Isoscapes 2011

Introduction to IsoMAP

Isoscapes Modeling, Analysis, and Prediction

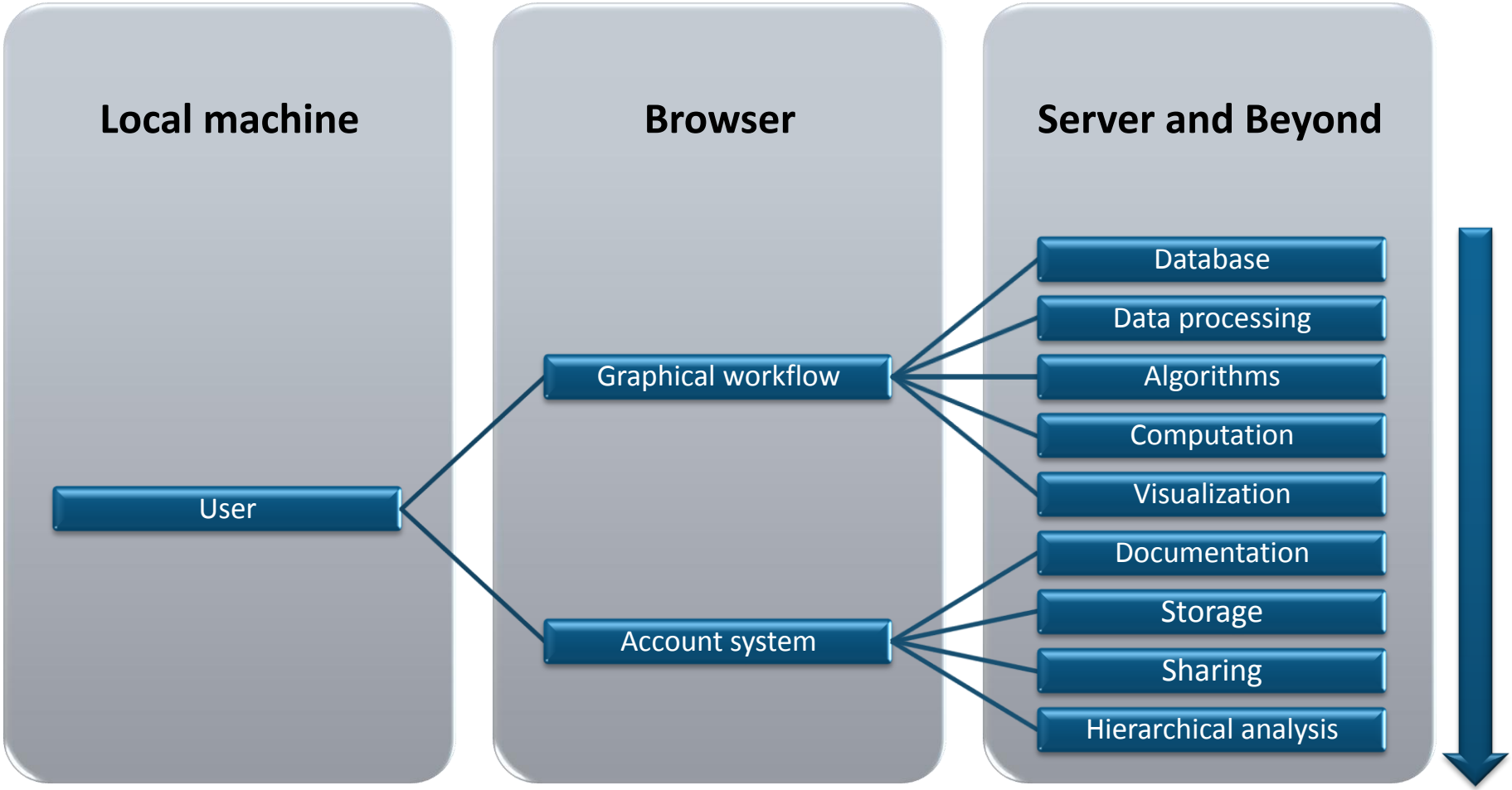
What is IsoMAP

- To the user, and online workspace for:
  - Accessing, manipulating, and analyzing, and modeling environmental isotope data
  - Creating derived data products (isoscapes)
  - Hierarchical modeling using isoscapes
  - Sharing and publishing isoscapes

What is IsoMAP

- Content
  - Current
    - Precipitation H and O
    - Geographic assignment with H and O
  - Near-term
    - Plant leaf water H and O
  - Long-term vision
    - Computational support framework accommodating many environmental geospatial data (isotopic and non-isotopic)

