Mind Your Metadata

Exploiting Semantics for Configuration, Adaptation, and Provenance in Scientific Workflows

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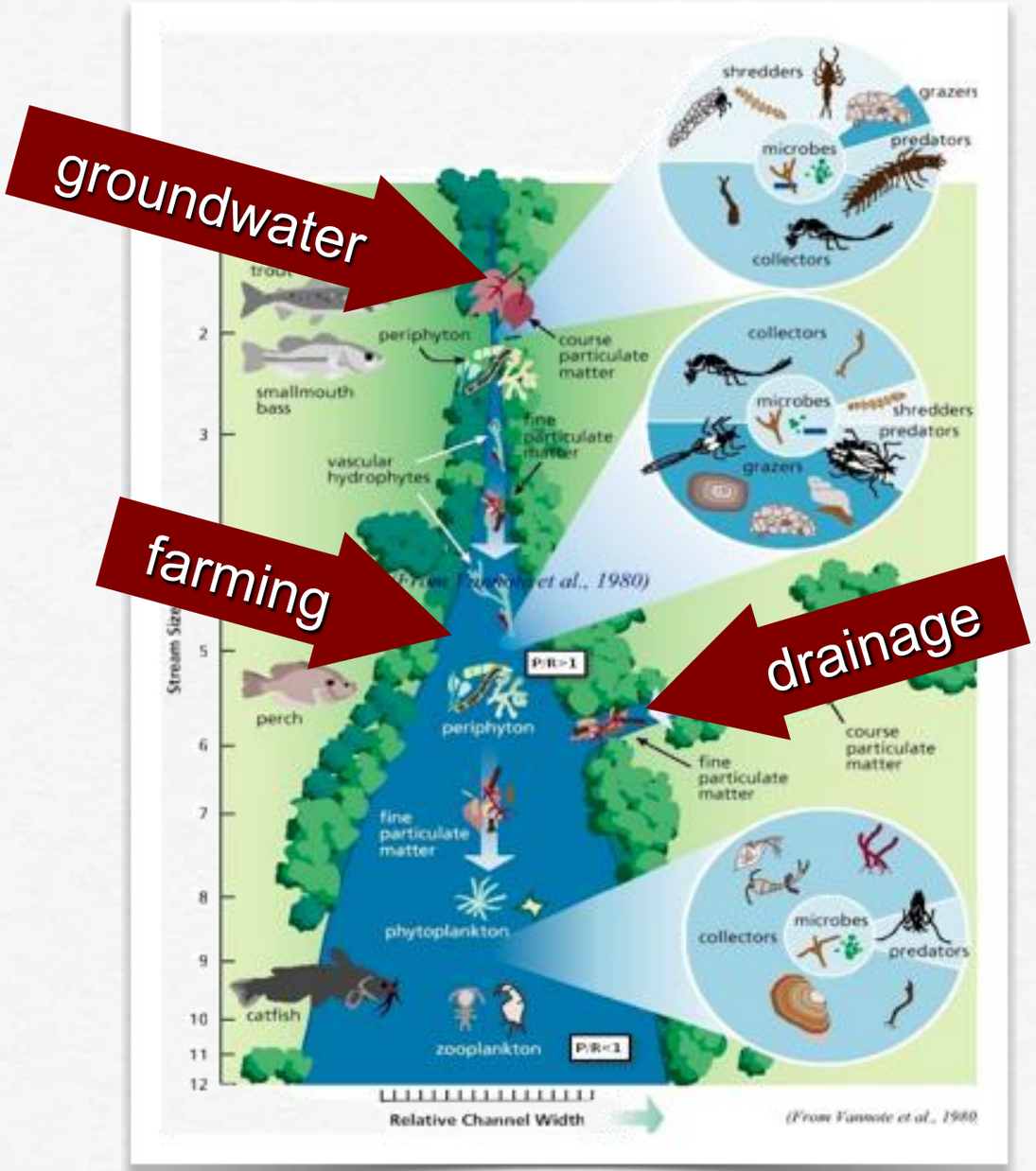
Sandra Villamizar

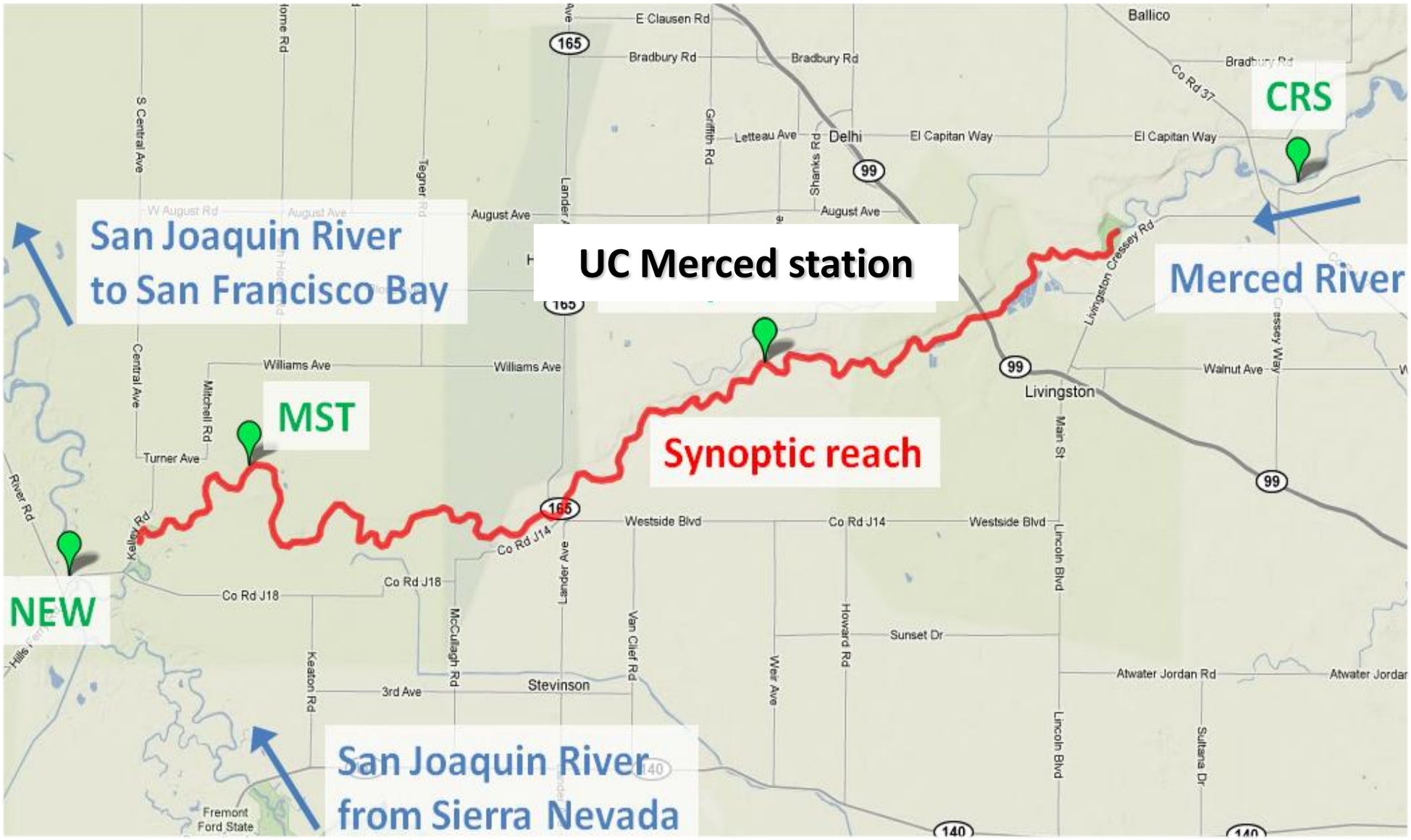
UC Merced

River Continuum vs Human Activities

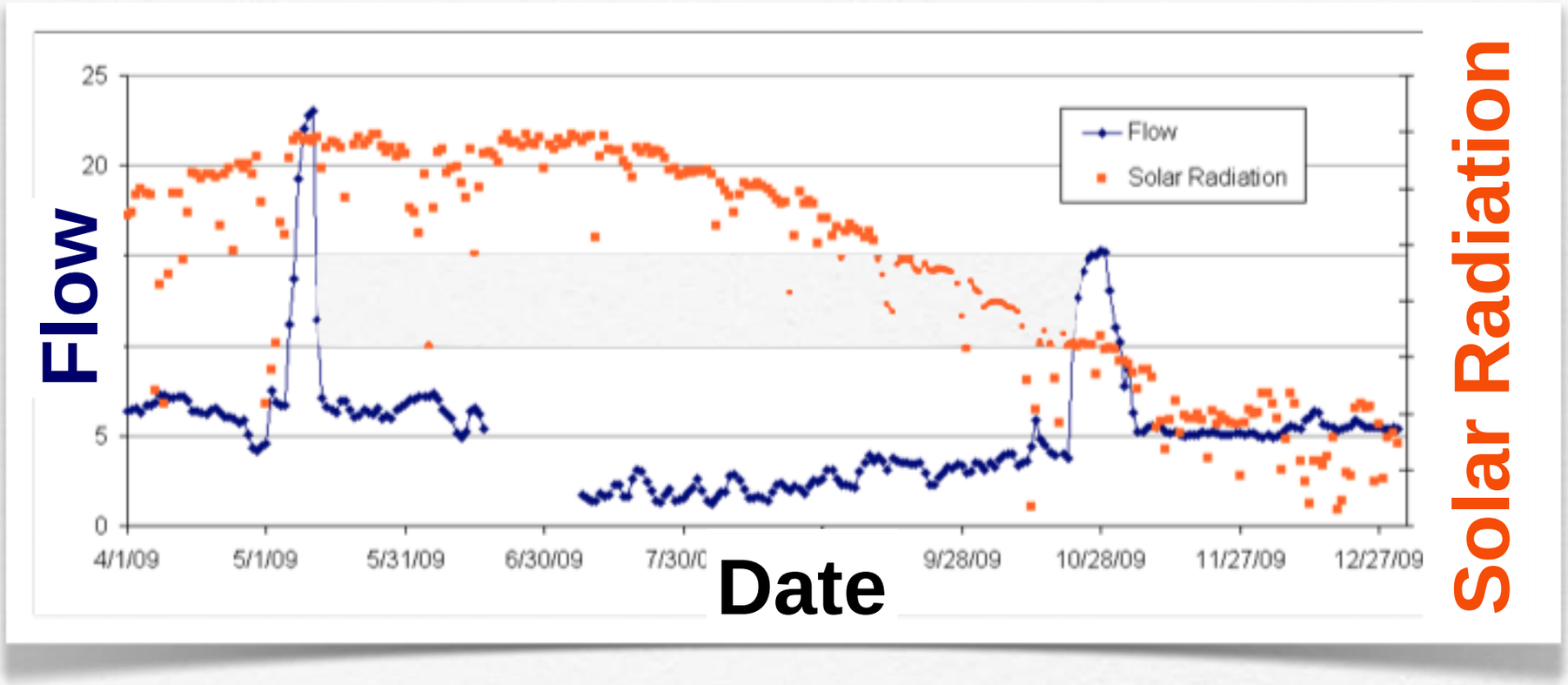
- River continuum: natural inputs, reactive transport
- Human intervention: Agricultural, industrial, municipal
- What management practices help/hurt?
- Can we restore natural behavior?



Case Study

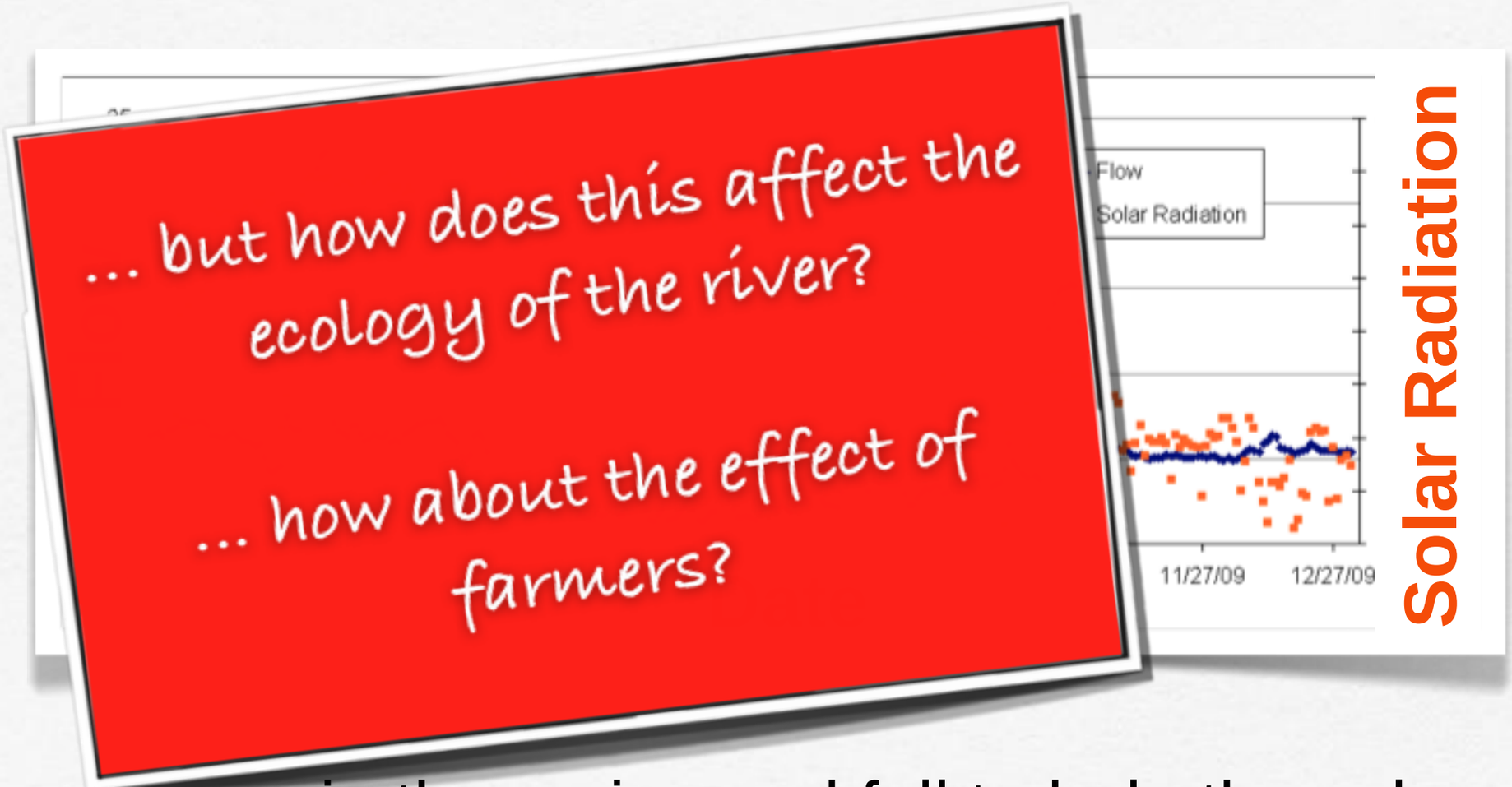

San Joaquin River
to San Francisco Bay
UC Merced station
Merced River
CRS
MST
Synoptic reach
NEW
San Joaquin River
from Sierra Nevada
Ballico
Delhi
Livingston
Stevinson
E Clausen Rd
Bradbury Rd
Letteau Ave
El Capitan Way
August Ave
Williams Ave
Turner Ave
Walnut Ave
Westside Blvd
Co Rd J14
Co Rd J18
Sunset Dr
Atwater Jordan Rd
3rd Ave
Co Rd 37
Livingston Cressey Rd
S Central Ave
Tegner Rd
Lander Ave
Griffith Rd
Shanks Rd
Mitchell Rd
Kelley Rd
River Rd
McCullagh Rd
Van Clief Rd
Weir Ave
Howard Rd
Lincoln Blvd
Main St
Keaton Rd
Sultana Dr
Fremont Ford State

