Introduction to Scientific Workflows

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What is a workflow?

How does climate affect productivity?
How could I test that?

Acquire data

What is a workflow?

Location: Pine Mountain
Methods: Protocol A
Plot size: 5m x 5m

SPEC	COV99	HGT99	COV00	HGT00	COV01	HGT01
Veg1	30	4	35	4.2	35	4.4
veg2	12	1.2	11	0.9	10	0.3
veg3	44	6.3	46	6.6	51	6.9
...						

Sensor Dataset

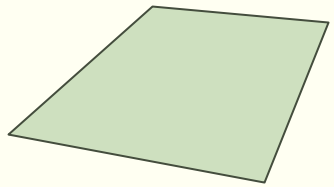


Image Dataset

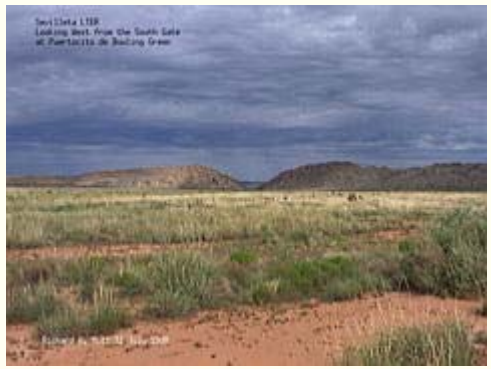
Weather Dataset

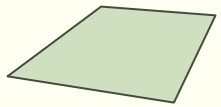
What is a workflow?

Search for compatible data

Location: White Mountain
Methods: Protocol B
Plot size: $1m^2$

TIME	BMASS
t1	323.1
t2	366.7
t3	383.2
…	





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→ **Conversion Analysis** → YYMMDD,443.5,YYMMDD, 454.8,YYMMDD, 462.8, …

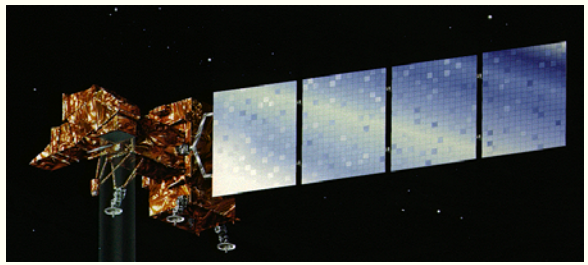
Location: White Mountain
Methods: Protocol B
Plot size: $1m^2$

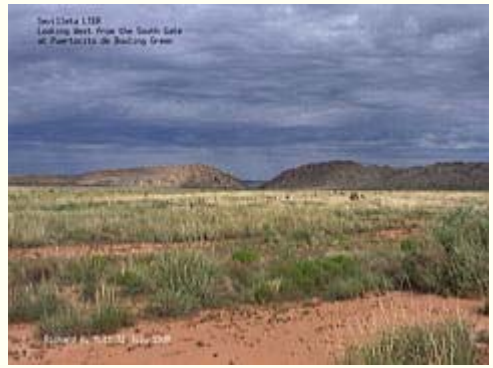
TIME	BMASS
t1	323.1
t2	366.7
t3	383.2
…	

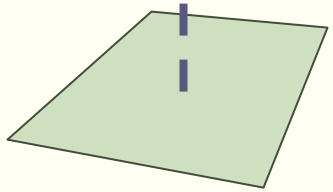
Data Integration:
Physical: file type
Logical: data organization
Semantic: space, time, methods

SITE	TIME	BMASS
PNM	t1	323.1
PNM	t2	366.7
WMT	t3	443.5
PNM	t4	383.2
WMT	t5	454.8
WMT	t6	462.8
…		

What is a workflow?







