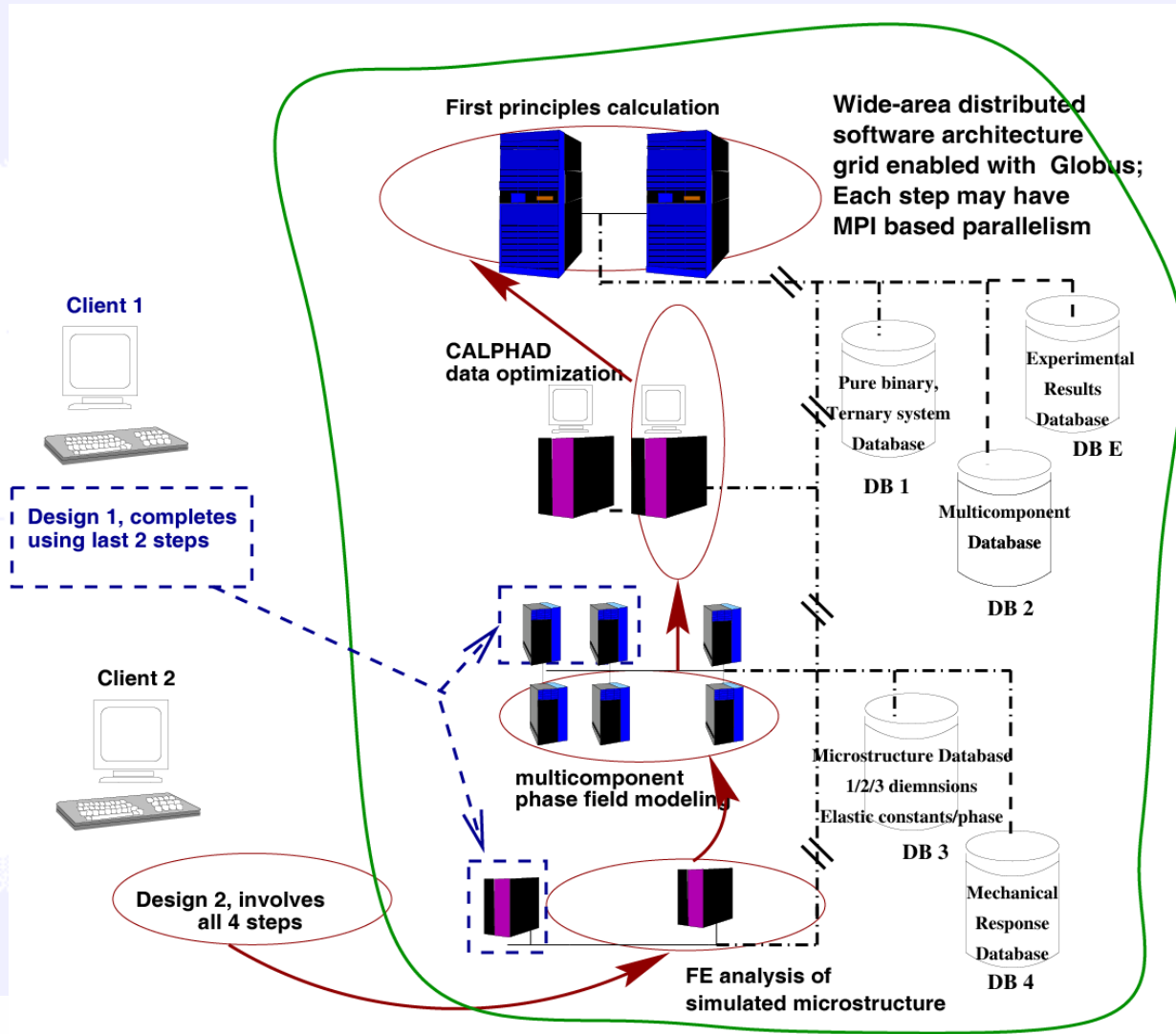DB 4

Team for the NSF ITR Project

- Zi-Kui Liu's group at Penn State (MSE)
- Long-Qing Chen's group at Penn State (MSE)
- Padma Raghavan's group at Penn State (CSE)
- Qiang Du's group at Penn State (Math)
- Jorge Sofo's group at Penn State (Physics)
- Chris Wolverton's group at Ford (*ab initio*)
- Steve Langer's group at NIST (OOF)