What is IsoMAP

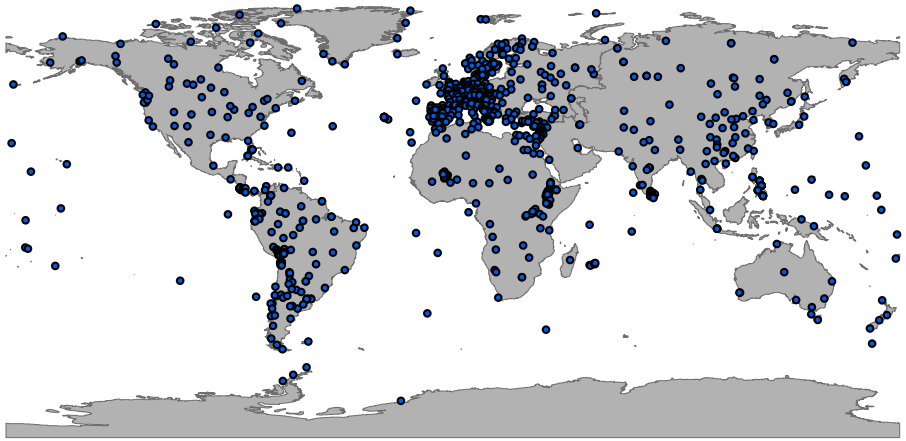


IsoMAP Database

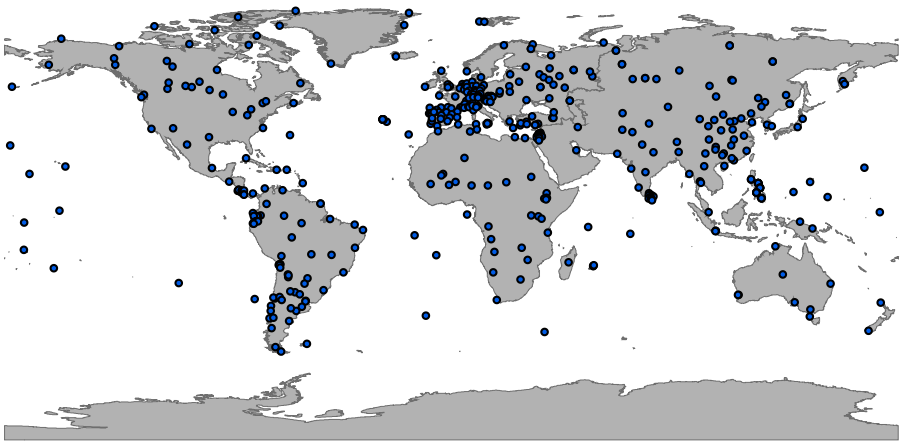
- Managed by IsoMAP team
- Vector (point) data
  - PostGIS spatial database (on PostgreSQL)
  - Almost 104,000 monthly entries from 899 sites
  - Precipitation stable isotope ratios
    - Current sources: GNIP, literature, colleagues
    - Near-term updates: USNIP, GNIP update, your contributions
  - Pre-processed climate and geography data
    - Station data native to GNIP network (WMO)
    - Extracted values from raster sources (ETOPO, PRISM, CRU)

IsoMAP Database

- Vector (point) data
  - IsoMAP DB is designed for flexibility



Waterisotopes.org



IsoMAP.org

IsoMAP Database

- Raster data
  - External data
    - CRU 2.1 climate (global continents, 0.5° resolution)
    - PRISM climate (contiguous USA, 2.5’ resolution)
    - ETOPO (global continents + oceans, 5’ resolution)
    - Latitude and longitude (global continents + oceans, 5’ resolution)
  - Internal data
    - Raster datasets produced in any IsoMAP job

Data Processing

- Driven by user input
  - Spatial
  - Temporal
  - Variables
- Spatial operations
  - Extract data within bounding box
  - Re-sample rasters to lowest common resolution

Data Processing

- Temporal data reduction
  - Reduce monthly values to temporal average for each station
    - Collapse to monthly means
    - Average across months
      - Precipitation-weighting for isotopes, unweighted for others
      - Weighting uses CRU precipitation to reduce missing data
  - Combine with time-independent variables

obs.txt

	A	B	C	D	E	F	G	H	I	J
1	ID	time	long	lat	y	Int	elev_e	lat_l^2	lat_abs(l)	
2	933	1	-106.7	52.2	-117.702	1	504	2724.84	52.2	
3	934	1	32.35	67.15	-70.1192	1	26	4509.122	67.15	
4	935	1	36.17	51.77	-69.4016	1	247	2680.133	51.77	
5	936	1	48.03	46.27	-105.139	1	18	2140.913	46.27	
6	937	1	49.63	58.6	-125.374	1	158	3433.96	58.6	
7	938	1	69.07	60.97	-103.338	1	40	3717.341	60.97	
8	939	1	78.37	55.37	-165.412	1	120	3065.837	55.37	
9	940	1	66.53	66.53	-164.732	1	16	4426.241	66.53	
10	941	1	113.13	54.62	-76.103	1	995	2983.344	54.62	
11	942	1	112.43	68.5	-90.0758	1	220	4692.25	68.5	
12	943	1	129.75	62.08	-120.855	1	103	3853.926	62.08	
13	944	1	158.75	52.97	-101.659	1	24	2805.821	52.97	
14	945	1	136.67	45.03	-48.2272	1	68	2027.701	45.03	
15	100400	1	11.56	78.15	-83.1892	1	7	6107.423	78.15	
16	100500	1	13.63	78.07	-66.5099	1	6	6094.925	78.07	
17	142700	1	6.57	58.1	-47.6676	1	13	3375.61	58.1	
18	206000	1	21.53	68.68	-117.198	1	403	4716.942	68.68	
19	307600	1	-3.7	58.38	-55.9084	1	155	3408.224	58.38	
20	348700	1	-1.08	52.88	-49.8177	1	60	2796.294	52.88	
21	353000	1	-0.25	52.16	-48.6854	1	30	2720.666	52.16	
22	365302	1	-1.1	51.6	-45.7484	1	48	2662.56	51.6	
23	395300	1	-10.25	51.93	-34.7911	1	9	2696.725	51.93	

Algorithms - Precipitation

- Precipitation modeling
  - (Geo)statistical code
    - Develop model
    - Apply model to predict (map)
  - Developed by Tonglin Zhang, Purdue Dept. of Statistics
    - Zhang et al., in prep.
    - Poster #26
    - isomapstat.pdf on your thumb drive

Algorithms - Precipitation

- Develop model
  - User specifies problem
    - Spatial
    - Temporal
    - Variables
  - Two models fit to resulting dataset
    - Multiple regression
    - Geostatistical (universal kriging)

Algorithms - Precipitation

- Multiple regression

$$Y(s) = x'(s)\beta + \epsilon(s) \qquad \epsilon(s) \sim^{iid} N(0, \sigma^2)$$

  - Fit β given isotope station data
  - Predict Y at unknown sites using gridded data

- Moran's I – test of global spatial autocorrelation in *ϵ(s)*

$$I = \frac{1}{S_0 b_2} \sum_{i=1}^{m} \sum_{j=1, j \neq i}^{m} w_{ij}(z_i - \bar{z})(z_j - \bar{z})$$