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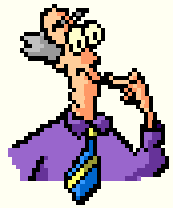
GIS Expert



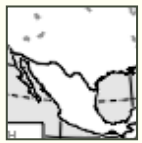
Sample 1, lat, long, presence

Sample 3, lat, long, absence

Sample 2, lat, long, presence

Biome

Elevation (m)



Mean annual temperature (C)

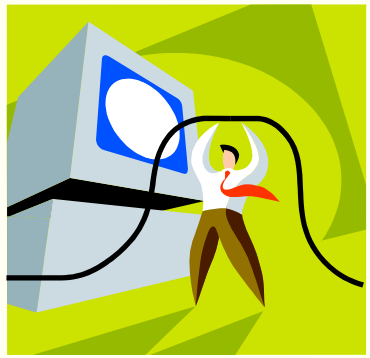
Integrated data:

323.1, biomeA, 2200m, 16C
366.7, biomeB, 2320m, 14C
443.5, biomeC, 1535m, 22C

What is a workflow?

Integrated data:

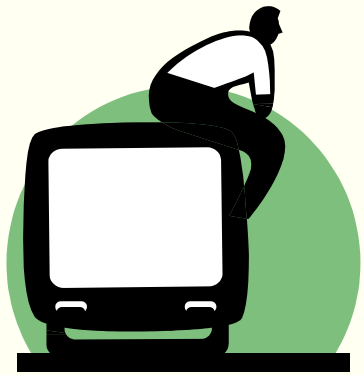
323.1, biomeA, 2200m, 16C
366.7, biomeB, 2320m, 14C
443.5, biomeC, 1535m, 22C



Big, ugly statistical program

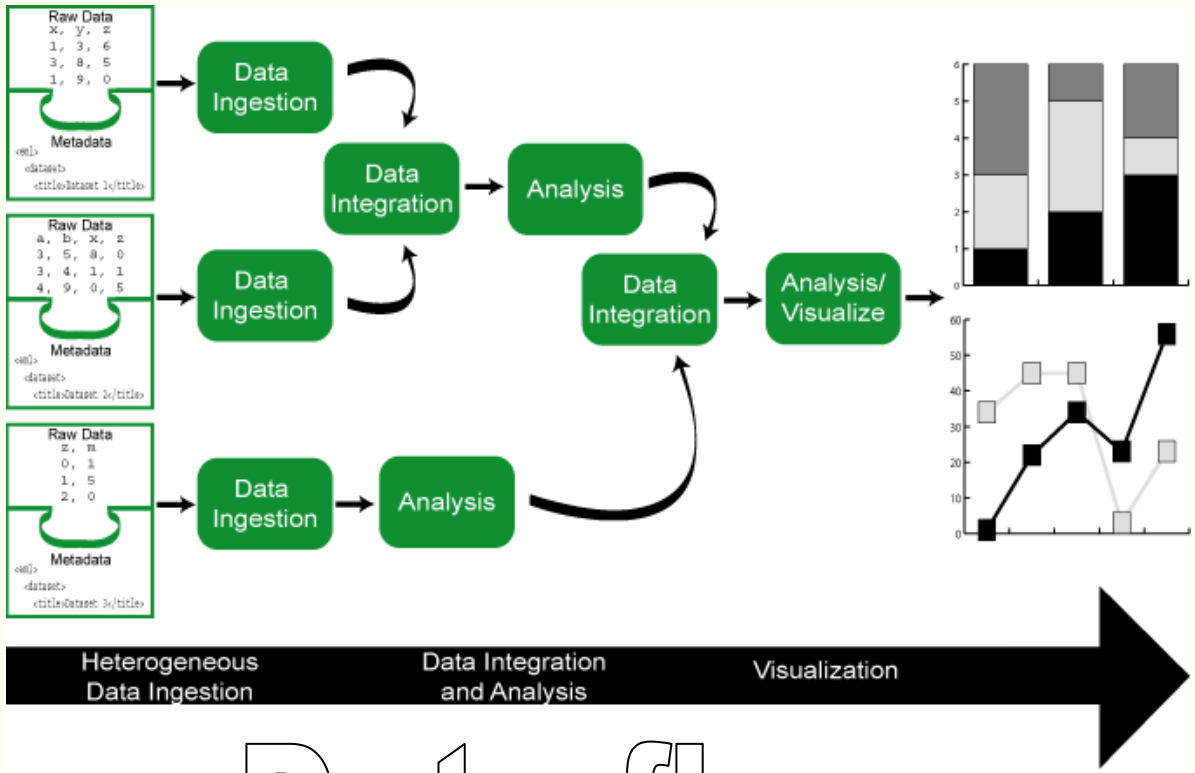
What is a workflow?