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Our Approach

- Develop a database for original data used in modeling

- Automate most technical procedures in modeling

- Stamp the details in data/weight/uncertainty/time selections in modeling

- Provide statistic analysis of model parameters

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Technical Approach
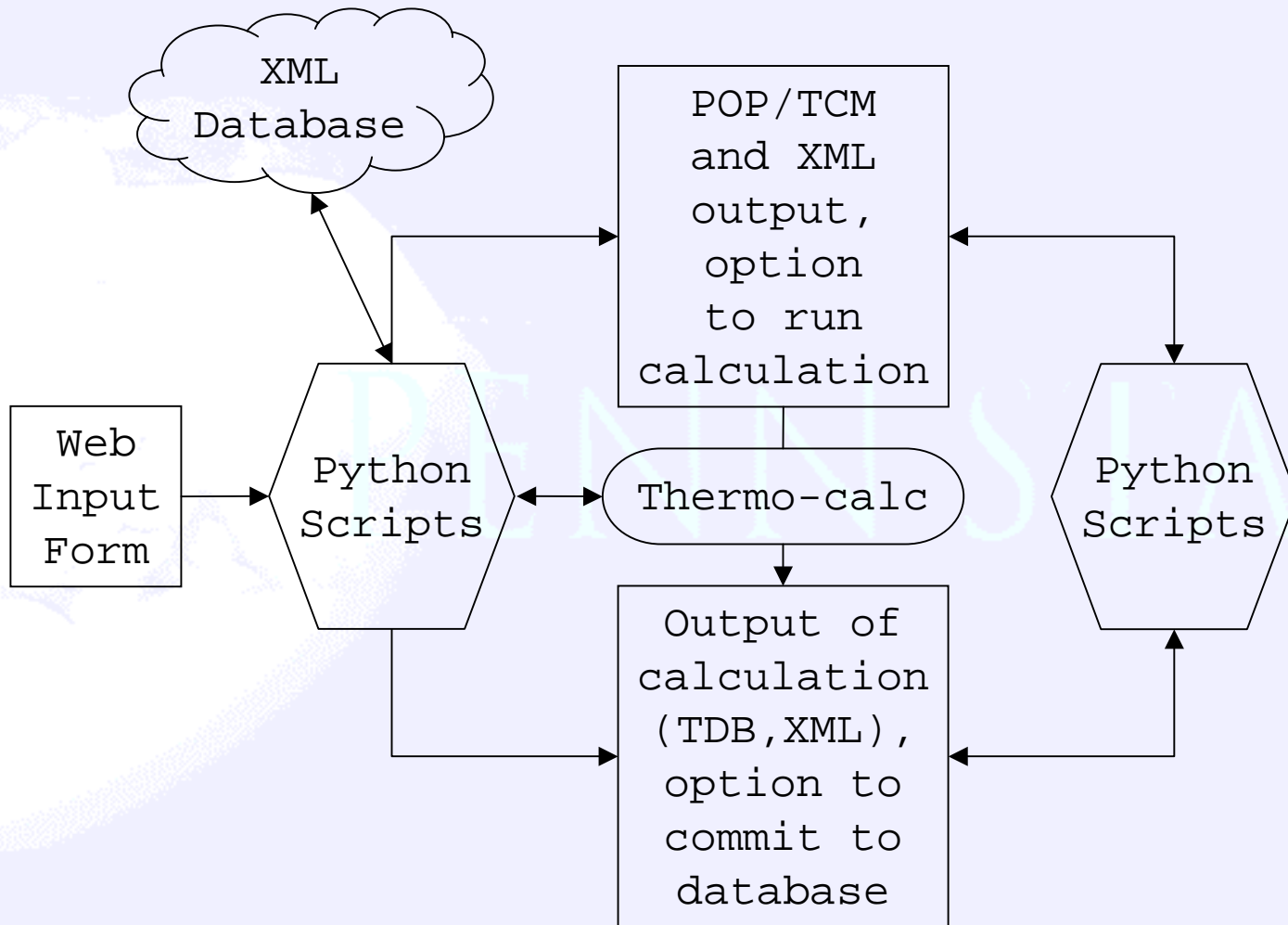
Python