Stream Metabolism Response to Human Disturbances



Pulse releases in the spring and fall to help the salmon runs

Stream Metabolism Response to Human Disturbances

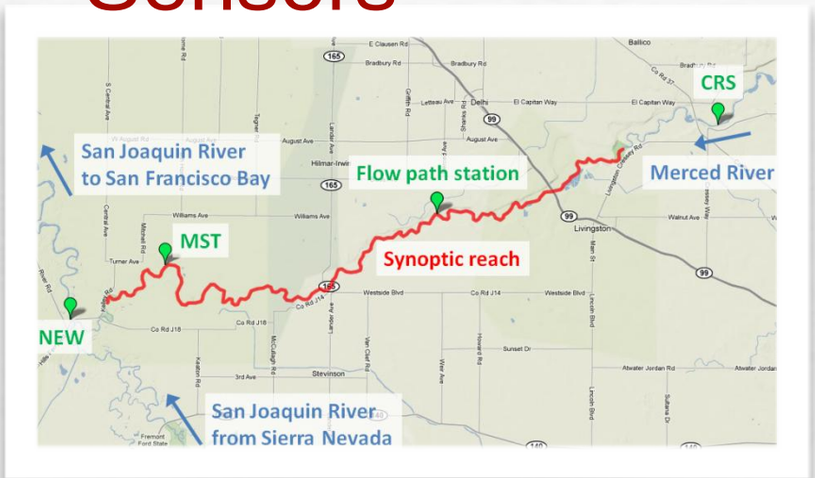


Pulse releases in the spring and fall to help the salmon runs

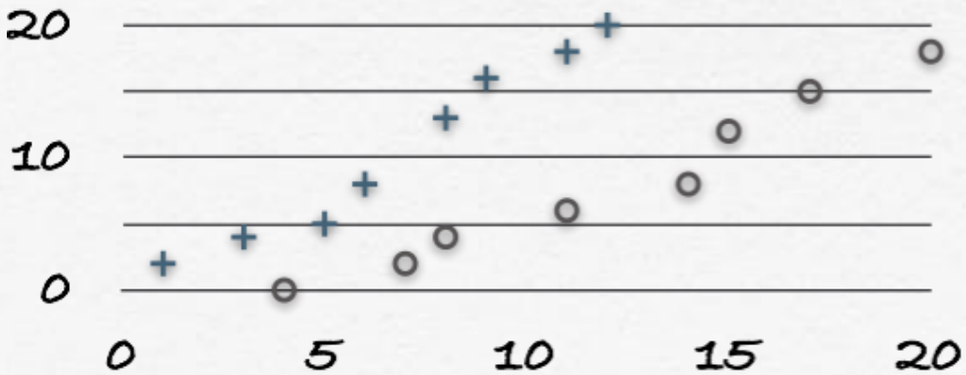
Aquatic Photosynthesis

Models of gross primary production (GPP), community respiration (CR24)

Sensors



Analysis

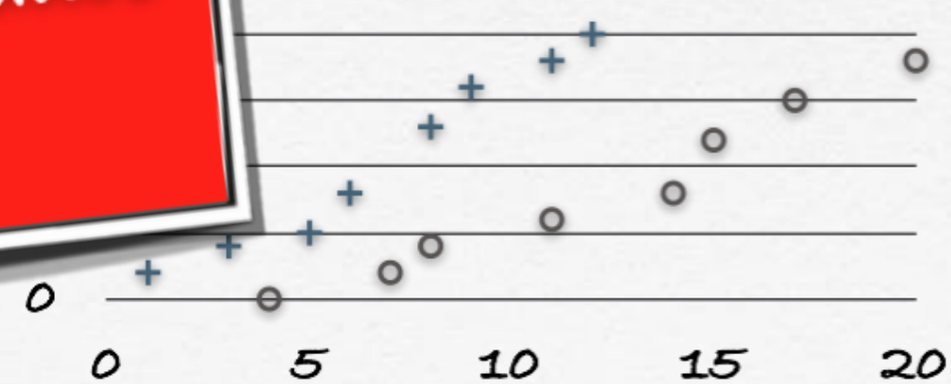


Aquatic Photosynthesis

Models of gross primary production (GPP), community respiration (CR24)

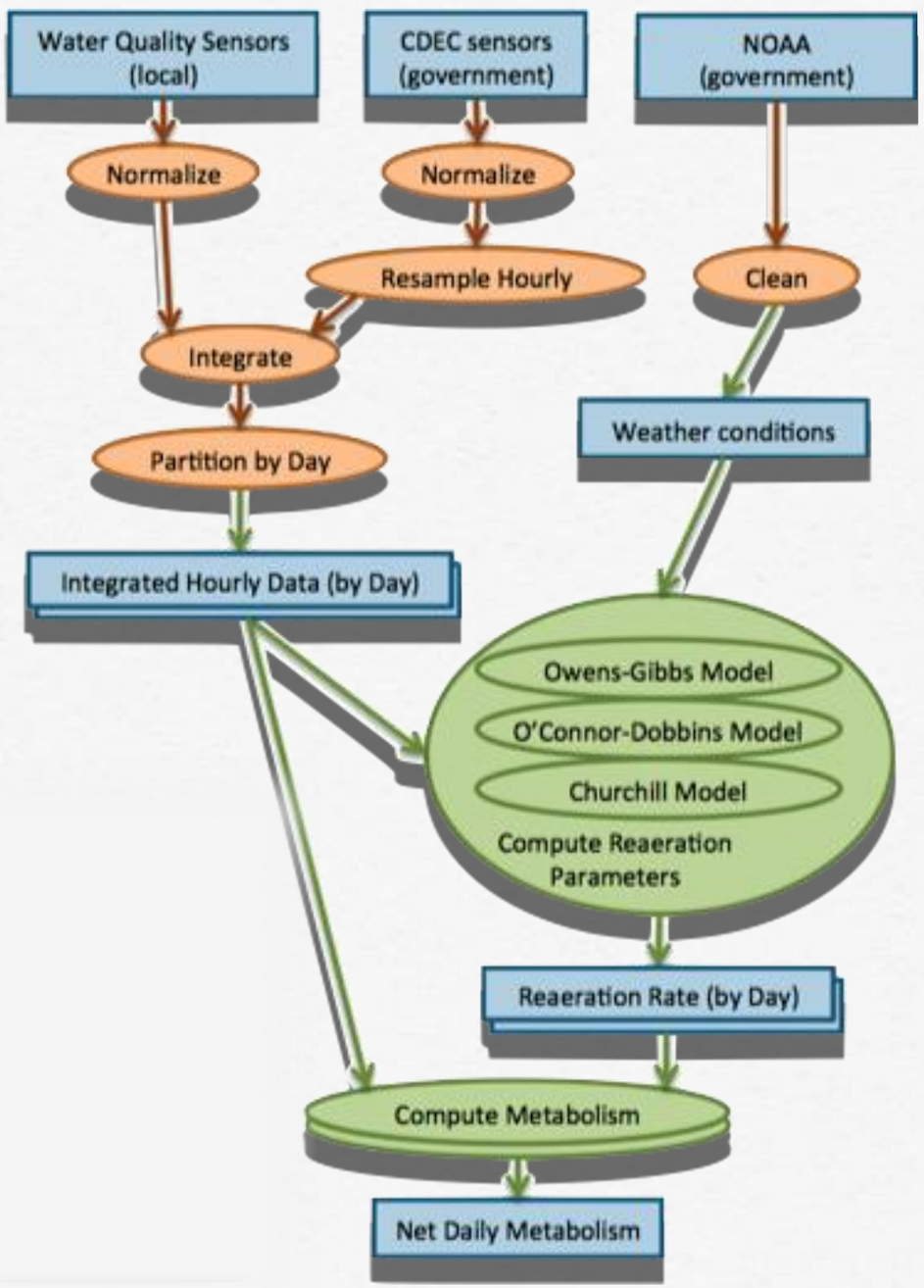
Sensors

Analysis



Analyses must be fast to produce actionable information

Workflow



Tom Harmon

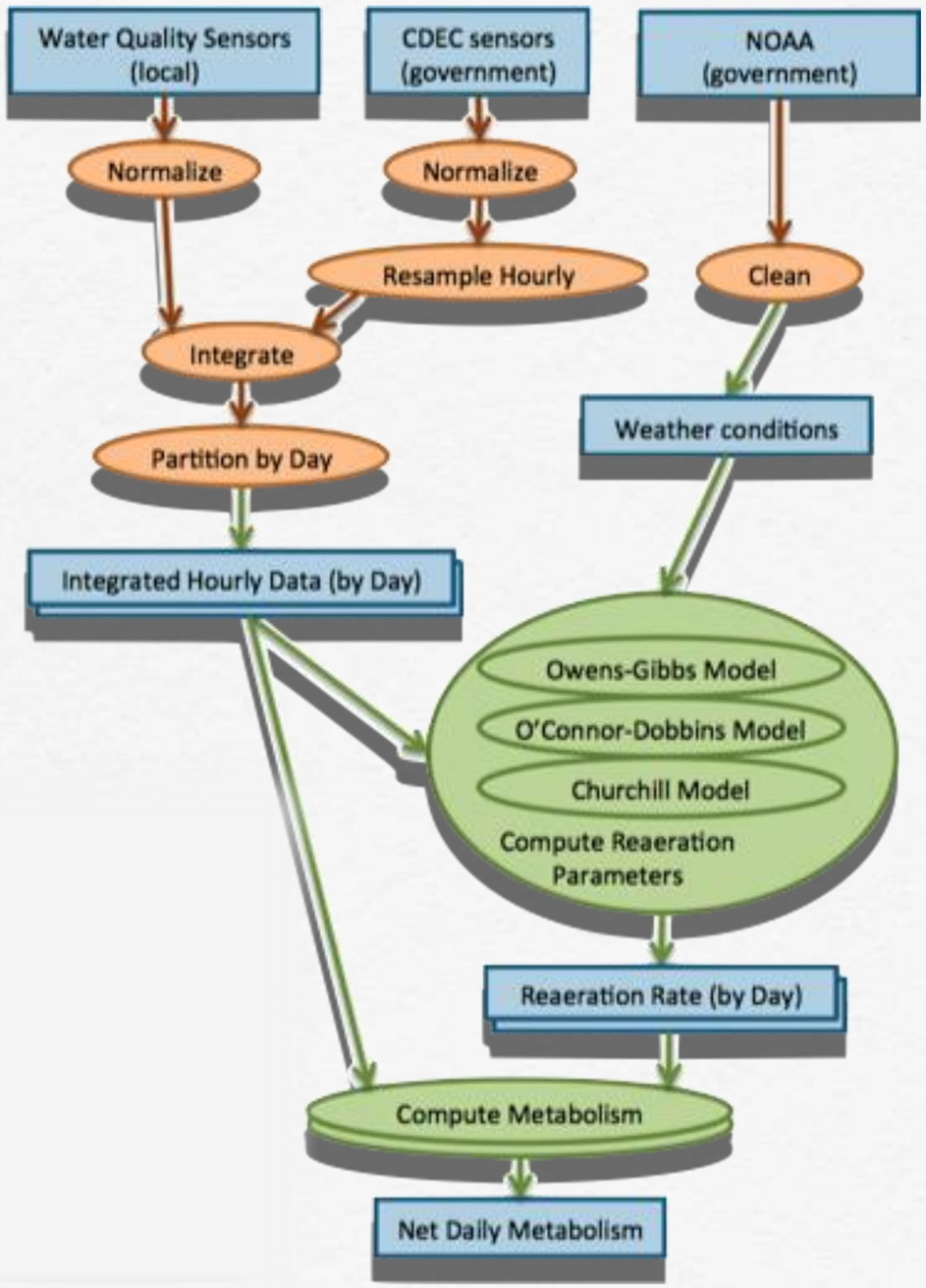
environmental systems

Vision: Automated & Fast

Reality: Difficult & Time Consuming

?