  - Used to assess whether spatial pattern remains after regression modeling

Algorithms - Precipitation

- Geostatistical model
  - Isotope value is considered a function of
    - Independent variables
    - Spatially autocorrelated residuals

$$Y^*(s_0) = E[Y(s_0)|Y] = x_0'\hat{\beta} + c_0' R_{\hat{\theta}}^{-1}(Y - X\hat{\beta})$$

  - Fit β and model for spatial covariance (c'_0, R_θ) given isotope station data
  - Predict Y at unknown sites using gridded data

Algorithms - Precipitation

- Uncertainty
  - Goodness of fit, parameter uncertainty and significance calculated for all models
  - Precision of estimates given as maps of standard deviations for predictions
    - Propagated from uncertainty in model parameters
    - For regression: model coefficients + error term
    - For geostatistics: model coefficients + spatially varying error term (function of station proximity)
      - Includes nugget

Algorithms - Precipitation

coeff.reg	moranI.reg	coeff.krig
mse.reg		mse.krig
R2.reg		
anova.reg		anova.krig
significance.reg		
estimate.reg		estimate.krig
predreg		predkrig
stdreg		stdkrig

Algorithms - Assignment

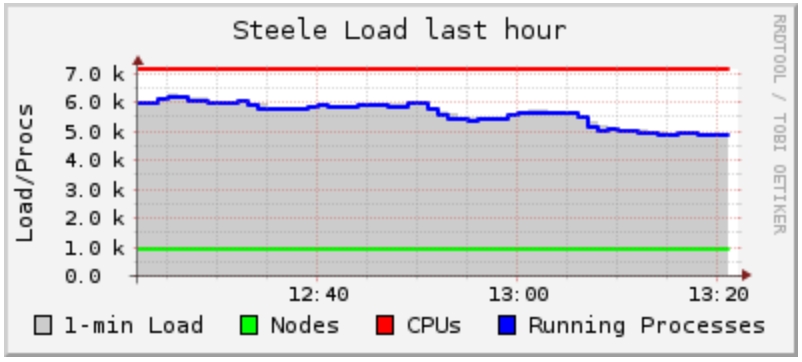
- Assignment modeling
  - Given precipitation isoscape and user-input sample value (+ uncertainties)
  - Calculate relative likelihood that sample originated from any pixel on map
- Simple Bayesian probabilistic calculation with non-informative priors

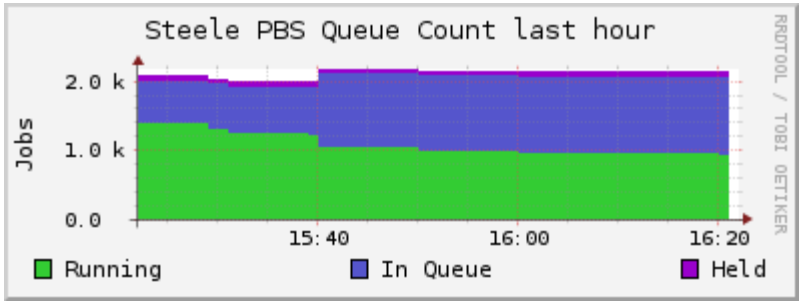
$$P(A_i|B) \approx L(y|\mu_i, \sigma_i^2) = \frac{1}{\sqrt{2\pi\sigma_i^2}} e^{-(y-\mu_i)^2/2\sigma_i^2}$$

  - As used in Kennedy et al. (2011, Forensic Science International), after Wunder (Isoscapes, elsewhere)

Computation

- IsoMAP jobs run on NSF-supported grid computing resources
  - Purdue's Steele cluster
    - 893 node, 7144 processor, 67 Teraflop cluster
  - File system network-mounted





Computation

- On submission
  - Job specifications sent to IsoMAP server
  - Server creates new job description, submits to Steele queue
  - Server monitors status
    - Submitted
    - Pending
    - Active
    - Done
  - Server post-processes results and registers them for display

Visualization

- Computational outputs in a range of custom formats
  - Supports flexibility, program I/O
- Data processing scripts convert output into accessible and standard formats
- Text parsing
  - Interpret statistical output
  - Generate graphics
  - Display

Model Information

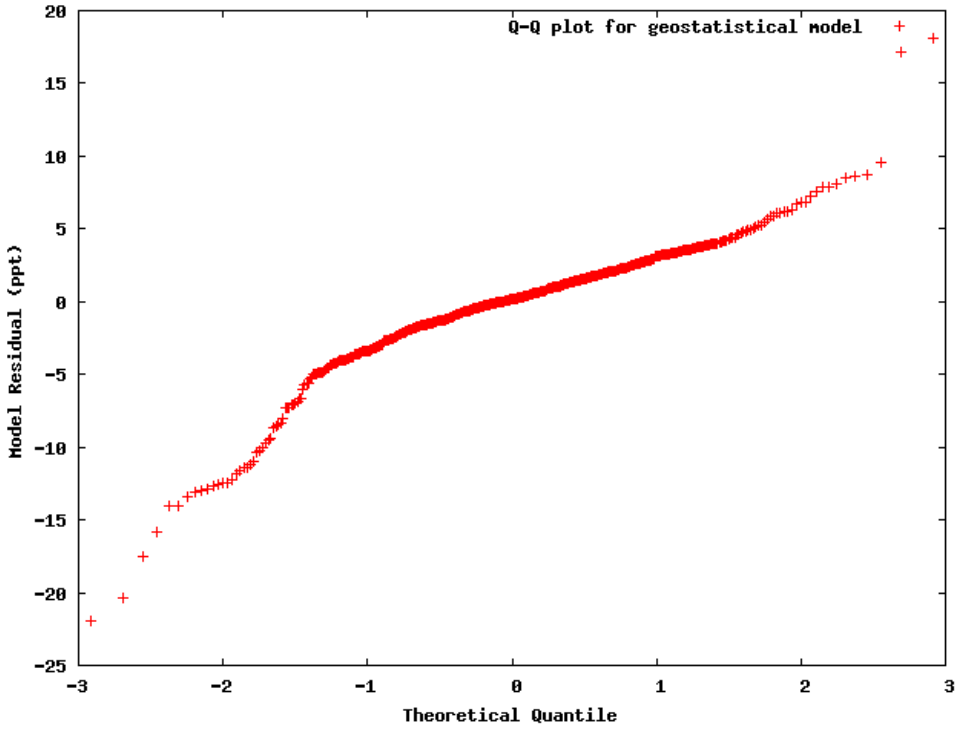
Model type: precipitation
Dependent variable: d2h
Longitude range: -180 to 180
Latitude range: -90 to 90
Year range: 1961 to 1999
Months range: 5, 6, 7, 8
Number of stations: 423
Independent variable 1 : minimum temperaturesquared
  variable source : cru_processed_point
Independent variable 2 : minimum temperature
  variable source : cru_processed_point
Independent variable 3 : precipitation
  variable source : cru_processed_point