: Script language
: Parsing, data treatment and optimizing
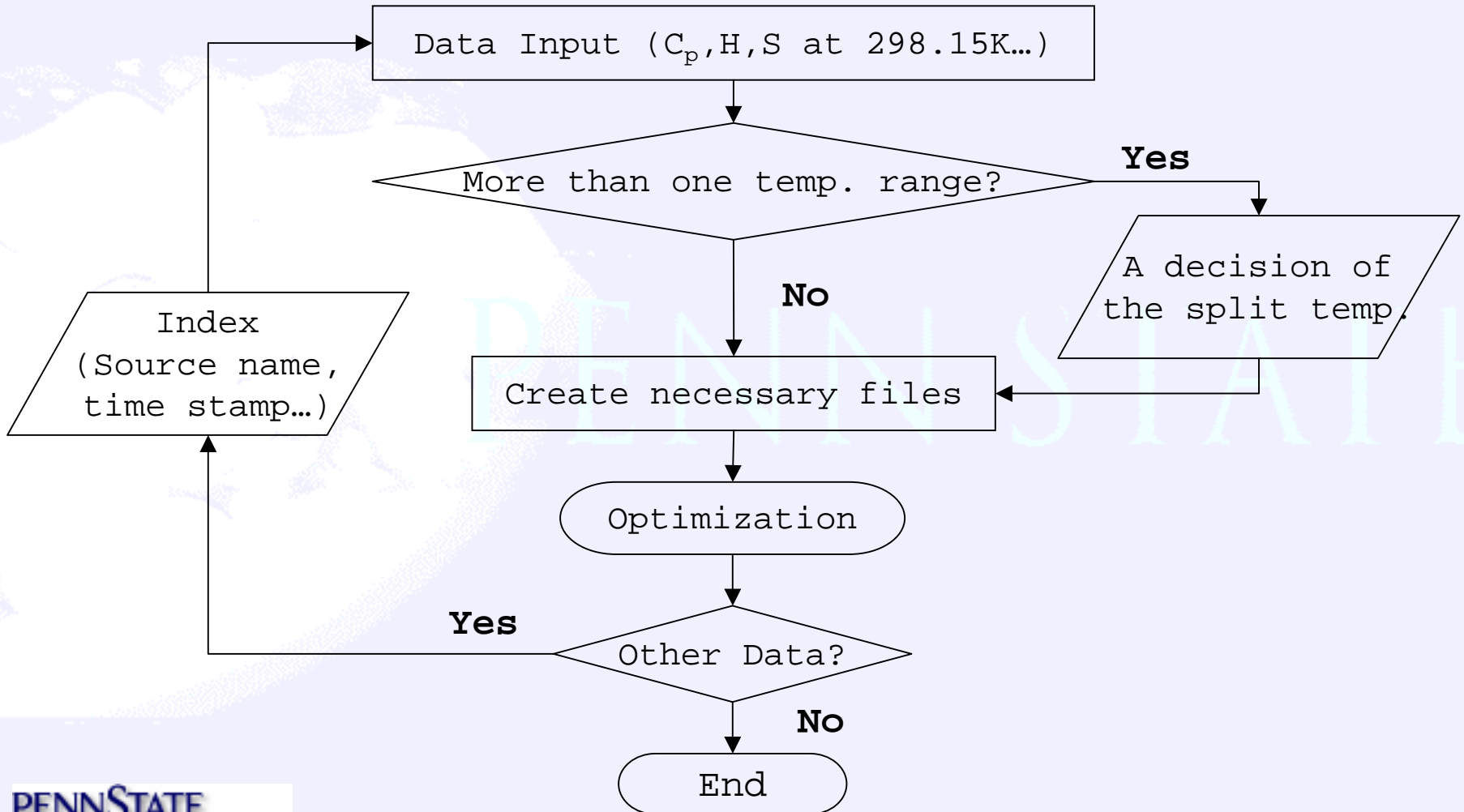: Installed as small packages

XML

: e**X**tensible **M**arkup **L**anguage
: Easily accessible through web interface
: Contains all the data

Technical Approach

Technical Approach

```
          ┌─────────────────────────────────────────────┐
   ┌─────►│ Data Input (C_p,H,S at 298.15K…)             │
   │      └─────────────────────────────────────────────┘
   │                         │
   │                         ▼
   │        ◇ More than one temp. range? ◇ ──── Yes ────┐
   │                         │                           │
   │                         │ No                        ▼
   │                         │              ╱ A decision of        ╱
   ╱ Index          ╱        │             ╱  the split temp.     ╱
  ╱ (Source name,  ╱        ▼
 ╱  time stamp…)  ╱  ┌───────────────────────┐ ◄──────────┘
                     │ Create necessary files│
                     └───────────────────────┘
                                 │
                                 ▼
                          ( Optimization )
                                 │
                                 ▼
   ◄── Yes ──── ◇ Other Data? ◇
                                 │ No
                                 ▼
                             ( End )
```

Summary

- We are just at the beginning and welcome any comments you can provide.

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