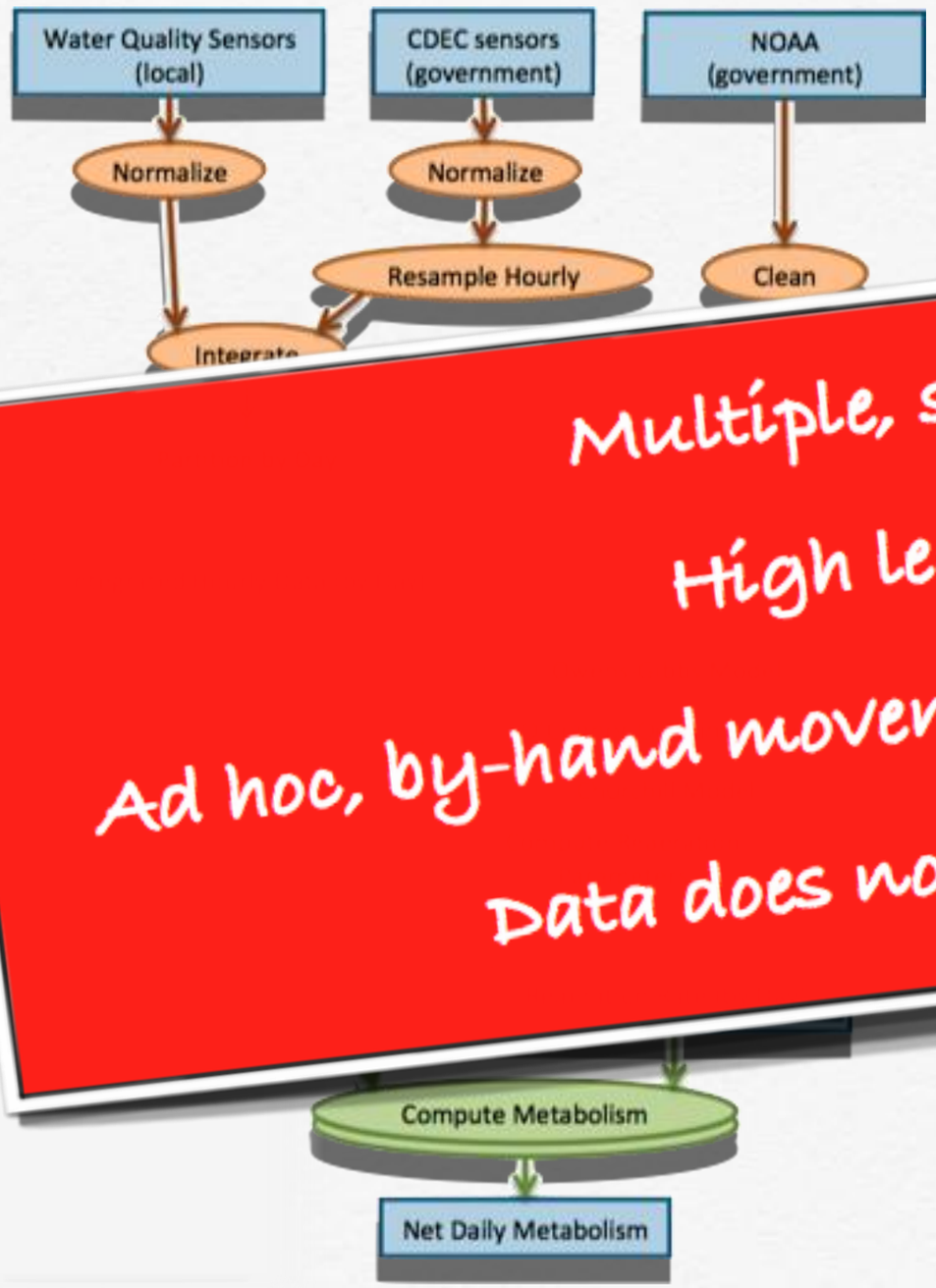
Current Method



Manual Data Preparation

Custom Scripts

Current Method



Manual

n

Scripts

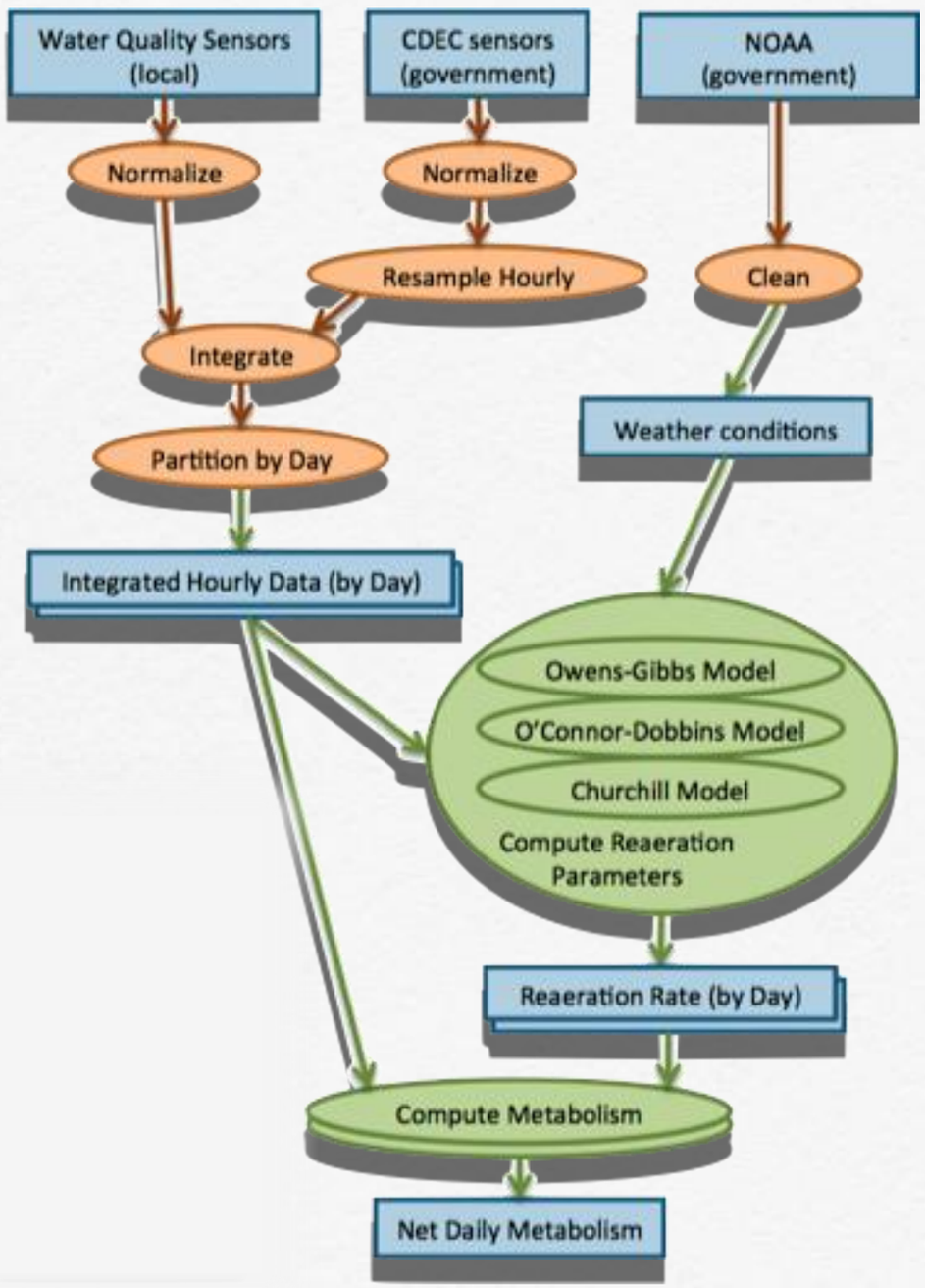
Multiple, separate tools

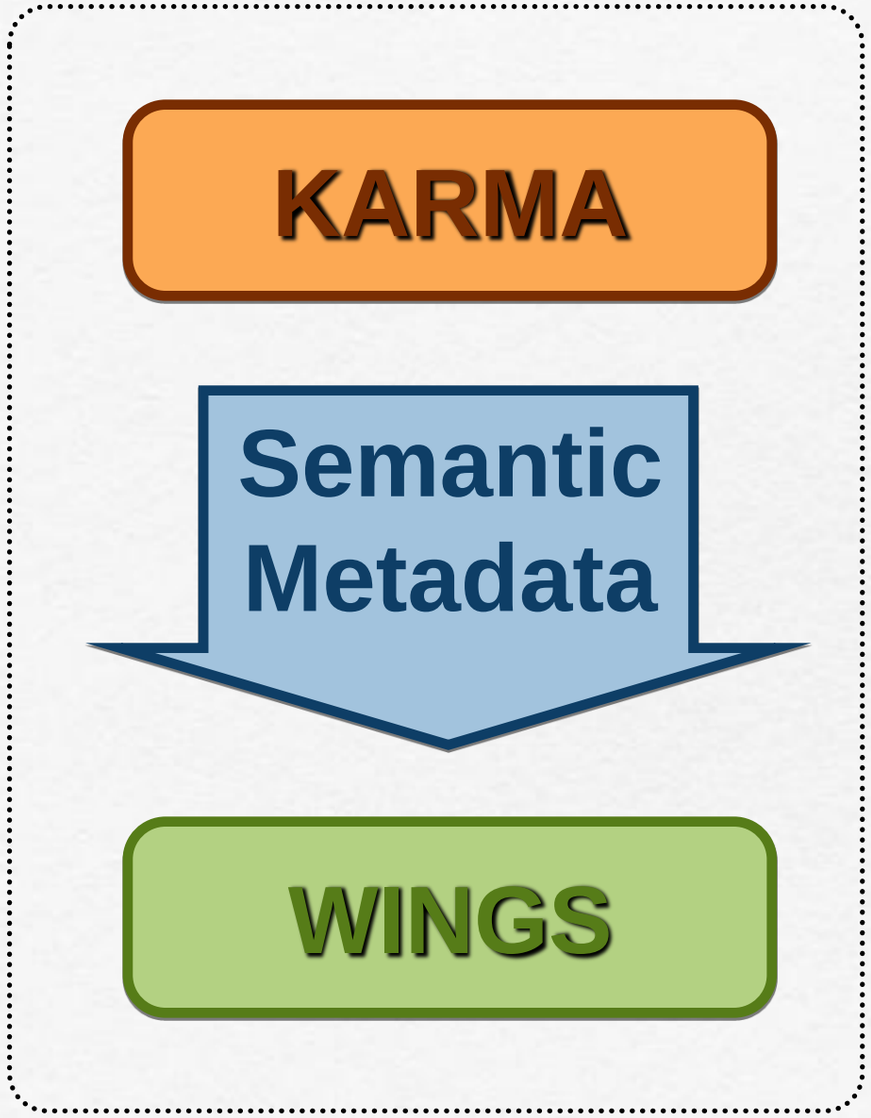
High learning costs

Ad hoc, by-hand movement of data & tool invocation

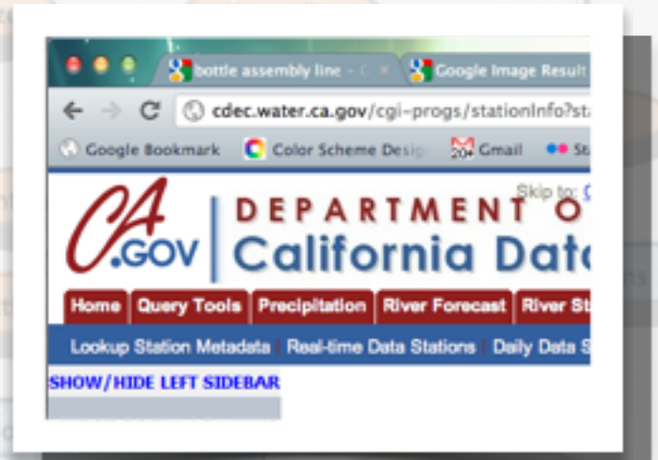
Data does not "flow" across tools

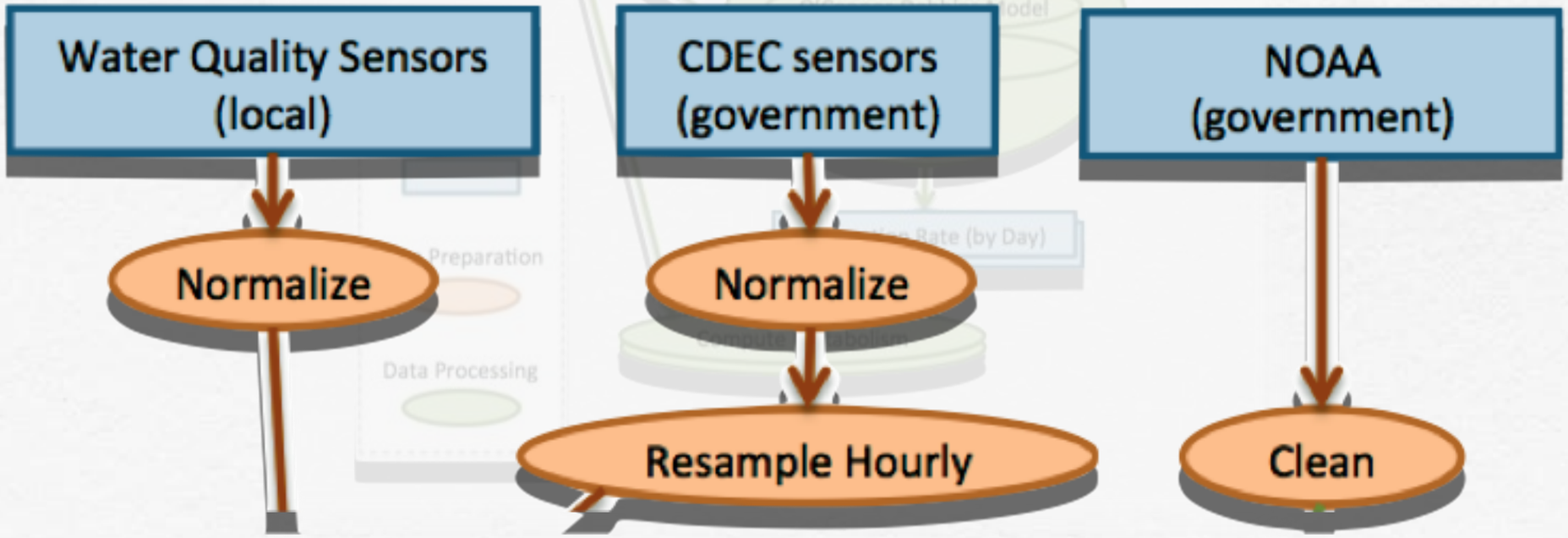
Our Approach





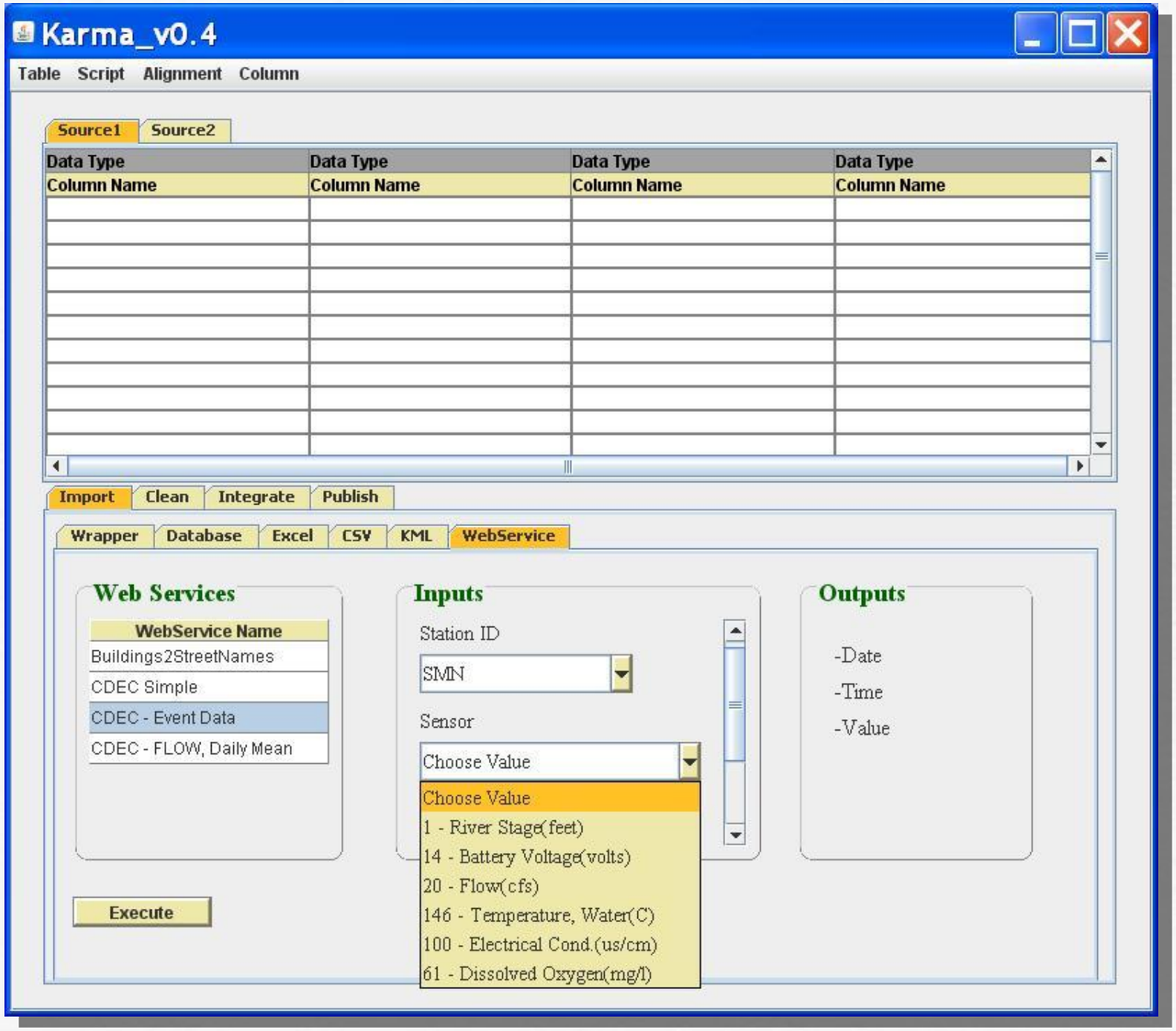
Data Sources





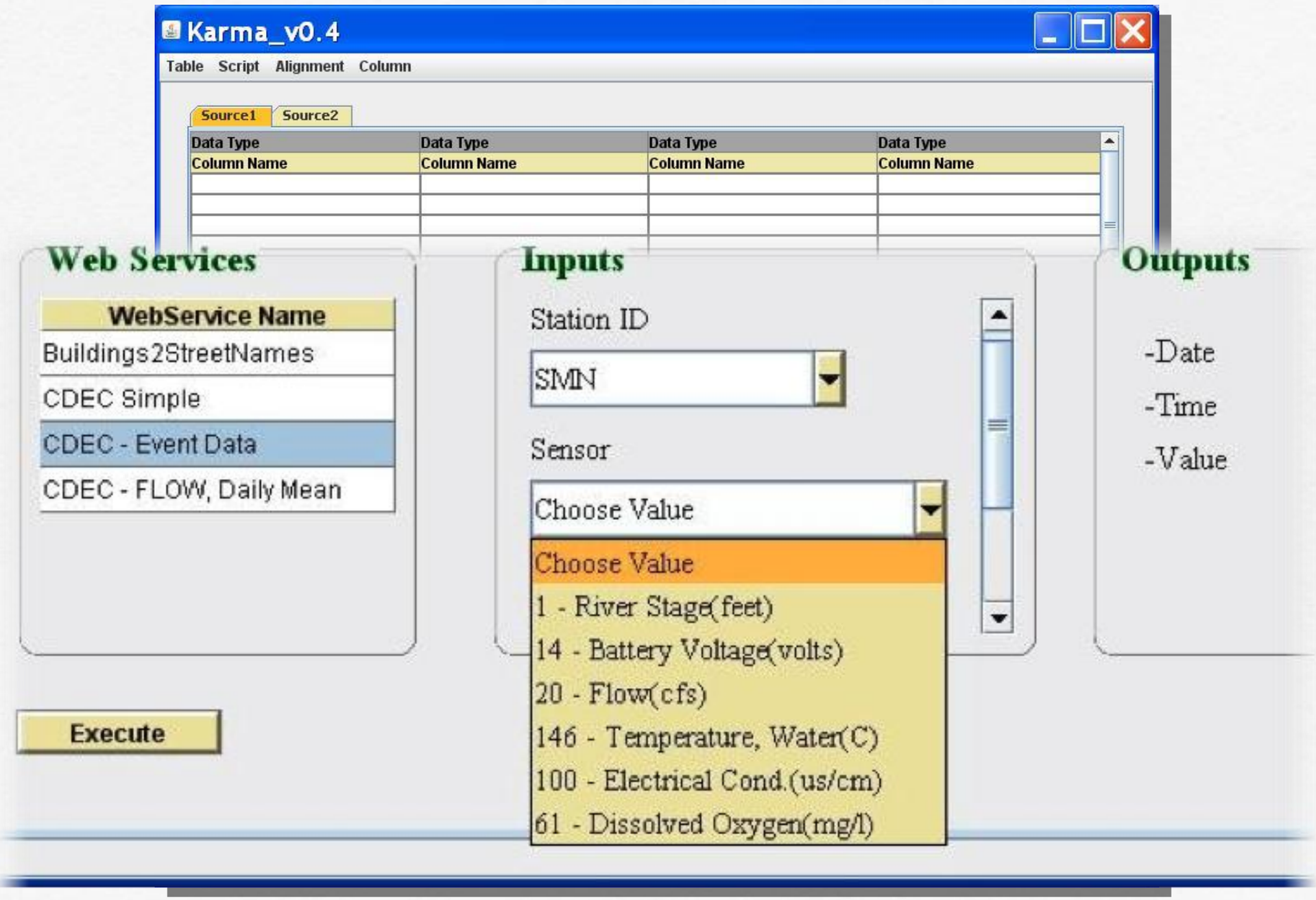
[Tuchinda et al TWEB'11; Tuchinda et al IUI'08, IUI'07]