Metadata XML download

Regression Model

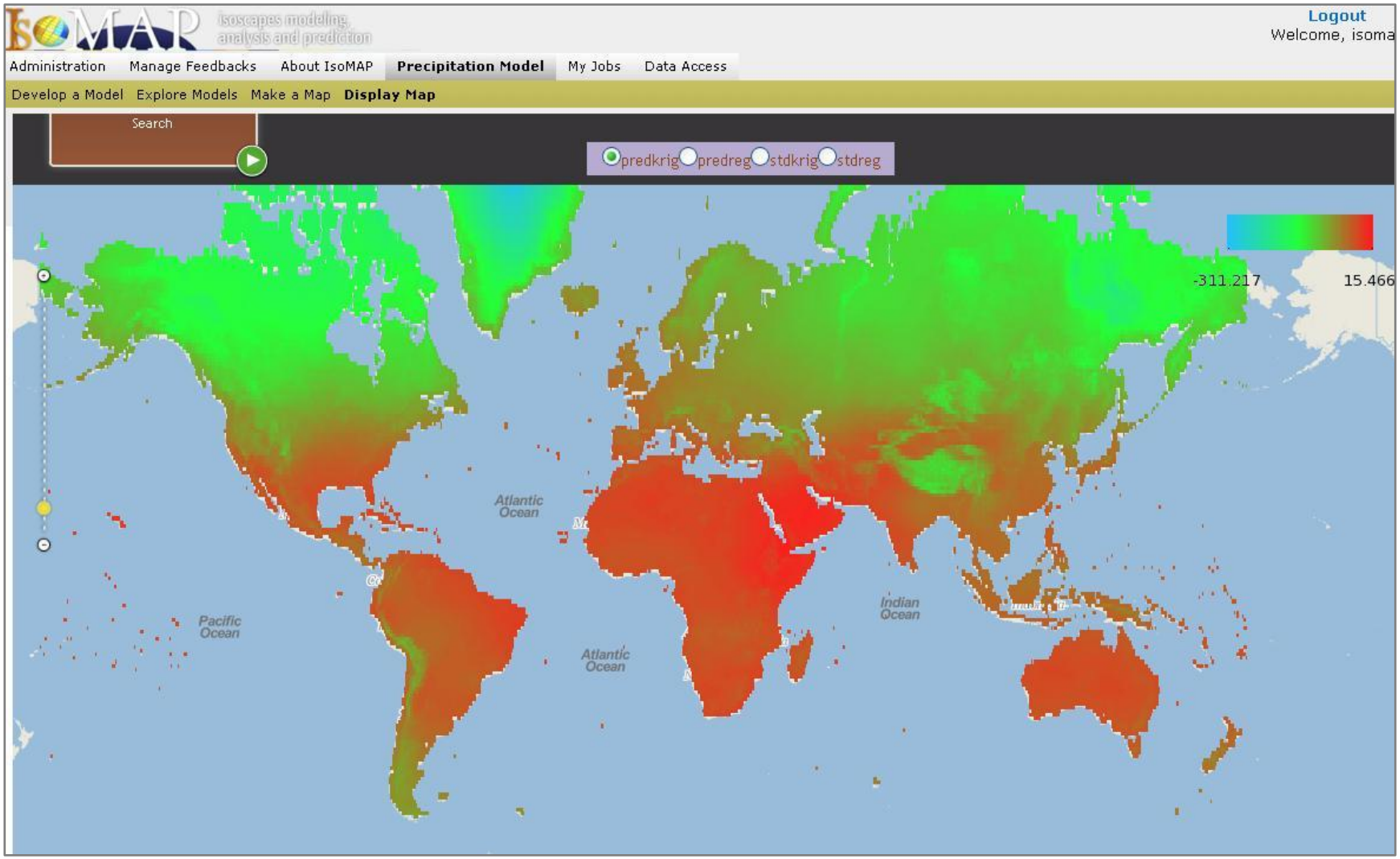
Anova

Variable	df	SS	MS	f-value	p-value
tmn_t^2	1	90527.3	90527.3	146.285	0
tmn_t	1	121889	121889	196.963	0
pre_p	1	5683.95	5683.95	9.18482	0.00259159
Error	419	259295	618.842	-	-
Total	422	477395	-	-	-