- What exactly did I do?
- Where did I put that piece of data?
- Who snatched the GIS expert away?
- Did I make that transformation before I…



What is a workflow?

Research Design



Reporting Sharing

Data flow

What is a workflow?

Data flow

Research Design

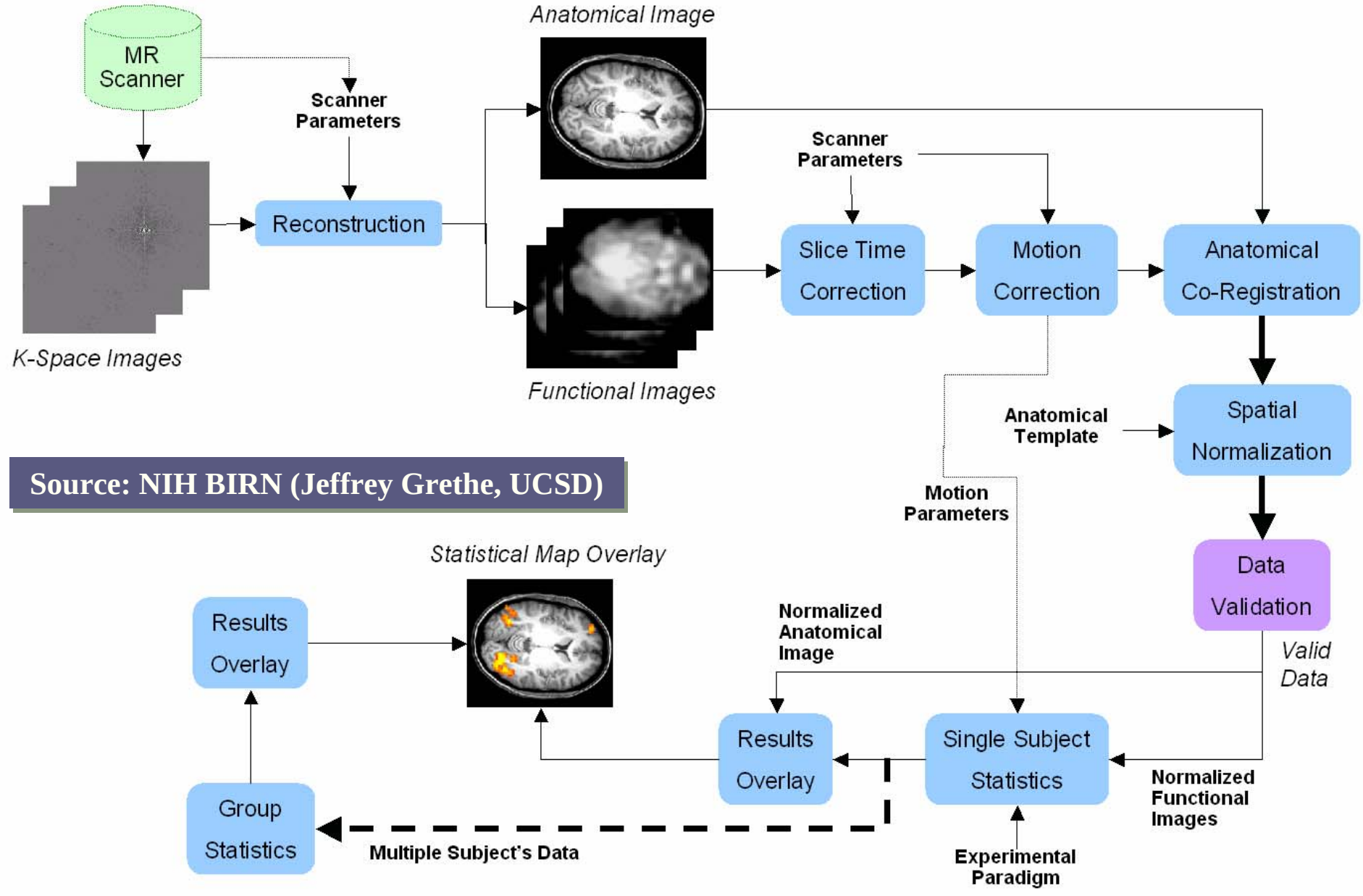
- Data discovery
- Analysis discovery
- Access to computational resources
- Automated data integration
- Automated transformation for analysis
- Workflow analysis