KARMA

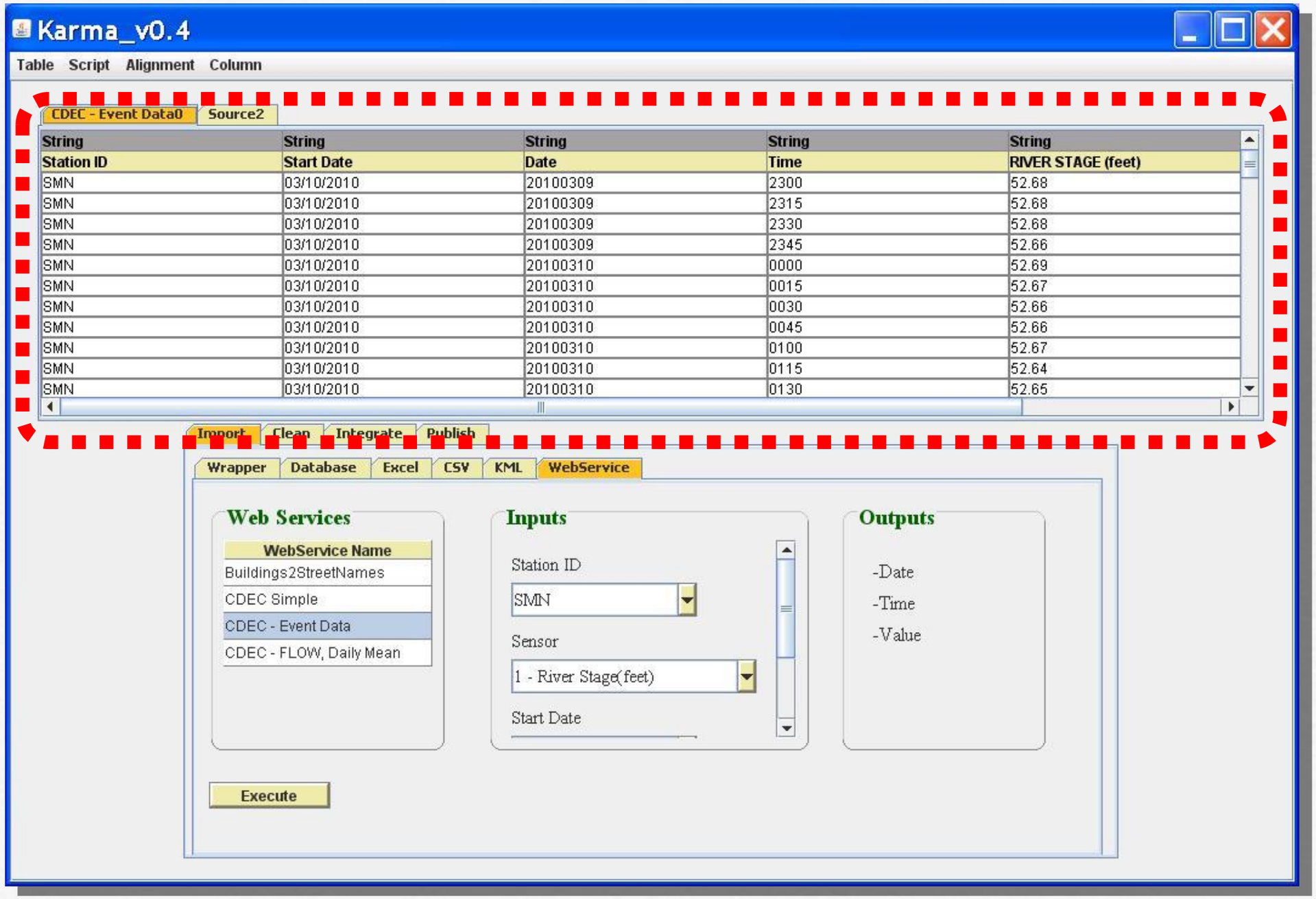


[Tuchinda et al TWEB'11; Tuchinda et al IUI'08, IUI'07]

KARMA



Data Import



String	String	String	String	String
Station ID	Start Date	Date	Time	RIVER STAGE (feet)
SMN	03/10/2010	20100309	2300	52.68
SMN	03/10/2010	20100309	2315	52.68
SMN	03/10/2010	20100309	2330	52.68
SMN	03/10/2010	20100309	2345	52.66
SMN	03/10/2010	20100310	0000	52.69
SMN	03/10/2010	20100310	0015	52.67
SMN	03/10/2010	20100310	0030	52.66
SMN	03/10/2010	20100310	0045	52.66
SMN	03/10/2010	20100310	0100	52.67
SMN	03/10/2010	20100310	0115	52.64
SMN	03/10/2010	20100310	0130	52.65

Need to Clean Data

Date	Time	RIVER STAGE (feet)
20100309	2300	52.68
20100309	2315	52.68

CDEC

timestamp	WXT510P
2010-03-10 00:00:00	760
2010-03-10 00:15:00	760

HYDROLAB

Date	Time	Temp	Cond
03/09/2010	23:00	13.4	1181.00
03/09/2010	23:15	13.4	1179.00

Required Format

Need to Clean Data

Date	Time	GE (feet)
20100309	2300	
20100309		

CDEC

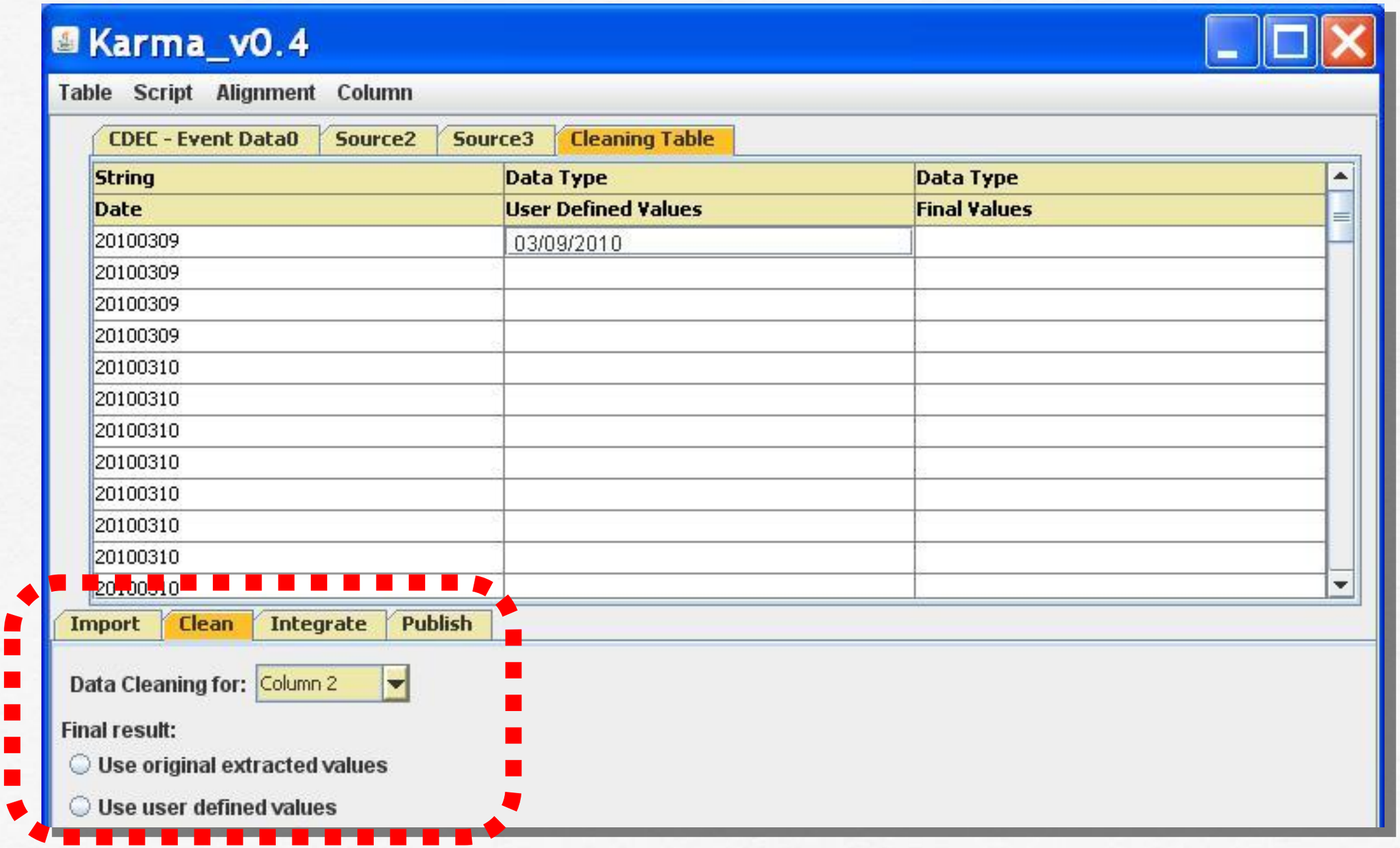
60 Files for 1 month!

HYDROLAB

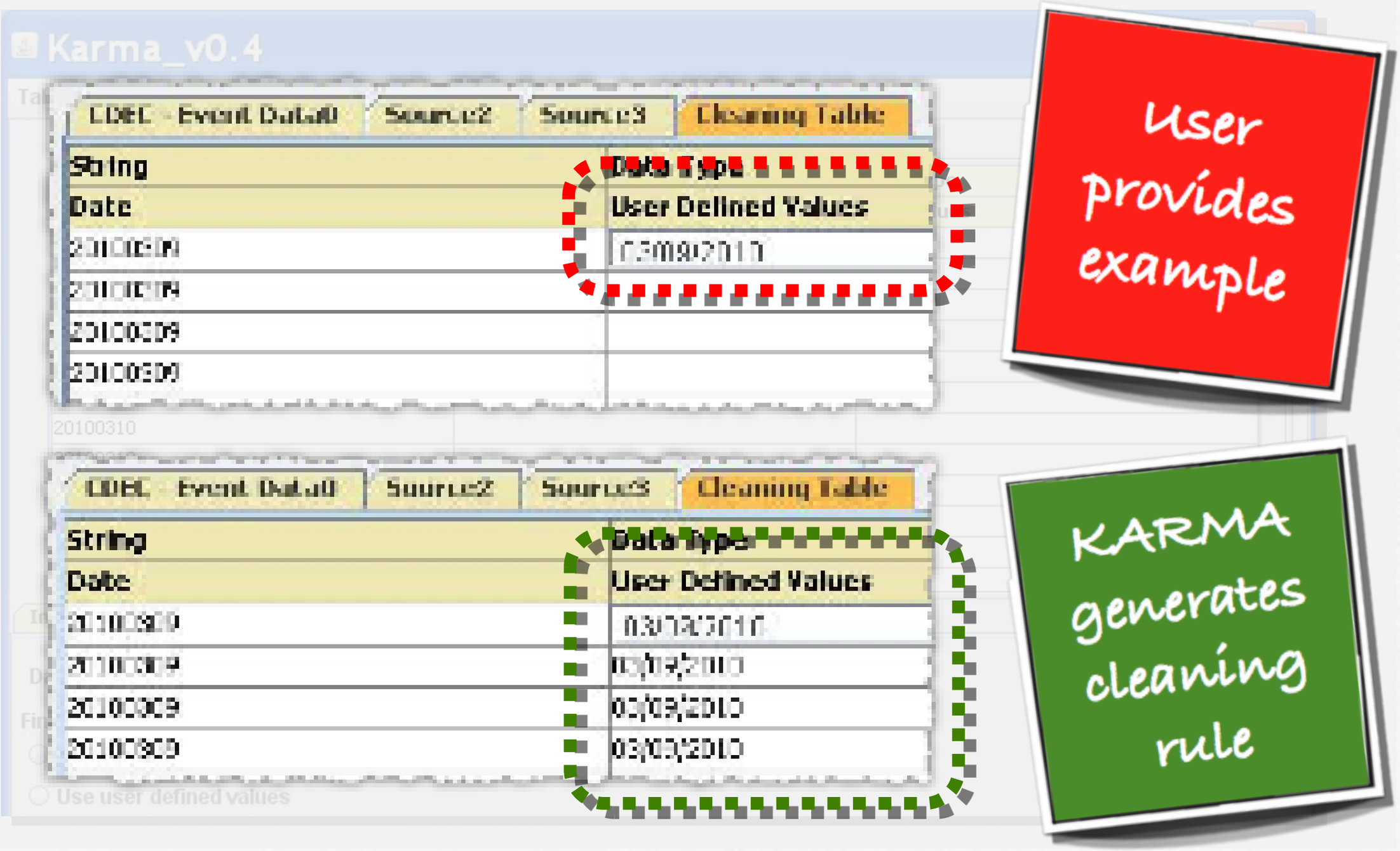
Date		Temp	Cond
03/09/2010	23:00	13.4	1181.00
03/09/2010	23:15	13.4	1179.00

Required Format

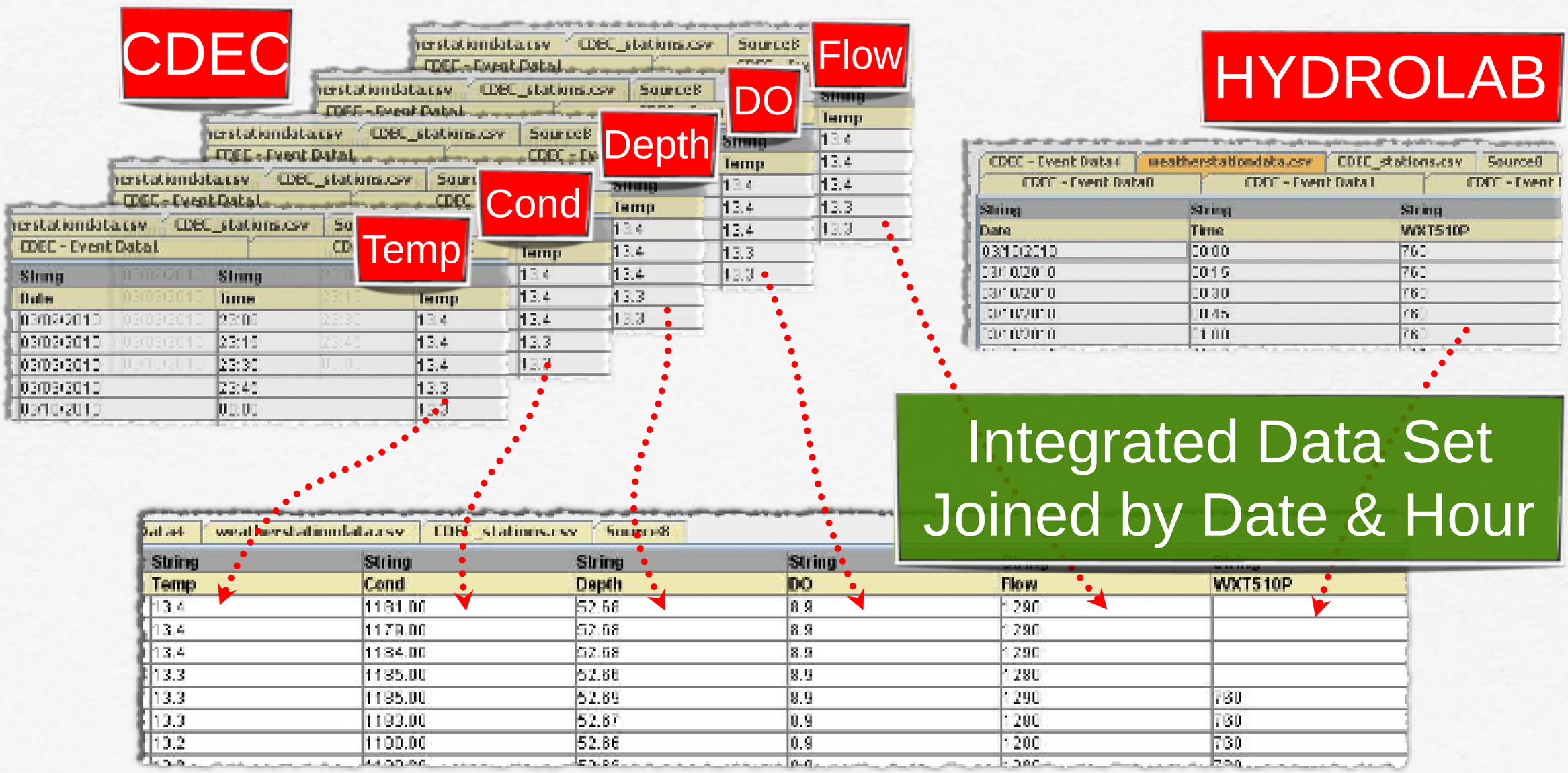
Data Cleaning with KARMA



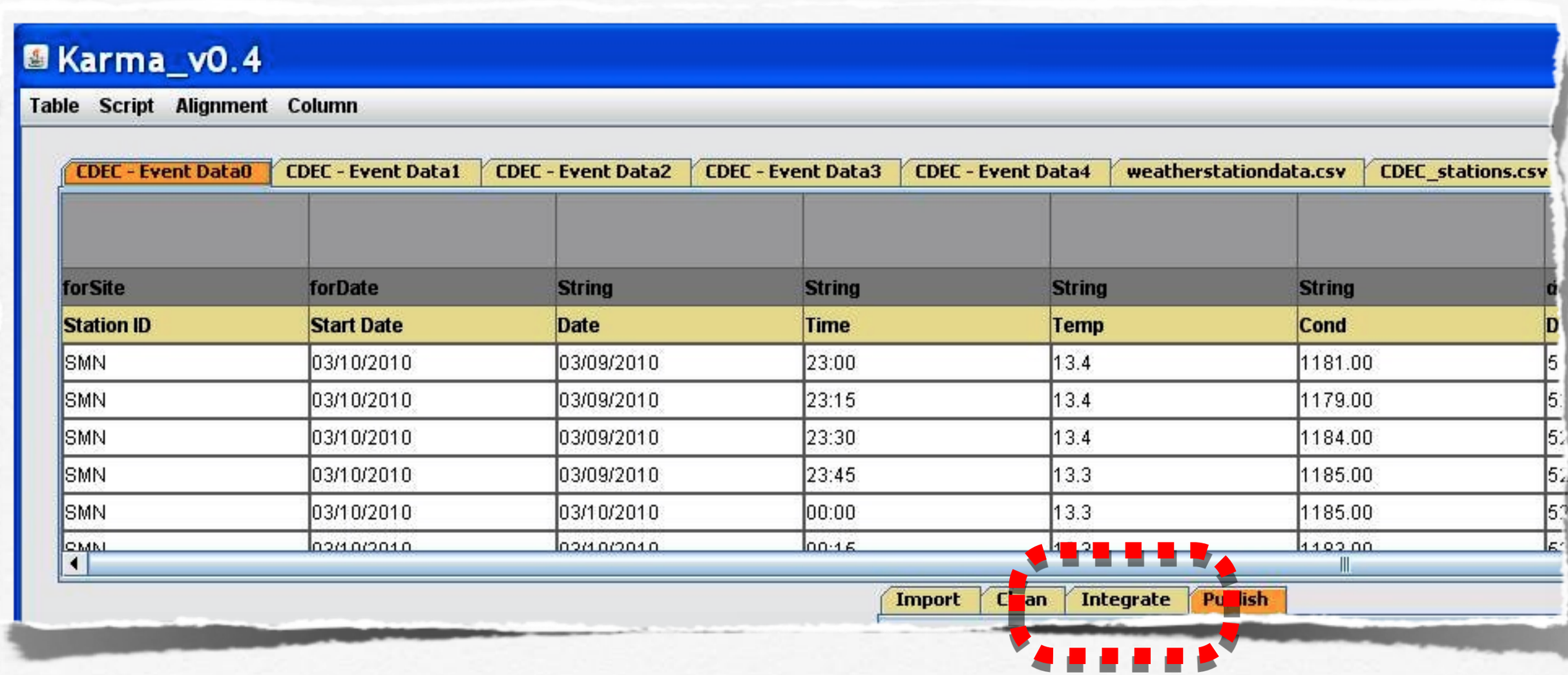
Data Cleaning with KARMA



Need to Integrate All the Sources



Integrated Dataset



forSite	forDate	String	String	String	String
Station ID	Start Date	Date	Time	Temp	Cond
SMN	03/10/2010	03/09/2010	23:00	13.4	1181.00
SMN	03/10/2010	03/09/2010	23:15	13.4	1179.00
SMN	03/10/2010	03/09/2010	23:30	13.4	1184.00
SMN	03/10/2010	03/09/2010	23:45	13.3	1185.00
SMN	03/10/2010	03/10/2010	00:00	13.3	1185.00