Visualization

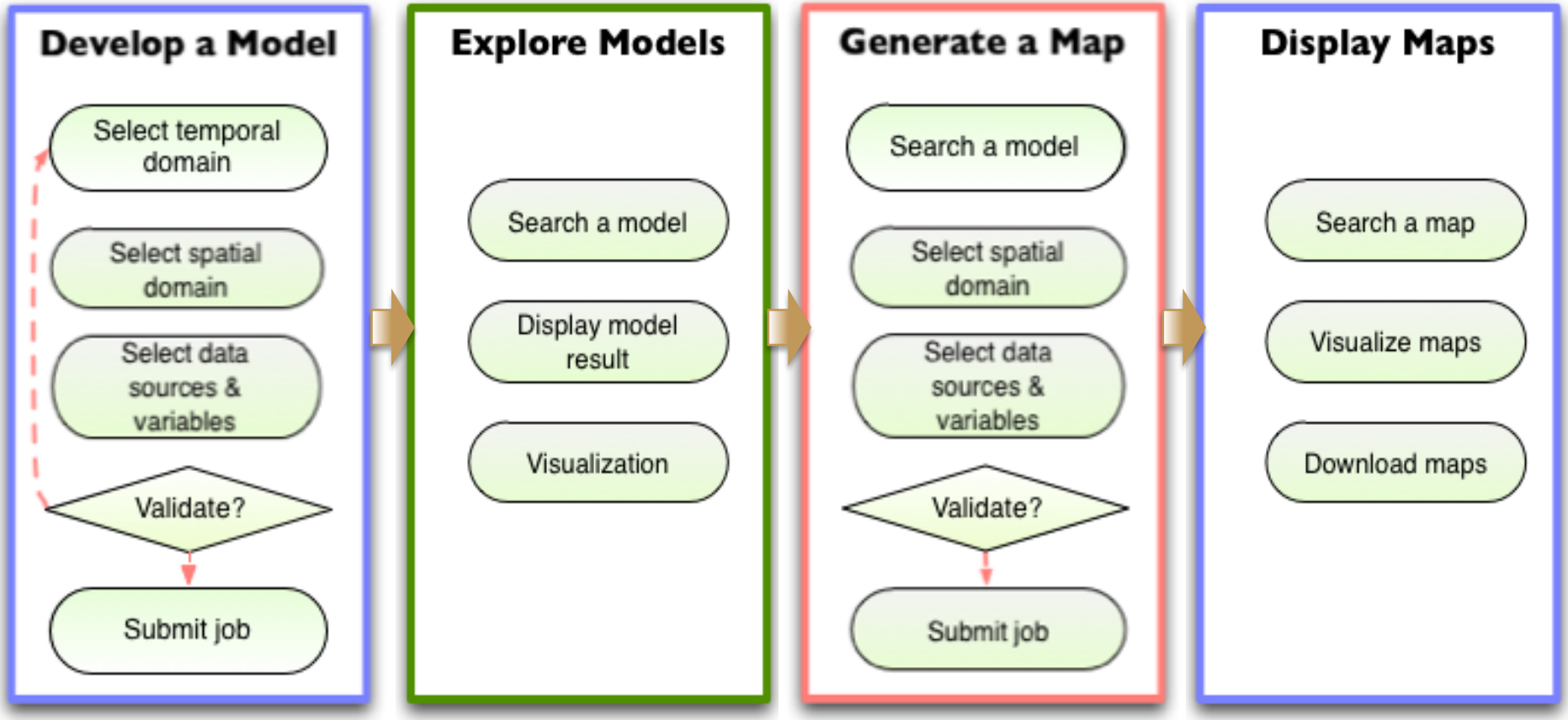
- File conversion
  - Tabular data -> raster
    - Arc ASCII
    - GeoTIFF
  - Display
    - Browser display using OpenLayers
    - Color map rescale on pan and zoom