Reporting
Sharing

Workflow sharing

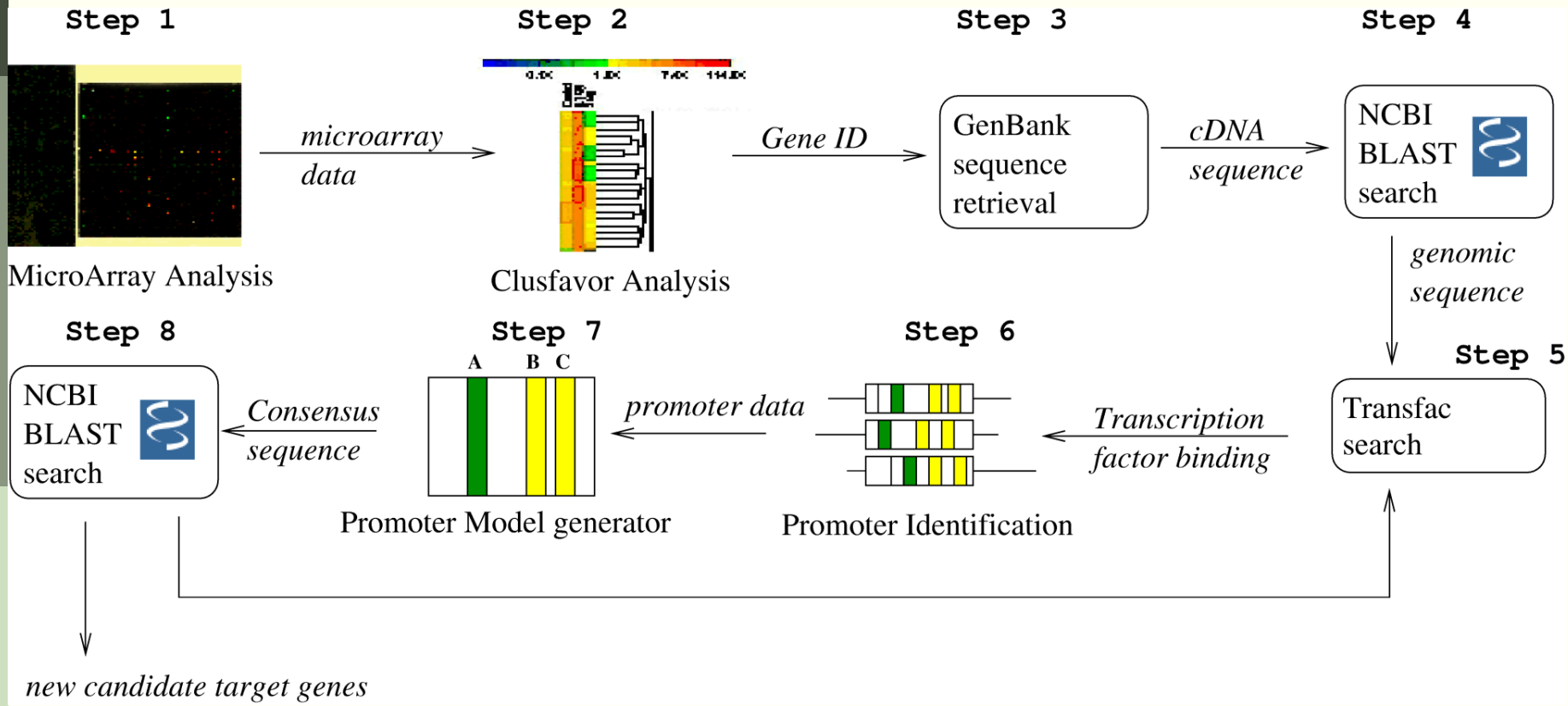
Workflow as methods metadata