KARMA Generates Data Processing Script

```
ImportWSSource("CDEC - Event Data","SMN","146","$1","$2");SetColumnName("CDEC
- Event Data0","4","Date");ApplyCleanRule("CDEC - Event
Data0","Date","20100309","03/09/2010");DeleteColumnCommand("Sensor");DeleteCo
lumnCommand("End Date");SetColumnName("CDEC - Event
Data0","3","Time");SetColumnName("CDEC - Event
Data0","4","Temp");ApplyCleanRule("CDEC - Event
Data0","Time","2300","23:00");SwitchToEmptySourceTab(1);ImportWSSource("CDEC
- Event Data","SMN","100","$1","$2");SetColumnName("CDEC - Event
Data1","4","Date");ApplyCleanRule("CDEC - Event
Data1","Date","20100309","03/09/2010");DeleteColumnCommand("Sensor");DeleteCo
lumnCommand("Start Date");DeleteColumnCommand("End Date");SetColumnName("CDEC
- Event Data1","2","Time");SetColumnName("CDEC - Event
Data1","3","Cond");ApplyCleanRule("CDEC - Event
Data1","Time","2300","23:00");SwitchToEmptySourceTab(2);ImportWSSource("CDEC
- Event Data","SMN","1","$1","$2");SetColumnName("CDEC - Event
Data2","4","Date");ApplyCleanRule("CDEC - Event
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lumnCommand("Start Date");DeleteColumnCommand("End Date");SetColumnName("CDEC
- Event Data2","2","Time");SetColumnName("CDEC - Event
Data2","3","Depth");ApplyCleanRule("CDEC - Event
Data2","Time","2300","23:00");SwitchToEmptySourceTab(3);ImportWSSource("CDEC
- Event Data","SMN","61","$1","$2");SetColumnName("CDEC - Event
Data3","4","Date");ApplyCleanRule("CDEC - Event
Data3","Date","20100309","03/09/2010");DeleteColumnCommand("Sensor");DeleteCo
lumnCommand("Start Date");DeleteColumnCommand("End Date");SetColumnName("CDEC
- Event Data3","2","Time");SetColumnName("CDEC - Event
Data3","3","DO");ApplyCleanRule("CDEC - Event
Data3","Time","2300","23:00");SwitchToEmptySourceTab(4);ImportWSSource("CDEC
- Event Data","SMN","20","$1","$2");SetColumnName("CDEC - Event
Data4","4","Date");ApplyCleanRule("CDEC - Event
Data4","Date","20100309","03/09/2010");DeleteColumnCommand("Sensor");DeleteCo
lumnCommand("Start Date");DeleteColumnCommand("End Date");SetColumnName("CDEC
- Event Data4","2","Time");SetColumnName("CDEC - Event
Data4","3","Flow");ApplyCleanRule("CDEC - Event
Data4","Time","2300","23:00");SwitchToSourceTab(0);join("CDEC - Event
Data0","CDEC - Event Data1","Cond");join("CDEC - Event Data0","CDEC - Event
Data2","Depth");join("CDEC - Event Data0","CDEC - Event
Data3","DO");join("CDEC - Event Data0","CDEC - Event
Data4","Flow");SwitchToEmptySourceTab(5);ImportCSVSource(".\\data\\CDEC_stati
ons.csv");ImportColumnFromCSV("Station
ID","0","true");ImportColumnFromCSV("Metadata","1","true");ImportColumnFromCS
V("Name","2","true");ImportColumnFromCSV("Elevation","3","true");ImportColumn
FromCSV("Latitude","4","true");ImportColumnFromCSV("Longitude","5","true");Sw
itchToSourceTab(0);join("CDEC - Event
Data0","CDEC_stations.csv","Latitude");join("CDEC - Event
Data0","CDEC_stations.csv","Longitude");PublishToWS("WINGS
Portal","TEST_CDEC_WEATHER_$3","CDEC - Event Data0");
```

KARMA Generates Data Processing Script

```
ImportWSSource("CDEC - Event Data","SMN","146","$1","$2");
SetColumnName("CDEC - Event Data0","4","Date");
ApplyCleanRule("CDEC - Event Data0","Date","20100309","03/09/2010");
DeleteColumnCommand("Sensor");
DeleteColumnCommand("End Date");
SetColumnName("CDEC - Event Data0","3","Time");
SetColumnName("CDEC - Event Data0","4","Temp");
ApplyCleanRule("CDEC - Event Data0","Time","2300","23:00");
SwitchToEmptySourceTab(1);
ImportWSSource("CDEC - Event Data","SMN","100","$1","$2");
SetColumnName("CDEC - Event Data1","4","Date");
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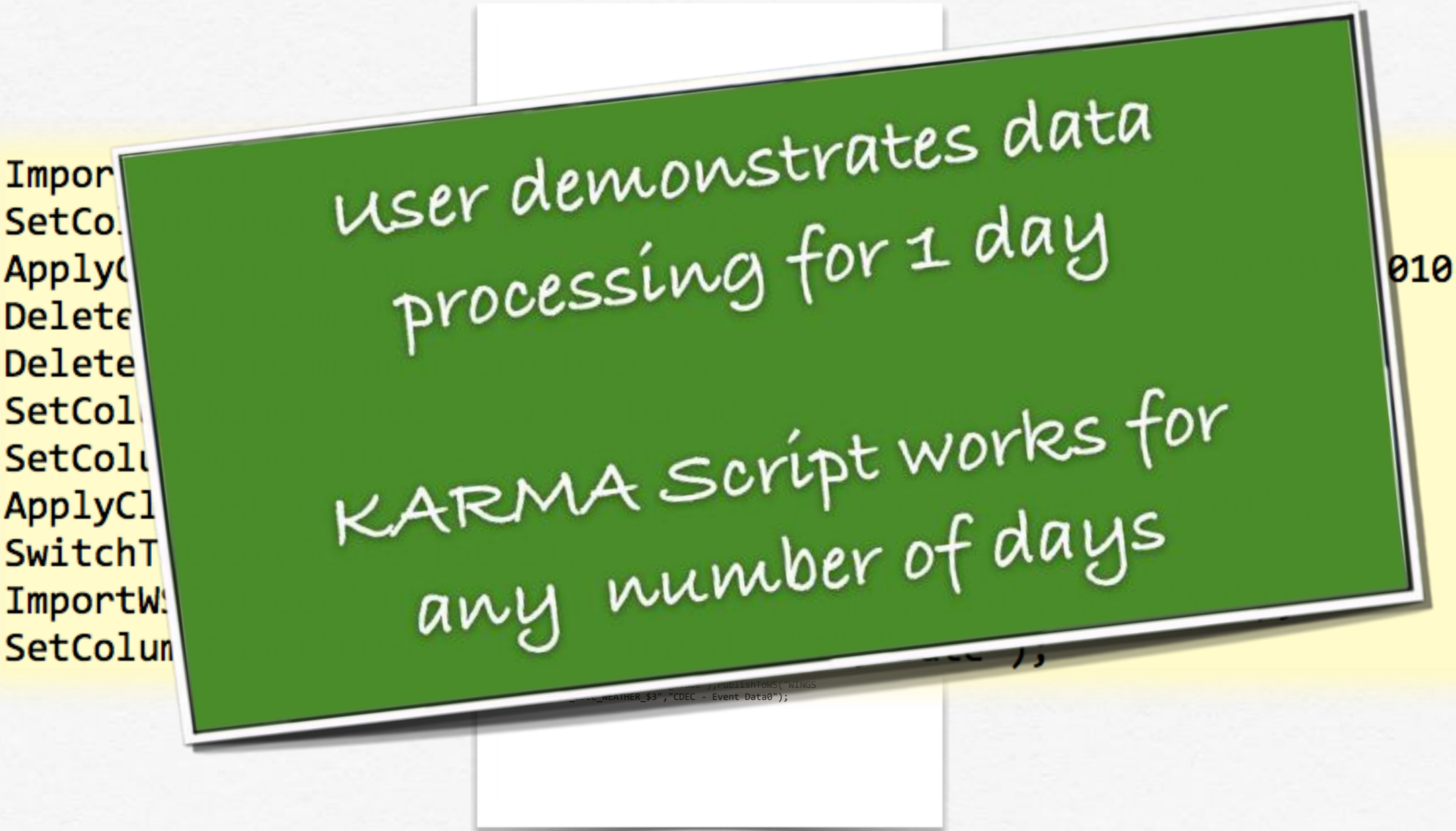
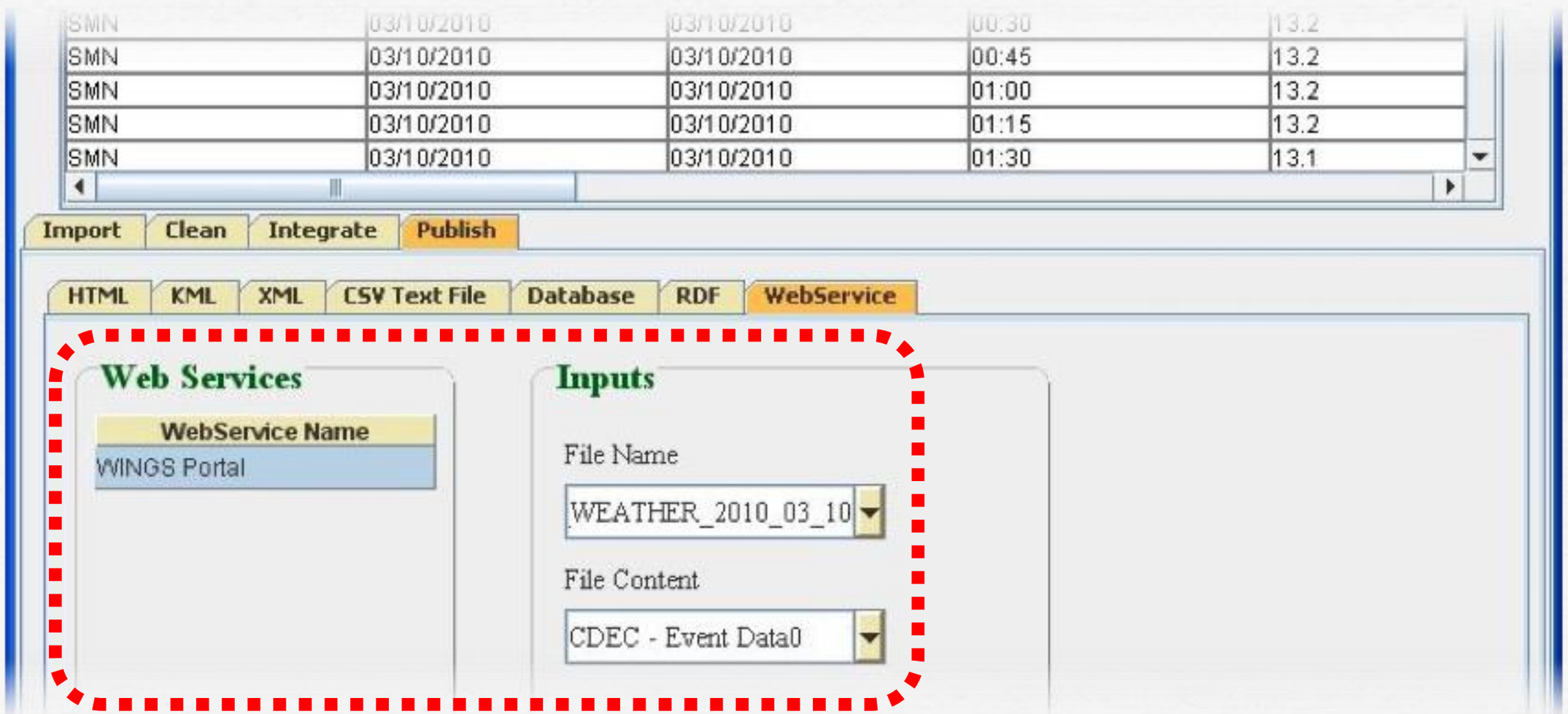
KARMA Generates Data Processing Script



Publishing Processed Data to WINGS



Semantic Metadata for Input Files

```xml
<?xml version="1.0" encoding="UTF-8" ?>

<rdf:RDF
   xml:base="http://www.isi.edu/dc/Water/library.owl#"
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
   xmlns:rdfs="http://www.w3.org/2000/01/rdf-schema#"
   xmlns:owl="http://www.w3.org/2002/07/owl#"
   xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
   xmlns:dc="http://www.isi.edu/dc/ontology.owl#"
   xmlns:dcdom="http://www.isi.edu/dc/Water/ontology.owl#"
   xmlns="http://www.isi.edu/dc/Water/library.owl#">

<dcdom:Daily_Sensor_Data rdf:ID="FILENAME">
   <dcdom:forDate rdf:datatype="http://www.w3.org/2001/XMLSchema#date">DATE</dcdom:forDate>
   <dcdom:forSite rdf:datatype="http://www.w3.org/2001/XMLSchema#string">STATIONID</dcdom:forSite>
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   <dcdom:siteLongitude rdf:datatype="http://www.w3.org/2001/XMLSchema#float">LONGITUDE</dcdom:siteLongitude>
   <dcdom:slope rdf:datatype="http://www.w3.org/2001/XMLSchema#float">SLOPE</dcdom:slope>
   <dcdom:velocity rdf:datatype="http://www.w3.org/2001/XMLSchema#float">VELOCITY</dcdom:velocity>
   <dcdom:depth rdf:datatype="http://www.w3.org/2001/XMLSchema#float">DEPTH</dcdom:depth>
   <dcdom:flow rdf:datatype="http://www.w3.org/2001/XMLSchema#float">FLOW</dcdom:flow>
   <dcdom:barpress rdf:datatype="http://www.w3.org/2001/XMLSchema#float">760</dcdom:barpress>
</dcdom:Daily_Sensor_Data>

</rdf:RDF>
```

Semantic Metadata for Input Files

```
<?xml version="1.0" encoding="UTF-8" ?>

<rdf:RDF
   xml:base="http://www.isi.edu/dc/Water/library
   xmlns:rdf="http://www.w3.org/1999/02/22-rdf-s
   xmlns:rdfs="http://www.w3.org/2000/01/rdf-sche
   xmlns:owl="http://www.w3.org/2002/07/owl#"
   xmlns:xsd="http://www.w3.org/2001/XMLSchema#"
   xmlns:dc="http://www.isi.edu/dc/ontology.owl#"
   xmlns:dcdom="http://www.isi.edu/dc/Water/ontol
   xmlns="http://www.isi.edu/dc/Water/library.owl#