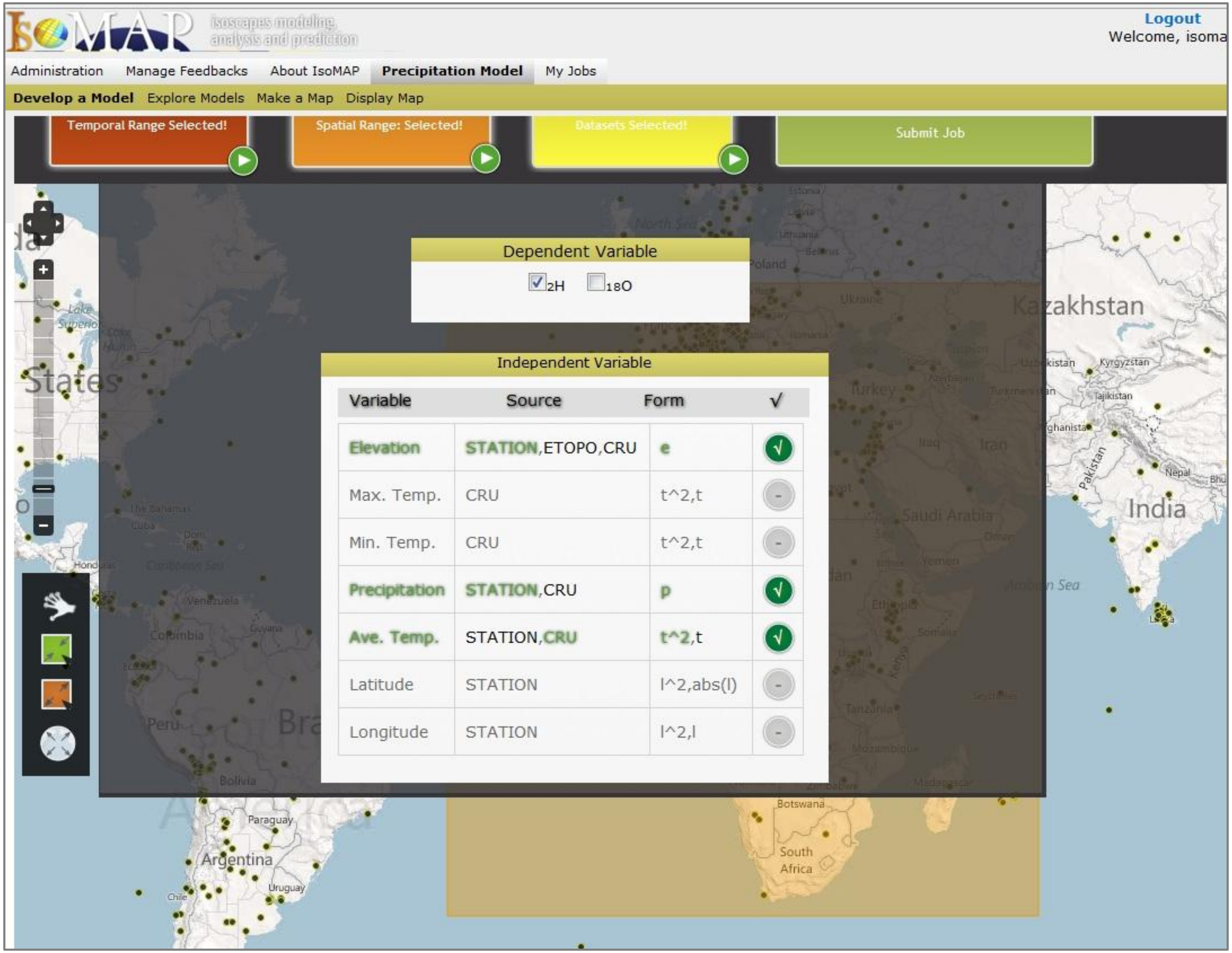

IsoMAP
isoscapes modeling, analysis and prediction
Logout
Welcome, isoma
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Data Access
Develop a Model
Explore Models
Make a Map
Display Map
Search
predkrig
predreg
stdkrig
stdreg
-311.217
15.466
Atlantic Ocean
Pacific Ocean
Atlantic Ocean
Indian Ocean