Functional MRI Analysis Workflow



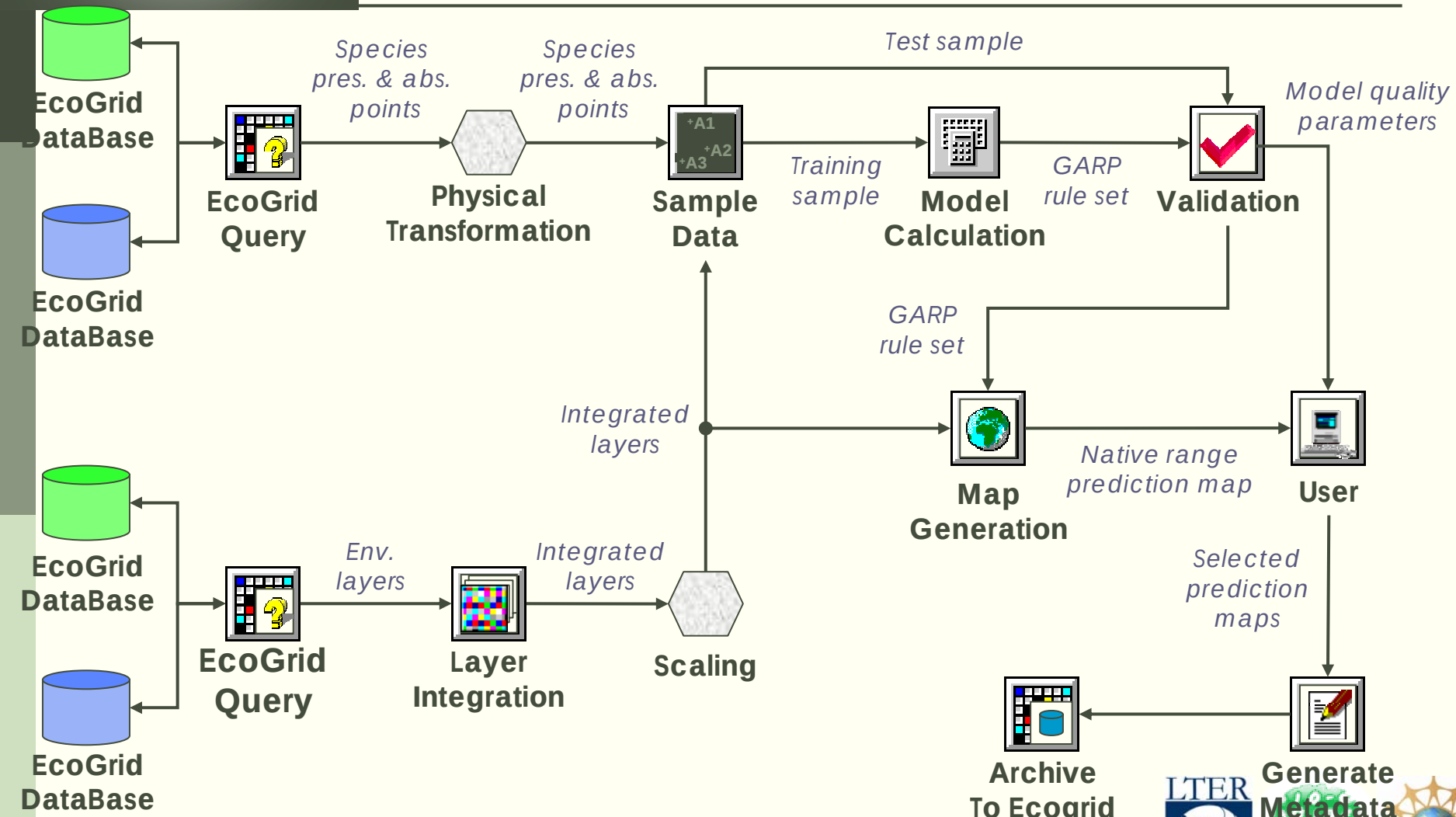
Source: NIH BIRN (Jeffrey Grethe, UCSD)