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   <dcdom:siteLongitude rdf:datatype="http://www.w3
   <dcdom:slope rdf:datatype="http://www.w3.org/2001/XMLSchema#float">SLOPE</dcdom:slope>
   <dcdom:velocity rdf:datatype="http://www.w3.org/2001/XMLSchema#float">VELOCITY</dcdom:velocity>
   <dcdom:depth rdf:datatype="http://www.w3.org/2001/XMLSchema#float">DEPTH</dcdom:depth>
   <dcdom:flow rdf:datatype="http://www.w3.org/2001/XMLSchema#float">FLOW</dcdom:flow>
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</dcdom:Daily_Sensor_Data>

</rdf:RDF>
```
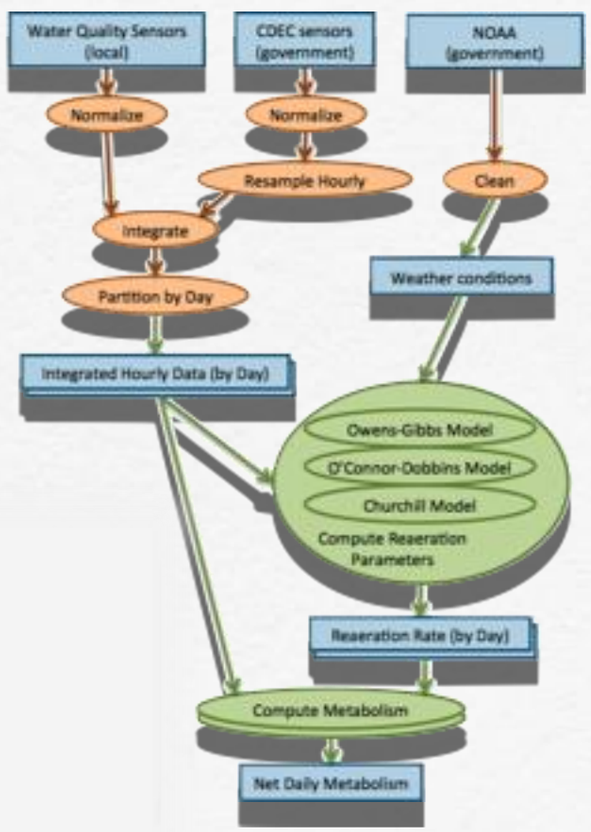
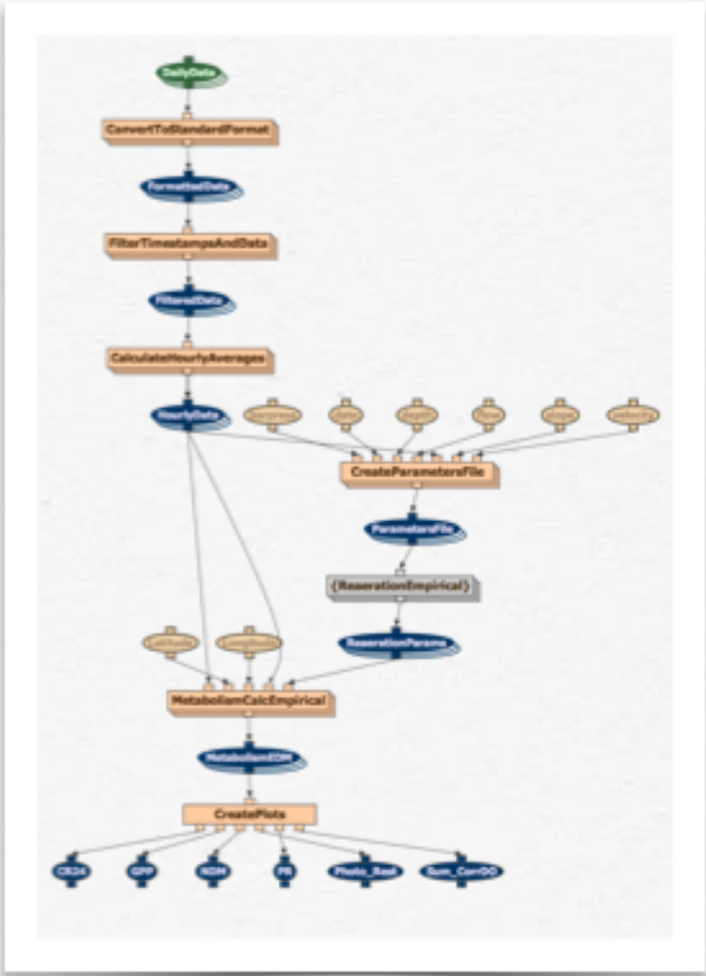

Automatically Generated by KARMA

[Gil et al JETAI'11; Gil et al IEEE-IS'11; Gil et al e-Science'09; Kim et al JCC'08]

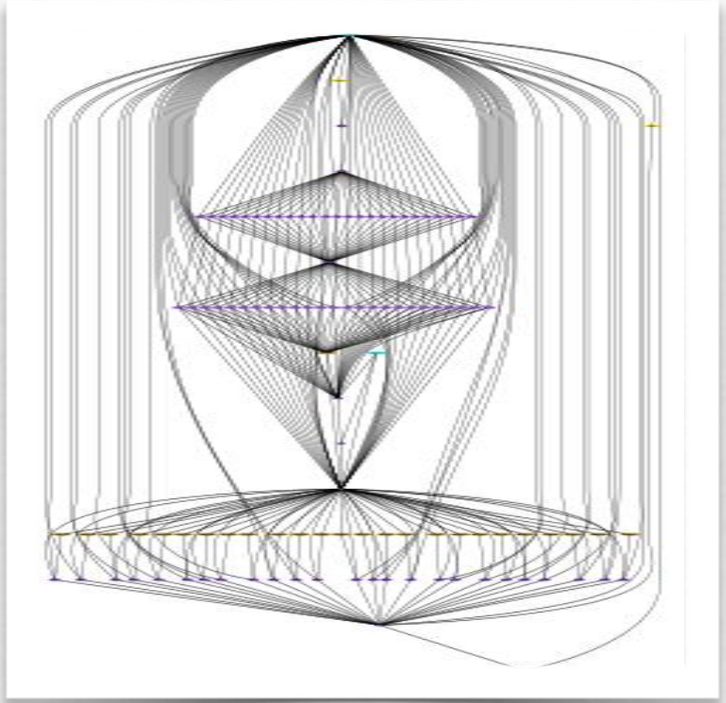
Workflows with WINGS



Conceptual workflow

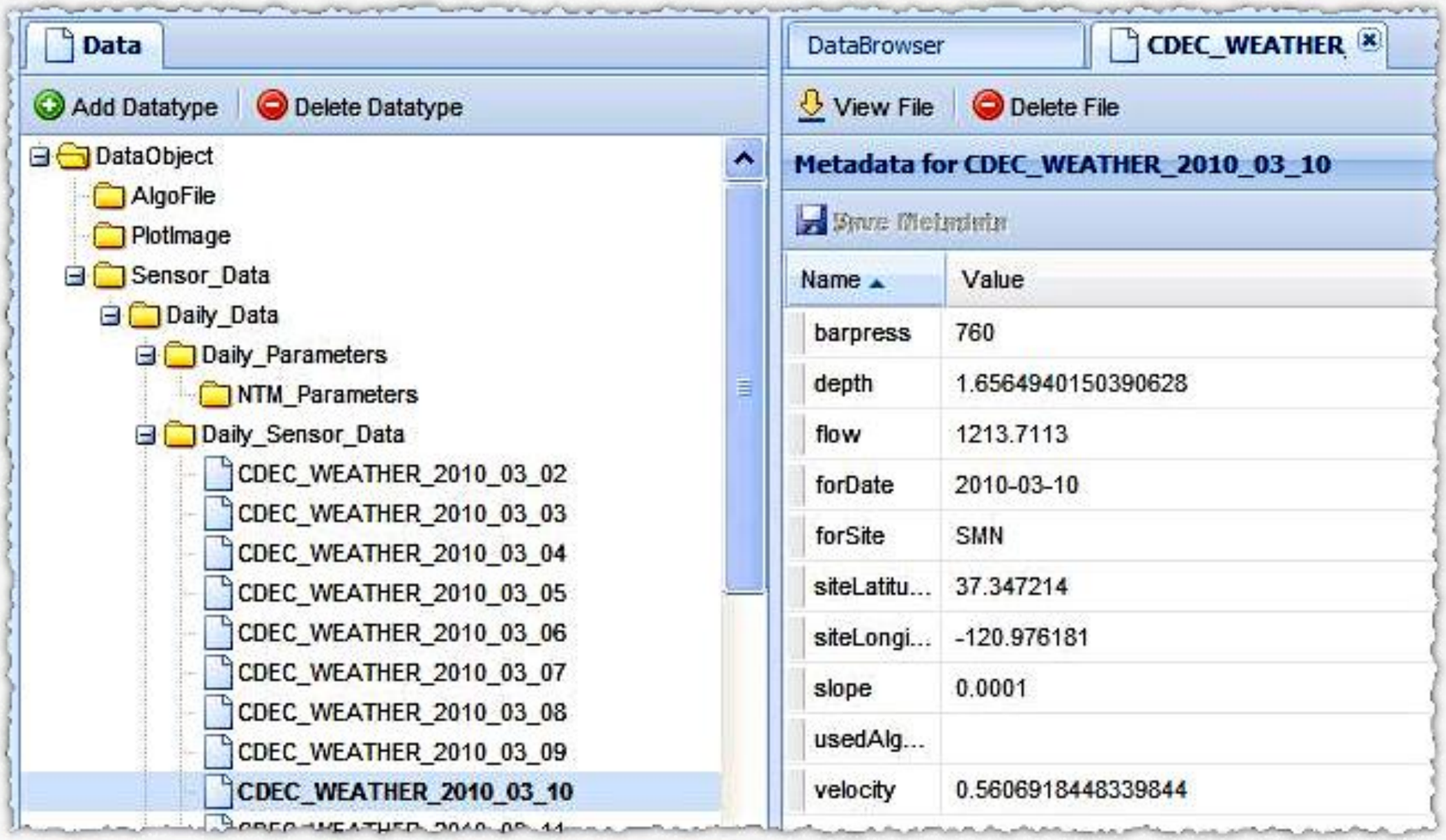


WINGS Workflow

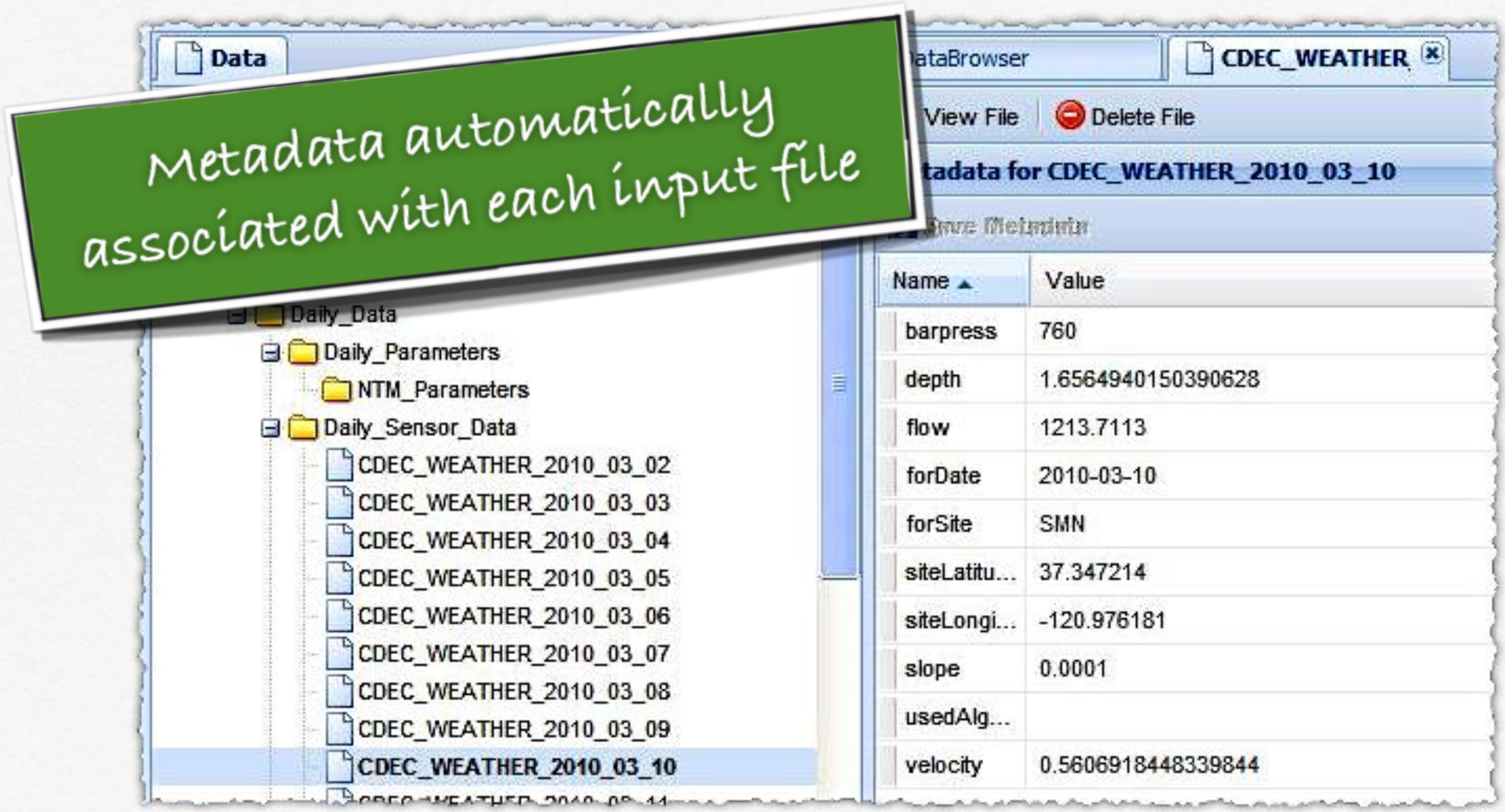


Workflow execution

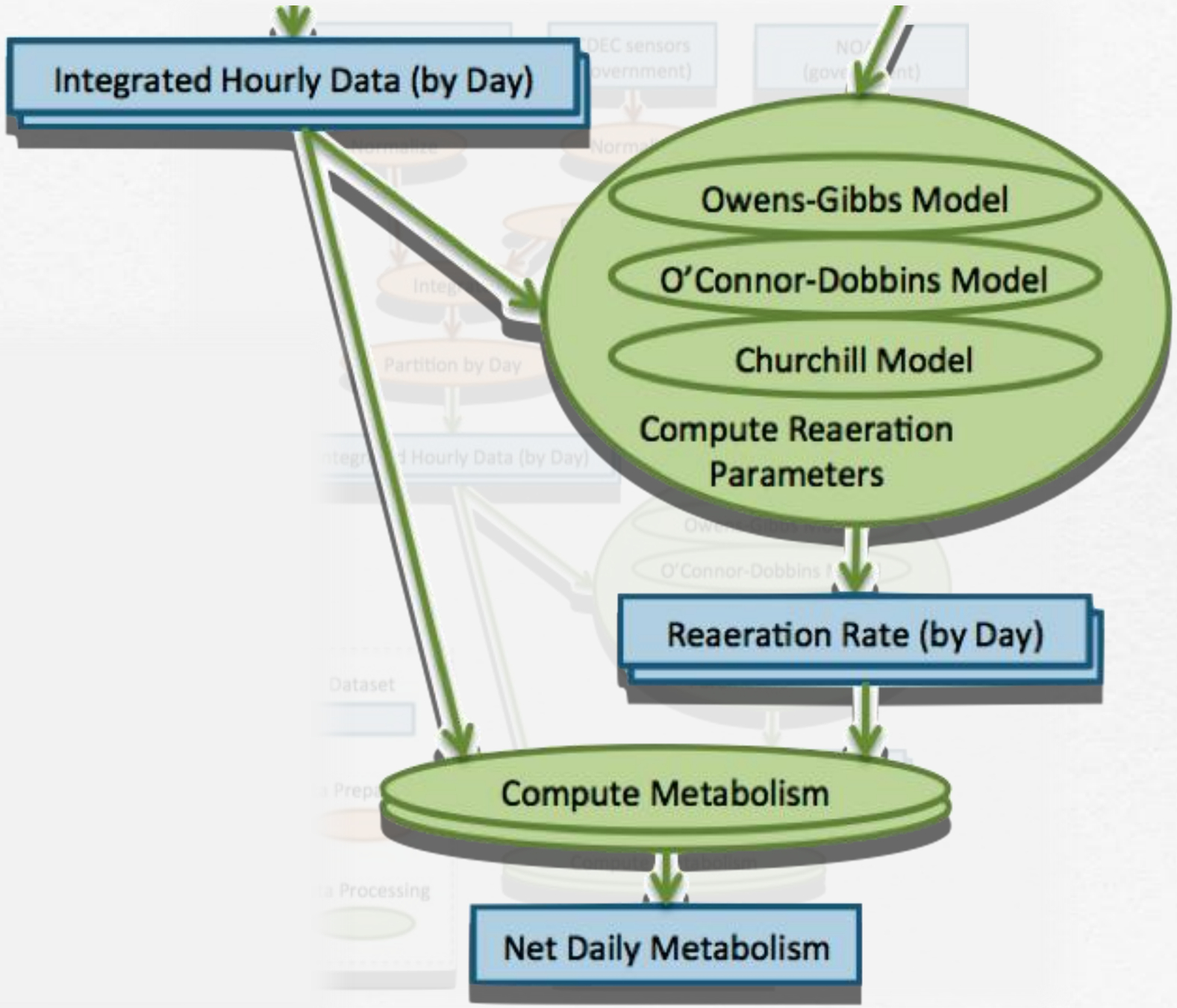
WINGS Received Metadata from KARMA



WINGS Received Metadata from KARMA



Workflow


Integrated Hourly Data (by Day)
Owens-Gibbs Model
O'Connor-Dobbins Model
Churchill Model
Compute Reaeration Parameters
Reaeration Rate (by Day)
Compute Metabolism
Net Daily Metabolism

Using Metadata in Workflow Execution

Metadata