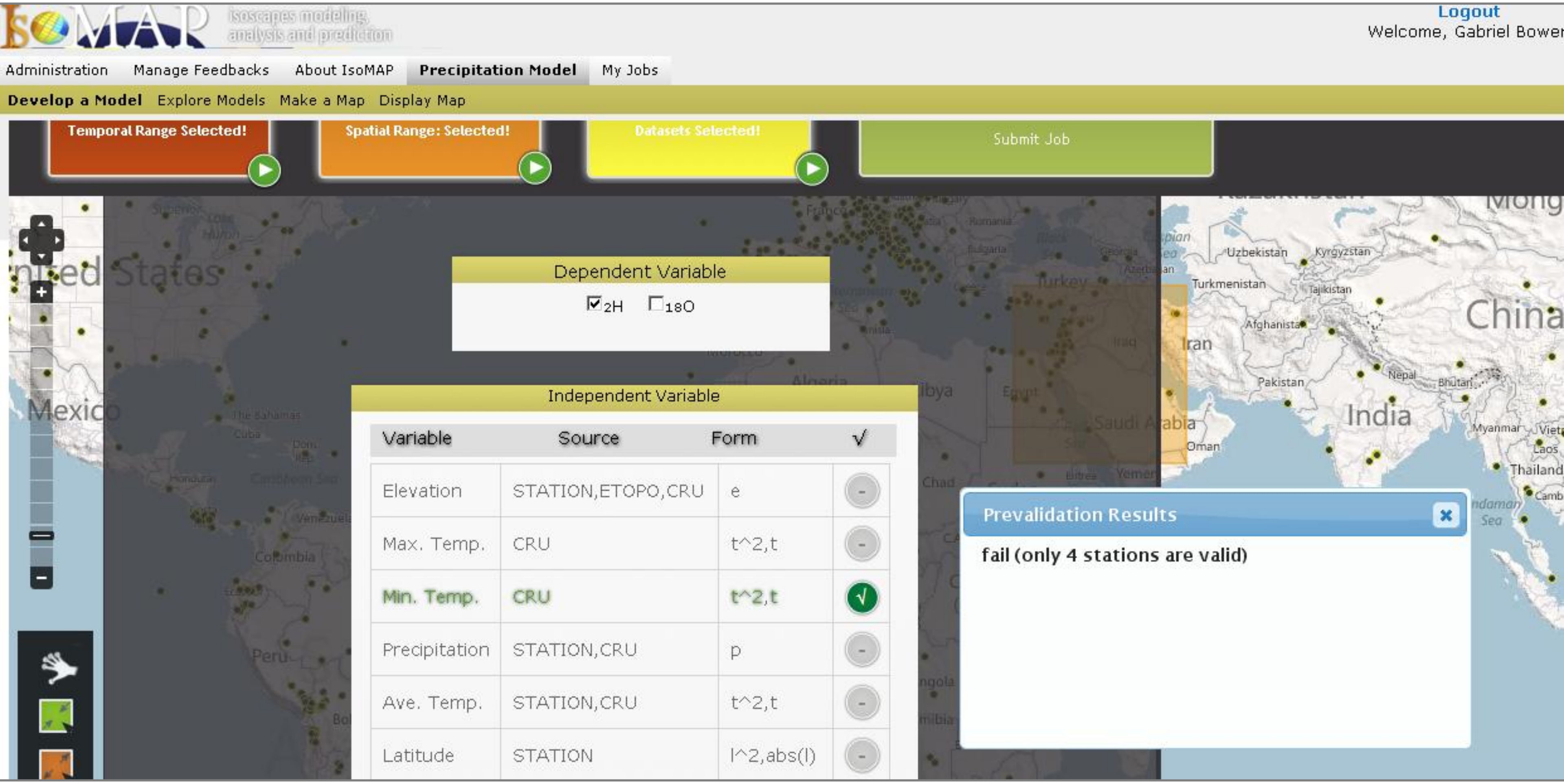
Graphical Workflow

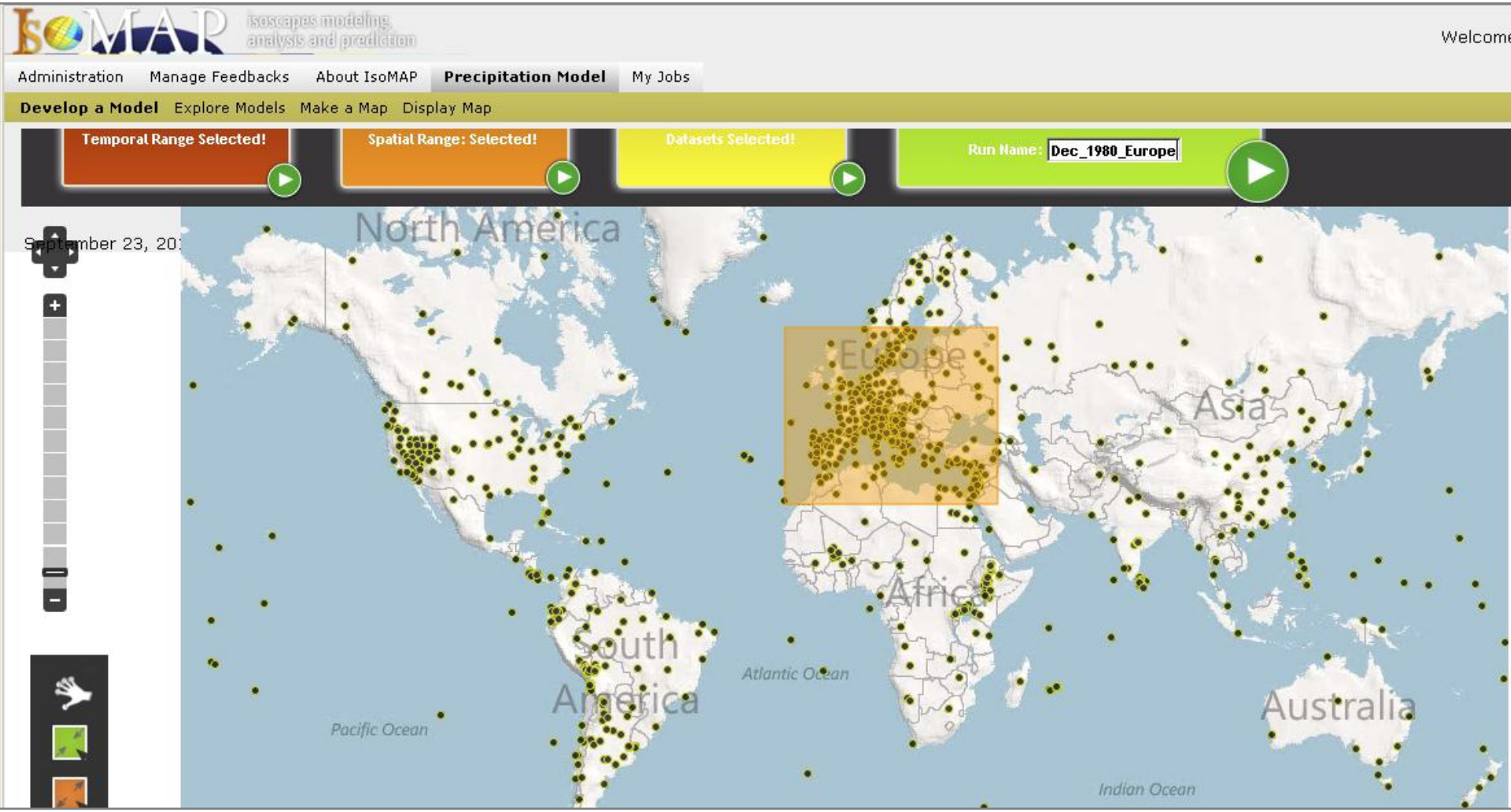
- Browser-based user interface
- Organizes and guides user through steps of developing analysis, finding and visualizing results
  - Ensures completeness
  - Validates user inputs
  - Provides feedback
- Consistent modular structure, look and feel for most implementations

Precipitation Modeling Workflow




isoscapes modeling, analysis and prediction
Logout
Welcome, isoma
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Develop a Model
Explore Models
Make a Map
Display Map
Temporal Range Selected!
Spatial Range: Selected!
Datasets Selected!
Submit Job
Dependent Variable
2H
18O
Independent Variable
Variable | Source | Form | √
Elevation | STATION,ETOPO,CRU | e | √
Max. Temp. | CRU | t^2,t | -
Min. Temp. | CRU | t^2,t | -
Precipitation | STATION,CRU | p | √
Ave. Temp. | STATION,CRU | t^2,t | √
Latitude | STATION | l^2,abs(l) | -
Longitude | STATION | l^2,l | -
Kazakhstan
India
Saudi Arabia
Turkey
Ukraine
Poland
Argentina
Paraguay
Uruguay
Bolivia
Peru
Colombia
Venezuela
South Africa
Botswana
States