Promoter Identification Workflow (PIW)

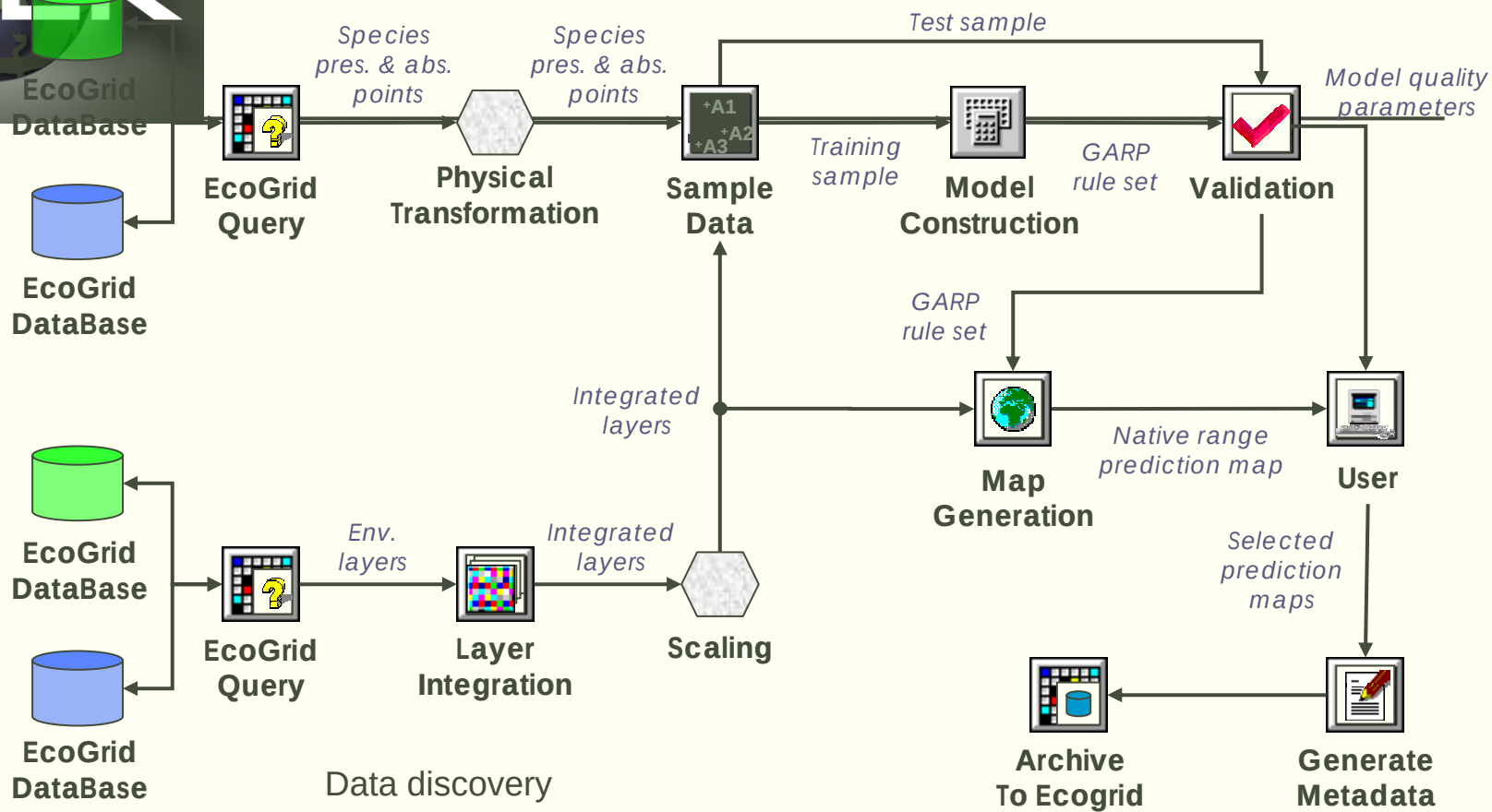


Source: Matt Coleman (LLNL)