```
<dcdom:Hydrolab_Sensor_Data rdf:ID="Hydrolab-CDEC-04272011">
   <dcdom:siteLong rdf:datatype="float">-120.931</dcdom:siteLongitude>
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   <dcdom:dateStart rdf:datatype="date">2011-04-27</dcdom:dateStart>
   <dcdom:forSite rdf:datatype="string">MST</dcdom:forSite>
   <dcdom:numberOfDayNights rdf:datatype="int">1</dcdom:numberOfDayNights>
   <dcdom:avgDepth rdf:datatype="float">4.523957</dcdom:avgDepth>
   <dcdom:avgFlow rdf:datatype="float">2399</dcdom:avgFlow>
</dcdom:Hydrolab_Sensor_Data>
```
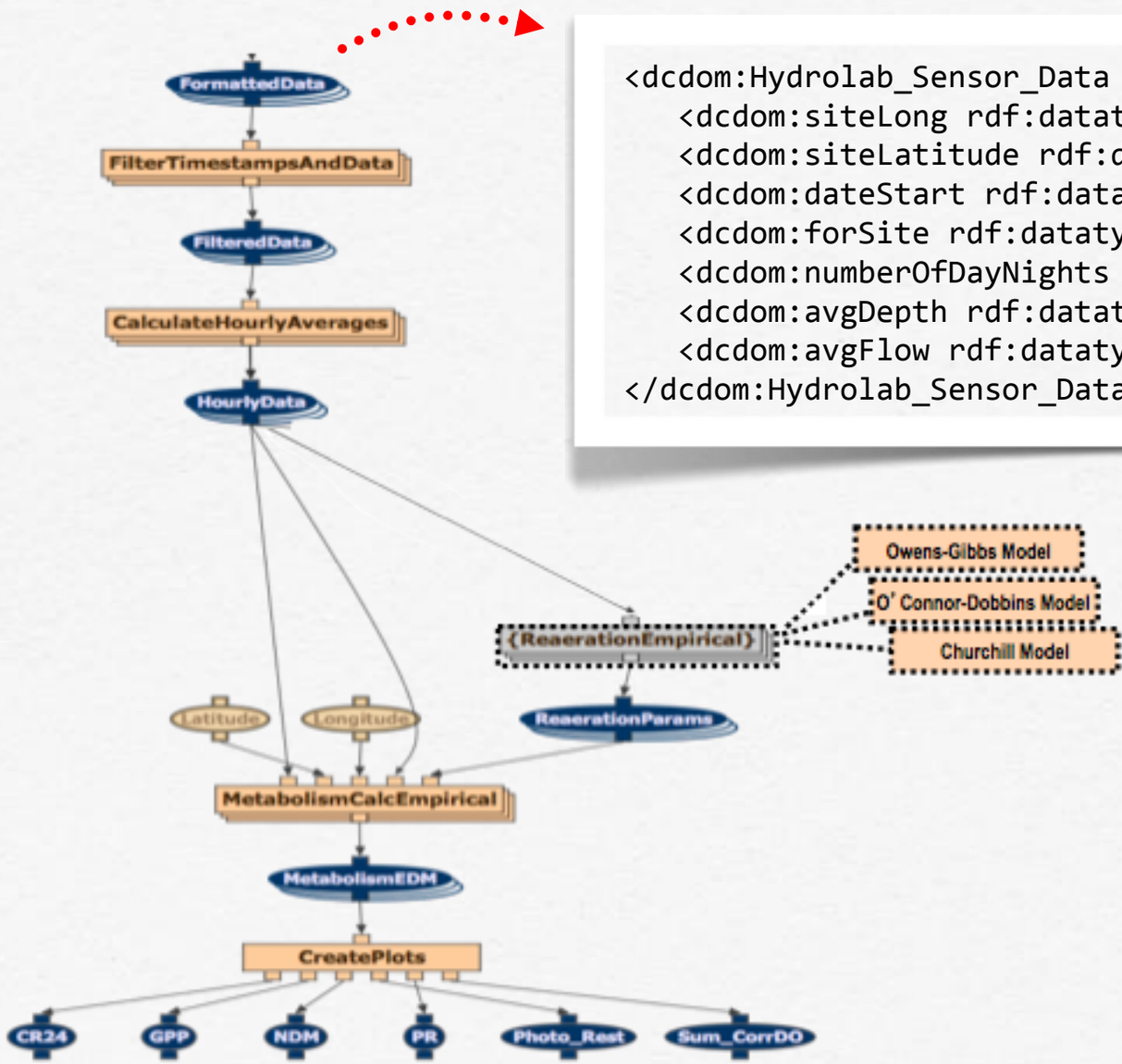
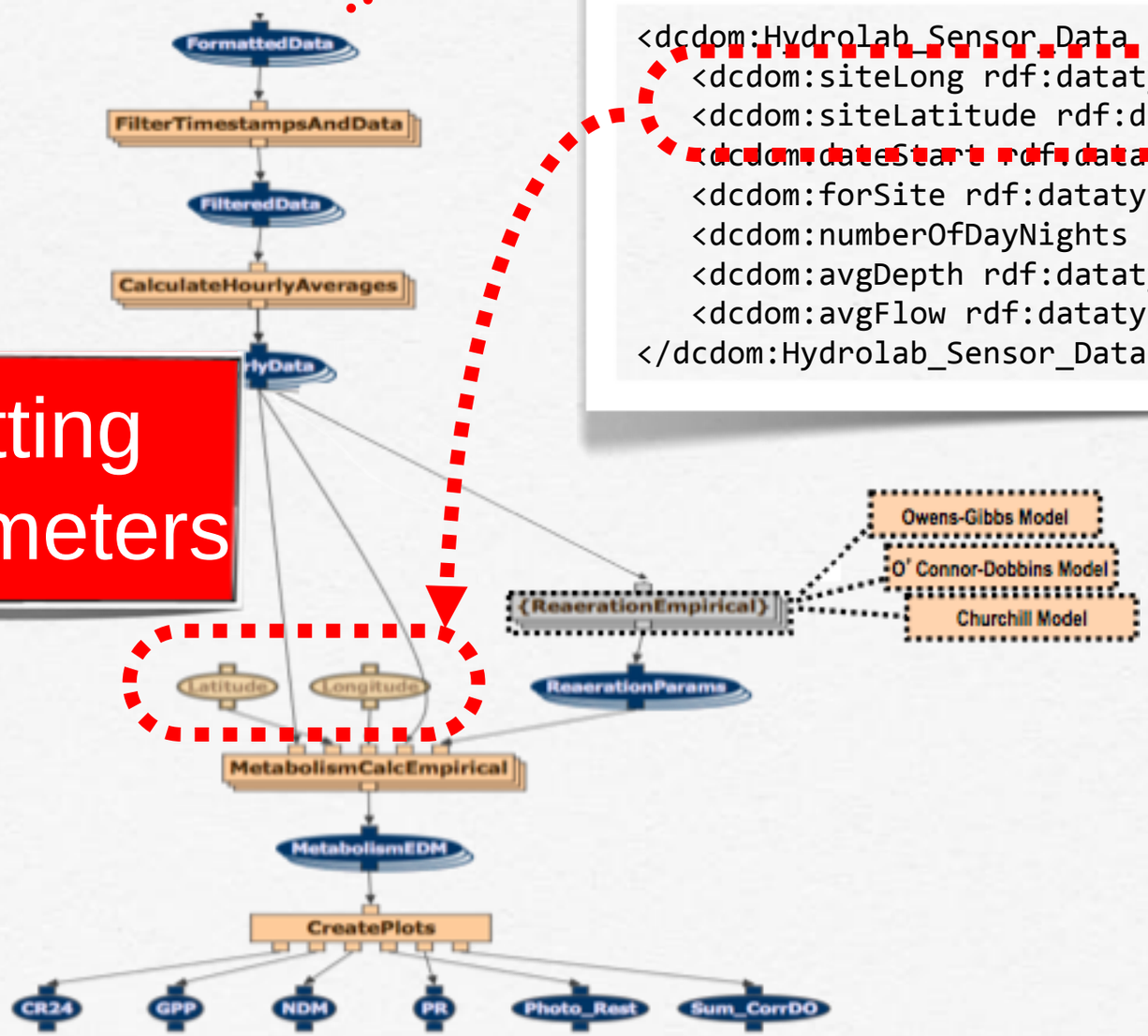



Using Metadata in Workflow Execution

Metadata

```
<dcdom:Hydrolab_Sensor_Data rdf:ID="Hydrolab-CDFC-04272011">
   <dcdom:siteLong rdf:datatype="float">-120.931</dcdom:siteLongitude>
   <dcdom:siteLatitude rdf:datatype="float">37.371</dcdom:siteLatitude>
   <dcdom:dateStart rdf:datatype="date">2011-04-27</dcdom:dateStart>
   <dcdom:forSite rdf:datatype="string">MST</dcdom:forSite>
   <dcdom:numberOfDayNights rdf:datatype="int">1</dcdom:numberOfDayNights>
   <dcdom:avgDepth rdf:datatype="float">4.523957</dcdom:avgDepth>
   <dcdom:avgFlow rdf:datatype="float">2399</dcdom:avgFlow>
</dcdom:Hydrolab_Sensor_Data>
```

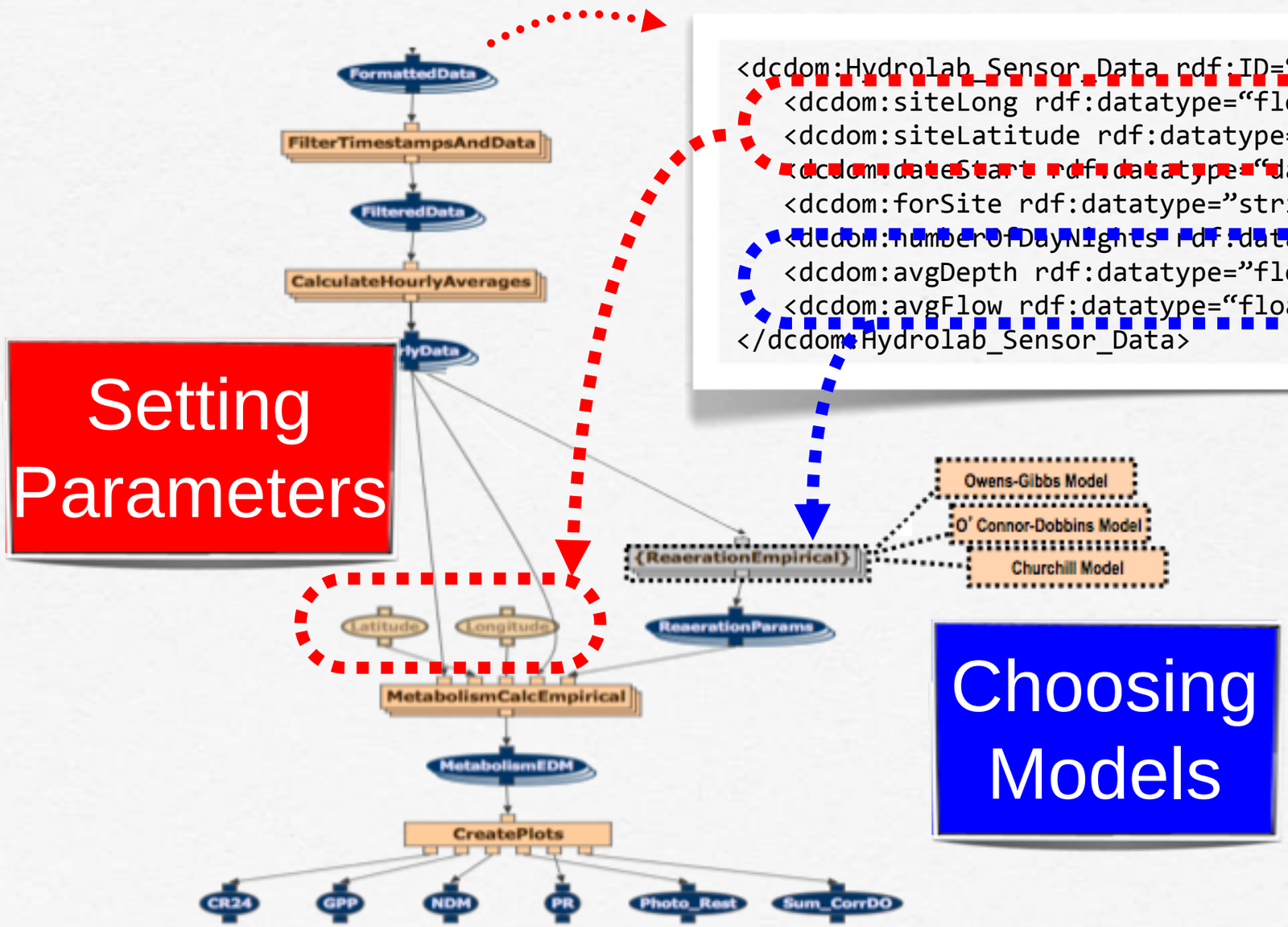
Setting Parameters



Using Metadata in Workflow Execution

Metadata