Species Distribution Workflow

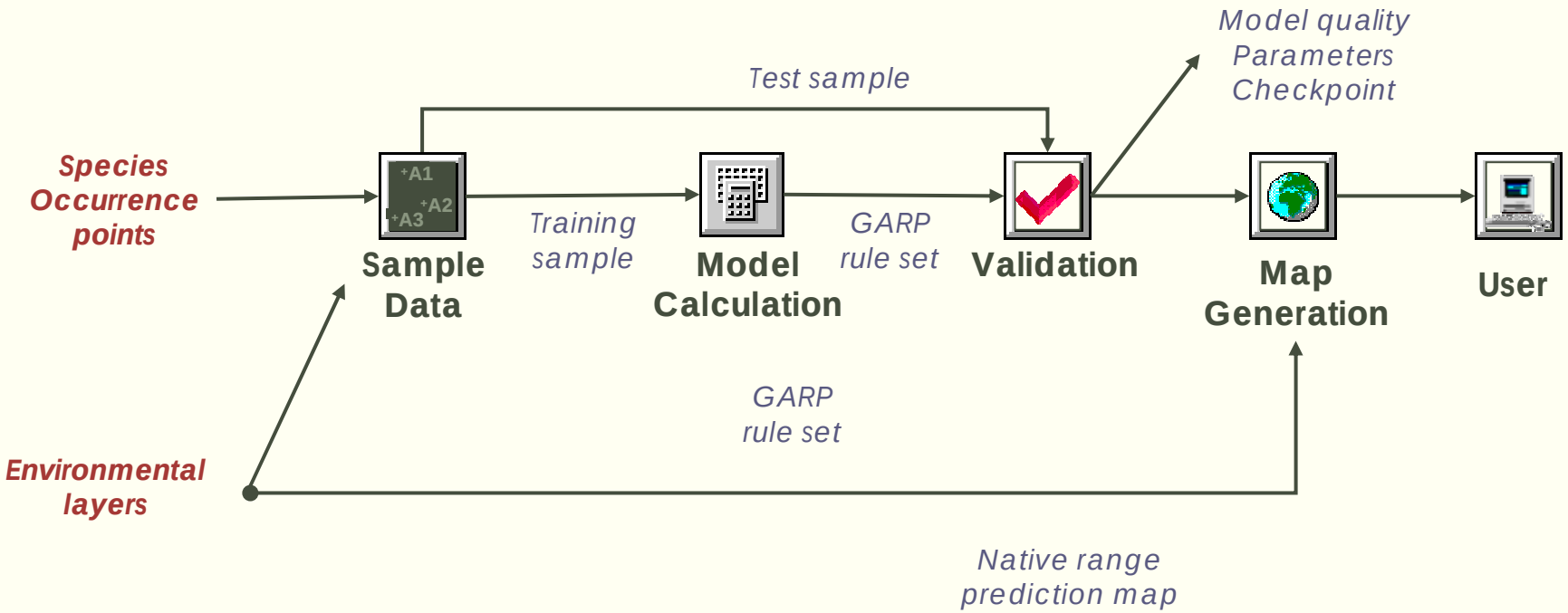


Species Distribution Workflow

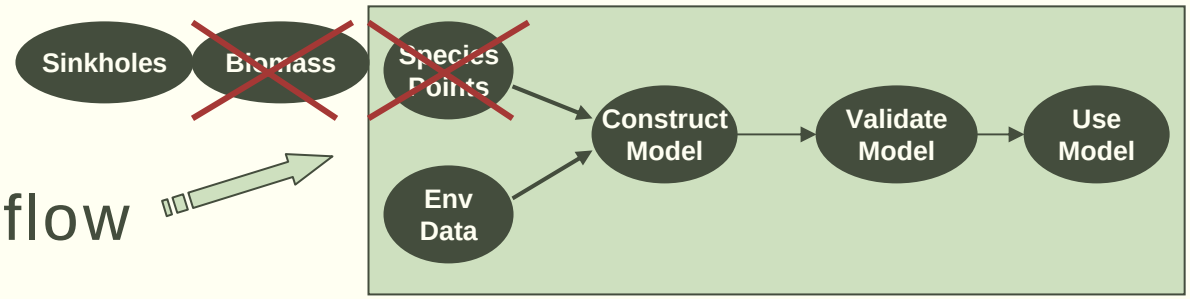


Data discovery
Analysis discovery
Access to computational resources
Workflow as methods metadata
Shared workflows
Automated data integration
Automated transformation for analysis
Workflow analysis

Abstract Workflow

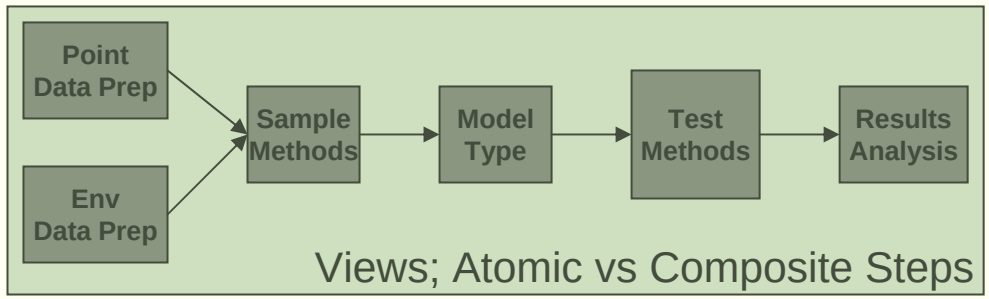


Hierarchical Workflows

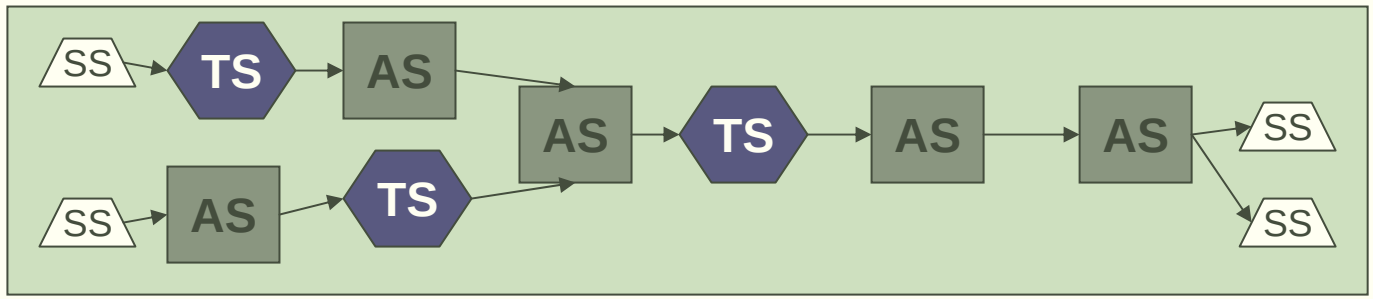


Conceptual Workflow

Abstract Workflow



Executable Workflow



- C — Concept
- AS — Analysis Step
- TS — Transformation Step
- SS — System Step

Workflow Reusability

- Reproduce/methods details
- Reuse within-discipline different data
- Reuse within-discipline different model/analyses
- Reuse between-discipline

Exercise: Conceptual and Abstract Workflows

1. Break into groups of 4
2. Pick a research topic
3. Construct an abstract workflow
4. Stop at 11:45
5. Group presentations

Acknowledgements

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