```
<dcdom:Hydrolab_Sensor_Data rdf:ID="Hydrolab-CDEC-04272011">
  <dcdom:siteLong rdf:datatype="float">-120.931</dcdom:siteLongitude>
  <dcdom:siteLatitude rdf:datatype="float">37.371</dcdom:siteLatitude>
  <dcdom:dateStart rdf:datatype="date">2011-04-27</dcdom:dateStart>
  <dcdom:forSite rdf:datatype="string">MST</dcdom:forSite>
  <dcdom:numberOfDayNights rdf:datatype="int">1</dcdom:numberOfDayNights>
  <dcdom:avgDepth rdf:datatype="float">4.523957</dcdom:avgDepth>
  <dcdom:avgFlow rdf:datatype="float">2399</dcdom:avgFlow>
</dcdom:Hydrolab_Sensor_Data>
```



Setting Parameters

Choosing Models

Workflow Results

http://seagull.isi.edu/marbles/wpaccessresults.html

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Run Workflows · Access Results · (PNG Image, 744x1180 pixels) · NSF FastLane :: Proposal Status

My Runs

Delete · Reload

Template	Progress	Start Time	End Time
AquaFlow-1 Run ID:64, Request ID:AquaFlow-1_Run_4d7a562851efe	Finished !	9:04:50 am, Mar 11, 2011	9:07:11 am, Mar 11, 2011

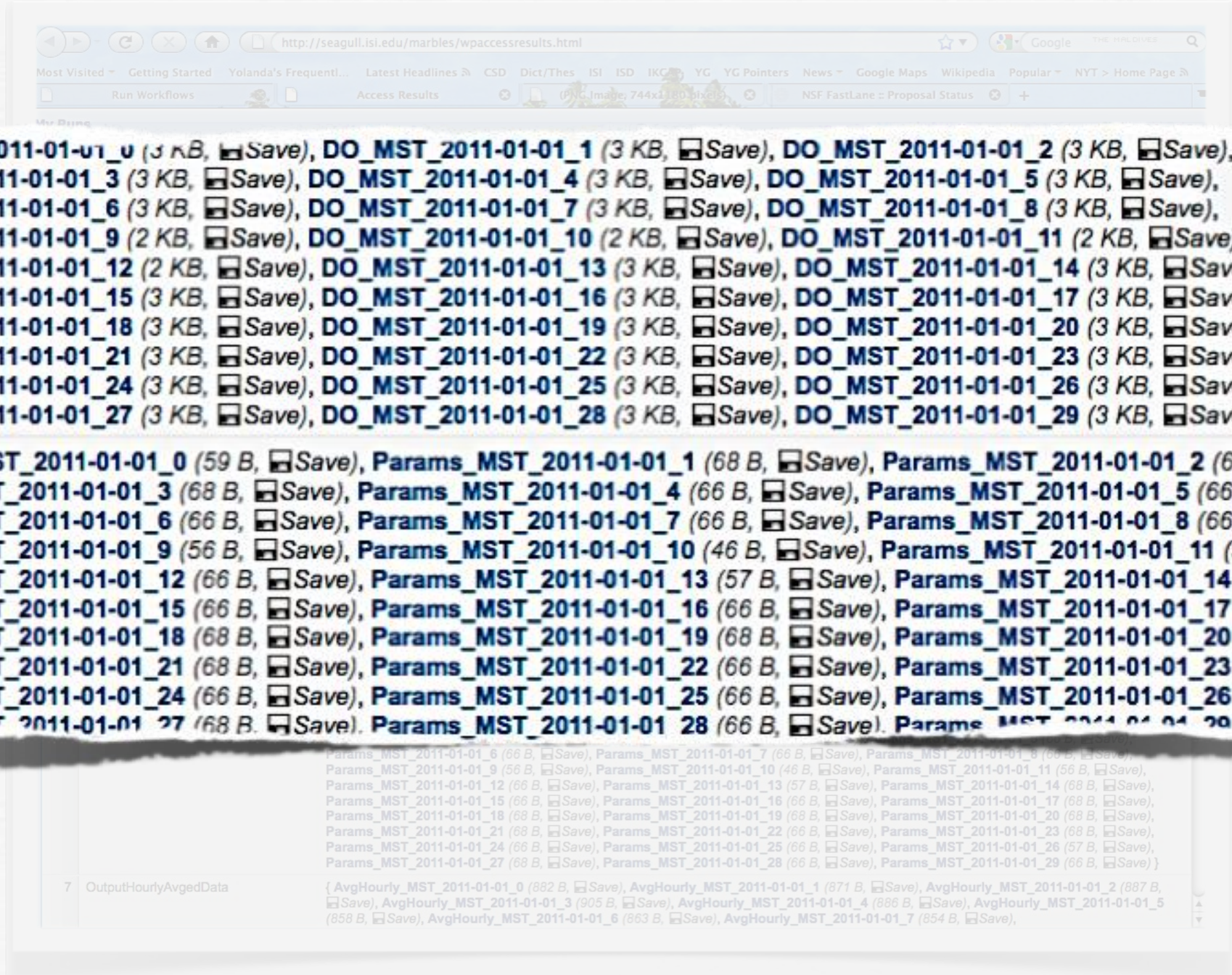
ResultBrowser · **AquaFlow-1_Run_4d7a**

Data · Run Log · Workflow · Documentation

Get HTML · Get RDF

	Variable	Bindings
	Data: Input (4)	
1	Hydrolab_Data	**Hydrolab_Jan_2011_NEXSENS_txt** *(168 KB)*
2	InputDepthFile	{ **depth_Jan_txt** *(57 B)* }
3	Latitude	{ **37.37** }
4	Longitude	{ **-120.93** }
	Data: Intermediate (7)	
5	MeanNightDO	{ **DO_MST_2011-01-01_0** *(3 KB, Save)*, **DO_MST_2011-01-01_1** *(3 KB, Save)*, **DO_MST_2011-01-01_2** *(3 KB, Save)*, **DO_MST_2011-01-01_3** *(3 KB, Save)*, **DO_MST_2011-01-01_4** *(3 KB, Save)*, **DO_MST_2011-01-01_5** *(3 KB, Save)*, **DO_MST_2011-01-01_6** *(3 KB, Save)*, **DO_MST_2011-01-01_7** *(3 KB, Save)*, **DO_MST_2011-01-01_8** *(3 KB, Save)*, **DO_MST_2011-01-01_9** *(2 KB, Save)*, **DO_MST_2011-01-01_10** *(2 KB, Save)*, **DO_MST_2011-01-01_11** *(2 KB, Save)*, **DO_MST_2011-01-01_12** *(2 KB, Save)*, **DO_MST_2011-01-01_13** *(3 KB, Save)*, **DO_MST_2011-01-01_14** *(3 KB, Save)*, **DO_MST_2011-01-01_15** *(3 KB, Save)*, **DO_MST_2011-01-01_16** *(3 KB, Save)*, **DO_MST_2011-01-01_17** *(3 KB, Save)*, **DO_MST_2011-01-01_18** *(3 KB, Save)*, **DO_MST_2011-01-01_19** *(3 KB, Save)*, **DO_MST_2011-01-01_20** *(3 KB, Save)*, **DO_MST_2011-01-01_21** *(3 KB, Save)*, **DO_MST_2011-01-01_22** *(3 KB, Save)*, **DO_MST_2011-01-01_23** *(3 KB, Save)*, **DO_MST_2011-01-01_24** *(3 KB, Save)*, **DO_MST_2011-01-01_25** *(3 KB, Save)*, **DO_MST_2011-01-01_26** *(3 KB, Save)*, **DO_MST_2011-01-01_27** *(3 KB, Save)*, **DO_MST_2011-01-01_28** *(3 KB, Save)*, **DO_MST_2011-01-01_29** *(3 KB, Save)* }
6	OutputDailyParams	{ **Params_MST_2011-01-01_0** *(59 B, Save)*, **Params_MST_2011-01-01_1** *(68 B, Save)*, **Params_MST_2011-01-01_2** *(66 B, Save)*, **Params_MST_2011-01-01_3** *(68 B, Save)*, **Params_MST_2011-01-01_4** *(66 B, Save)*, **Params_MST_2011-01-01_5** *(66 B, Save)*, **Params_MST_2011-01-01_6** *(66 B, Save)*, **Params_MST_2011-01-01_7** *(66 B, Save)*, **Params_MST_2011-01-01_8** *(66 B, Save)*, **Params_MST_2011-01-01_9** *(56 B, Save)*, **Params_MST_2011-01-01_10** *(46 B, Save)*, **Params_MST_2011-01-01_11** *(56 B, Save)*, **Params_MST_2011-01-01_12** *(66 B, Save)*, **Params_MST_2011-01-01_13** *(57 B, Save)*, **Params_MST_2011-01-01_14** *(68 B, Save)*, **Params_MST_2011-01-01_15** *(66 B, Save)*, **Params_MST_2011-01-01_16** *(66 B, Save)*, **Params_MST_2011-01-01_17** *(68 B, Save)*, **Params_MST_2011-01-01_18** *(68 B, Save)*, **Params_MST_2011-01-01_19** *(68 B, Save)*, **Params_MST_2011-01-01_20** *(68 B, Save)*, **Params_MST_2011-01-01_21** *(68 B, Save)*, **Params_MST_2011-01-01_22** *(66 B, Save)*, **Params_MST_2011-01-01_23** *(68 B, Save)*, **Params_MST_2011-01-01_24** *(66 B, Save)*, **Params_MST_2011-01-01_25** *(66 B, Save)*, **Params_MST_2011-01-01_26** *(57 B, Save)*, **Params_MST_2011-01-01_27** *(68 B, Save)*, **Params_MST_2011-01-01_28** *(66 B, Save)*, **Params_MST_2011-01-01_29** *(66 B, Save)* }
7	OutputHourlyAvgedData	{ **AvgHourly_MST_2011-01-01_0** *(882 B, Save)*, **AvgHourly_MST_2011-01-01_1** *(871 B, Save)*, **AvgHourly_MST_2011-01-01_2** *(887 B, Save)*, **AvgHourly_MST_2011-01-01_3** *(905 B, Save)*, **AvgHourly_MST_2011-01-01_4** *(886 B, Save)*, **AvgHourly_MST_2011-01-01_5** *(858 B, Save)*, **AvgHourly_MST_2011-01-01_6** *(863 B, Save)*, **AvgHourly_MST_2011-01-01_7** *(854 B, Save)*,

Workflow Results



Workflow Results Have Metadata

WINGS automatically generates metadata for each output file

```
<dcdom:Metabolism_Results  rdf:ID="Metabolism_Results-CDEC-04272011">
   <dcdom:siteLong rdf:datatype="float">-120.931</dcdom:siteLongitude>
   <dcdom:siteLatitude rdf:datatype="float">37.371</dcdom:siteLatitude>
   <dcdom:dateStart rdf:datatype="date">2011-04-27</dcdom:dateStart>
   <dcdom:forSite rdf:datatype="string">MST</dcdom:forSite>
   <dcdom:numberOfDayNights rdf:datatype="int">1</dcdom:numberOfDayNights>
   <dcdom:avgDepth rdf:datatype="float">4.523957</dcdom:avgDepth>
   <dcdom:avgFlow rdf:datatype="float">2399</dcdom:avgFlow>
</dcdom: Metabolism_Results>
```

WINGS Generates Provenance Metadata

```
SELECT ?url WHERE {
?data dcdom:usedAlgorithm dcdom:ODM .
?data rdf:type dcdom:Metabolism_Estimates .
?data wflow:hasLocation ?url
}
```

Metadata for Metabolism_SMN_2010_03_03Z_ODM

Save Metadata

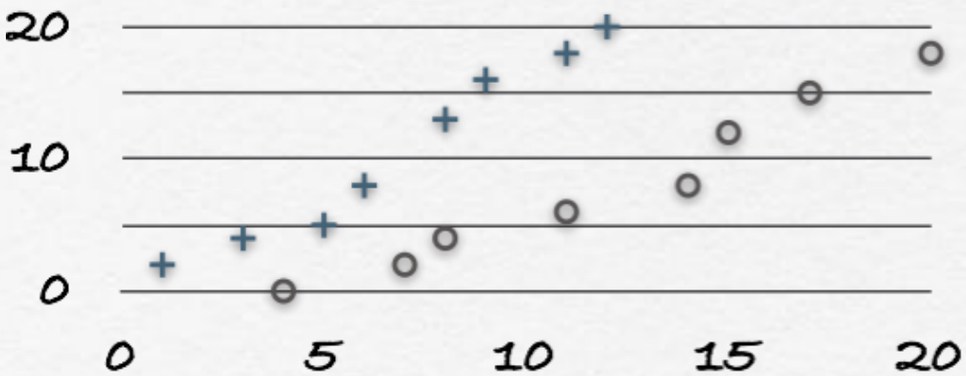
Name	Value
velocity	0.66163415
usedAlgorithm	dcdom:ODM
slope	1.0E-4
siteLongitude	-120.97618
siteLatitude	37.347214
forSite	SMN
forDate	2010-03-03Z
flow	1581.6842
depth	1.0403947

Aquatic Photosynthesis

Models of gross primary production (GPP), community respiration (CR24)

Sensors

Analysis

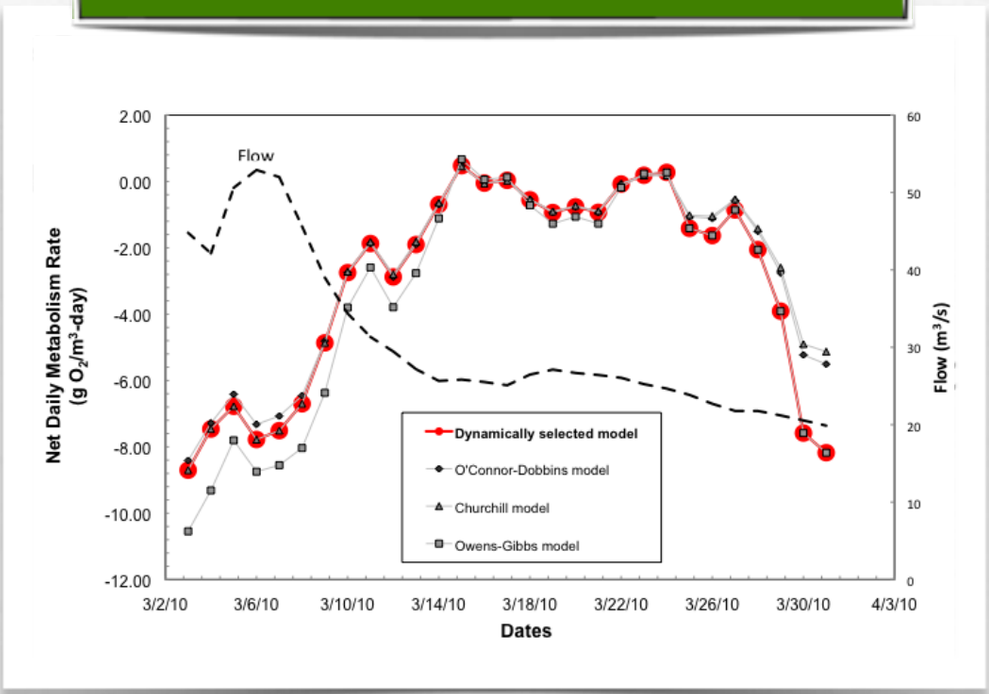


Aquatic Photosynthesis

Models of gross primary production (GPP), community respiration (CR24)

Sensors

Workflow Results



Aquatic Photosynthesis

Models of gross primary production (GPP), community respiration (CR24)

Sensors

Workflow Results

Summary

- Tools for end-users
- End to end support
- Data import, cleaning, integration
- Automated workflow execution
- Captures metadata provenance

Related Work

- Data integration:
  Data Wrangler [Kandel et al 2011]
  Google Refine [Huynh et al]
- Workflow systems:
  VisTrails [Howe et al 2008],
  Kepler [Barseghian et al 2010]
- Many tools generate provenance metadata, often in RDF
  - None generate other kinds of metadata
  - None use metadata to configure models

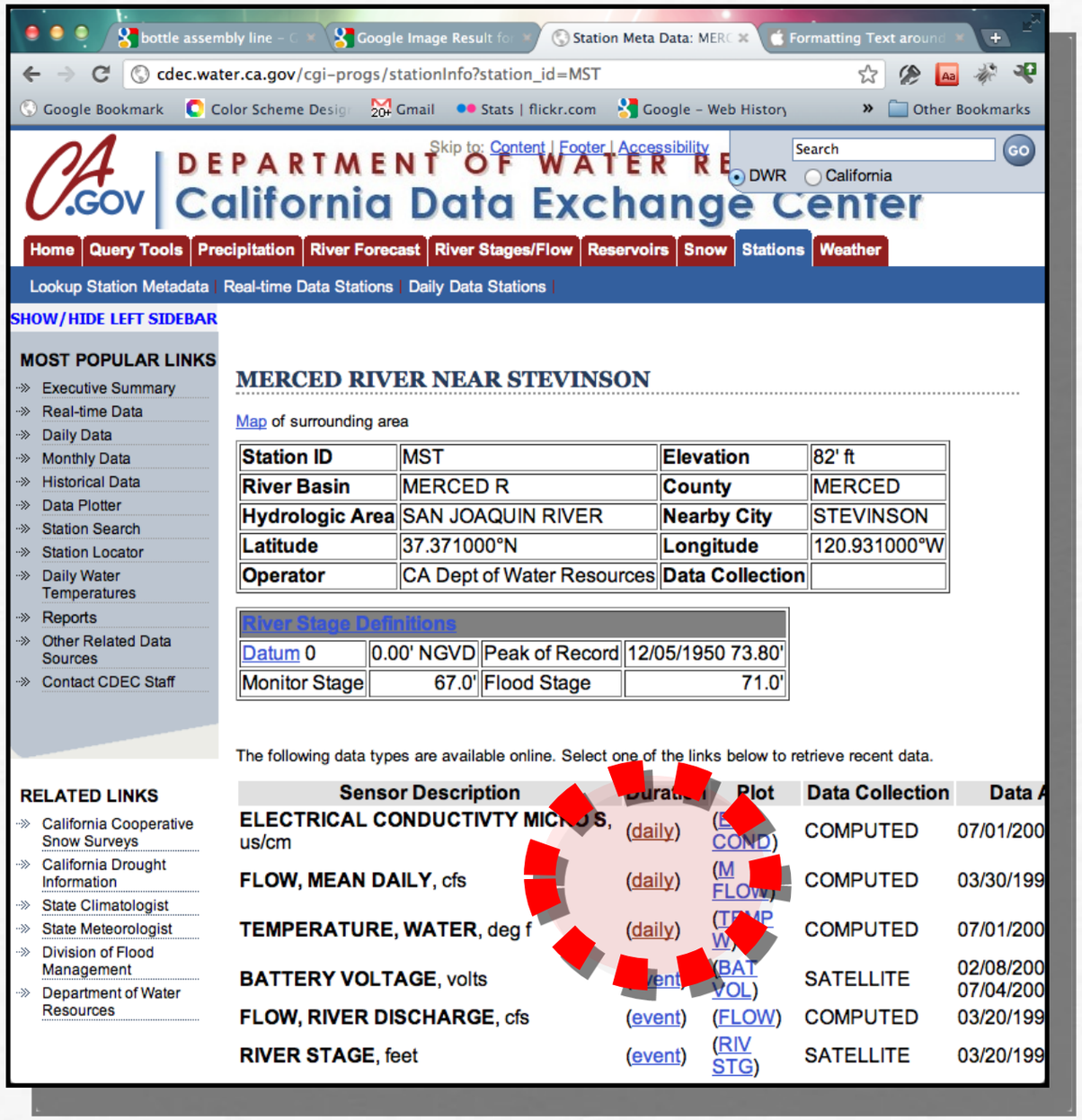
California's Central Valley Water Project

Complex network of rivers, reservoirs, canals, groundwater basins

Grand/Long-range vision

–Observe, model, manage water resources to optimize stream ecology while sustaining society's water needs

California Data Exchange Center



California Data Exchange Center

Date	Time	TempF
20091020	0	65.2
20091020	100	64.9
20091020	200	64.5
20091020	300	64.2
20091020	400	63.8
20091020	500	63.4
20091020	600	63.1
20091020	700	62.8
20091020	800	62.7
20091020	900	62.8
20091020	1000	63.2
20091020	1100	63.9
20091020	1200	64.6