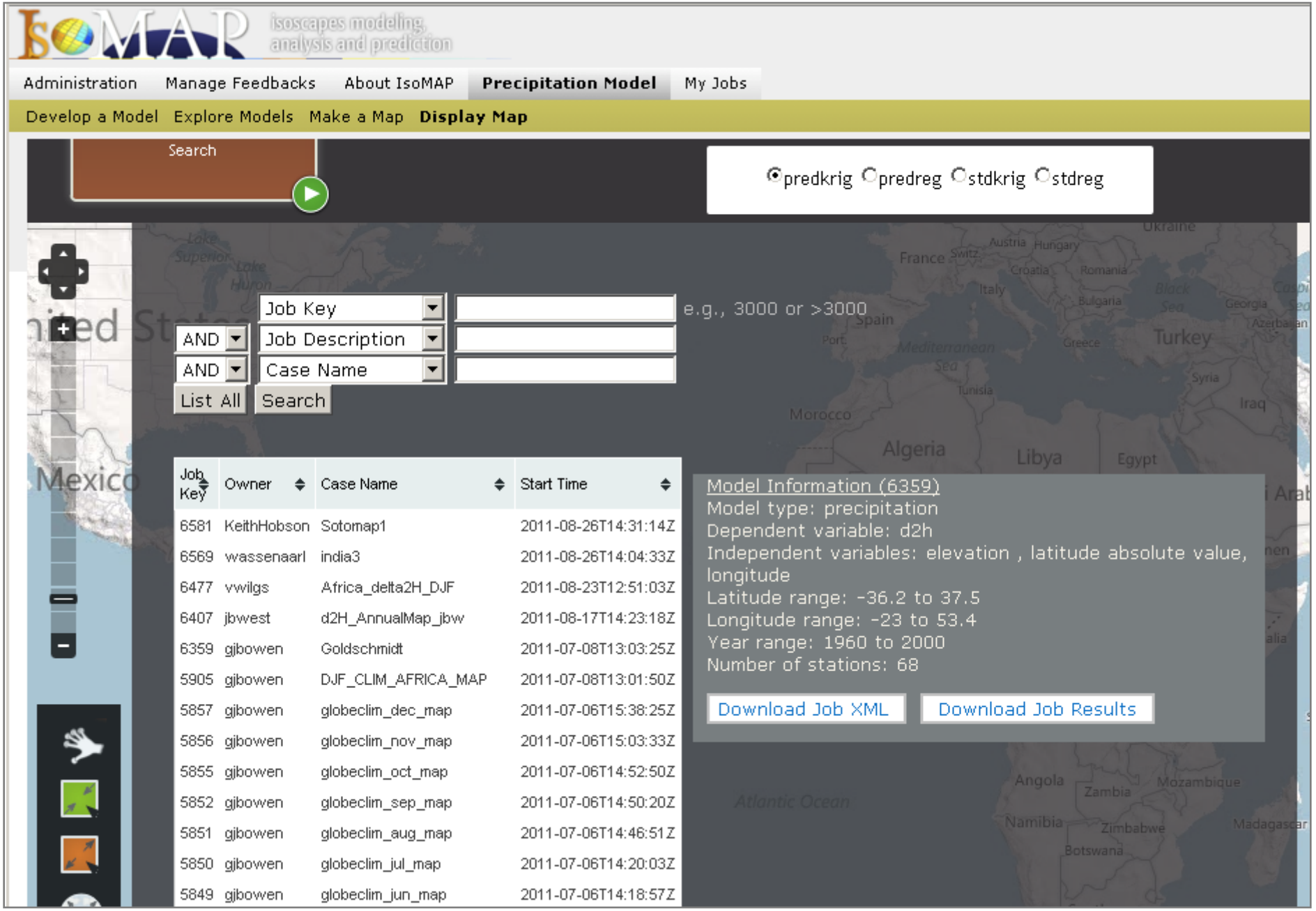

IsoMAP
isoscapes modeling, analysis and prediction
Logout
Welcome, Gabriel Bowen
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Develop a Model
Explore Models
Make a Map
Display Map
Temporal Range Selected!
Spatial Range: Selected!
Datasets Selected!
Submit Job
Dependent Variable
2H
18O
Independent Variable
Variable | Source | Form | √
Elevation | STATION,ETOPO,CRU | e
Max. Temp. | CRU | t^2,t
Min. Temp. | CRU | t^2,t
Precipitation | STATION,CRU | p
Ave. Temp. | STATION,CRU | t^2,t
Latitude | STATION | l^2,abs(l)
Prevalidation Results
fail (only 4 stations are valid)
Mexico
China
India
Iran
Saudi Arabia
Pakistan
Afghanistan
Turkmenistan
Uzbekistan
Kyrgyzstan
Tajikistan
Nepal
Oman
Thailand
Peru
Colombia


IsoMAP
isoscapes modeling, analysis and prediction
Welcome
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Develop a Model
Explore Models
Make a Map
Display Map
Temporal Range Selected!
Spatial Range: Selected!
Datasets Selected!
Run Name: Dec_1980_Europe
North America
Europe
Asia
Africa
South America
Australia
Atlantic Ocean
Pacific Ocean
Indian Ocean

Documentation

- IsoMAP keeps track of what you have done
- Metadata.xml
  - Job specifications
  - Summary of extracted/reduced datasets
  - Computational details
  - Key results
- Home-grown format
  - Designed to offer value to user, and
  - Serve as an information “payload” within the IsoMAP system

```
- <isomap_predictionfit>
  - <job_info>
      <jobkey>6359</jobkey>
      <description>describe this run</description>
      <job_stage>model_prediction</job_stage>
      <model_type>precipitation</model_type>
      <isotope>d2h</isotope>
      <formula/>
      <author>gjbowen</author>
      <access>private</access>
    - <tags>
        <tag source="user">killme</tag>
        <tag source="system">ui_testing</tag>
      </tags>
      <template_key stage="model_fitting">5903</template_key>
    </job_info>
  - <spatial>
      <proj4>+proj=longlat +ellps=wgs84 +datum=wgs84 +no_defs</proj4>
      <upper_longitude>53.4</upper_longitude>
      <lower_longitude>-23</lower_longitude>
      <upper_latitude>37.5</upper_latitude>
      <lower_latitude>-36.2</lower_latitude>
    </spatial>
  - <temporal>
      <upper_year>2000</upper_year>
      <lower_year>1960</lower_year>
      <time_mode>synoptic</time_mode>
      <month>1</month>
      <month>2</month>
      <month>12</month>
    </temporal>
  - <point_data>
```


IsoMAP
isoscapes modeling, analysis and prediction
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Develop a Model
Explore Models
Make a Map
Display Map
Search
predkrig
predreg
stdkrig
stdreg
Job Key
e.g., 3000 or >3000
AND
Job Description
AND
Case Name
List All
Search
Job Key
Owner
Case Name
Start Time
6581 KeithHobson Sotomap1 2011-08-26T14:31:14Z
6569 wassenaarl india3 2011-08-26T14:04:33Z
6477 vwilgs Africa_delta2H_DJF 2011-08-23T12:51:03Z
6407 jbwest d2H_AnnualMap_jbw 2011-08-17T14:23:18Z
6359 gjbowen Goldschmidt 2011-07-08T13:03:25Z
5905 gjbowen DJF_CLIM_AFRICA_MAP 2011-07-08T13:01:50Z
5857 gjbowen globeclim_dec_map 2011-07-06T15:38:25Z
5856 gjbowen globeclim_nov_map 2011-07-06T15:03:33Z
5855 gjbowen globeclim_oct_map 2011-07-06T14:52:50Z
5852 gjbowen globeclim_sep_map 2011-07-06T14:50:20Z
5851 gjbowen globeclim_aug_map 2011-07-06T14:46:51Z
5850 gjbowen globeclim_jul_map 2011-07-06T14:20:03Z
5849 gjbowen globeclim_jun_map 2011-07-06T14:18:57Z
Model Information (6359)
Model type: precipitation
Dependent variable: d2h
Independent variables: elevation , latitude absolute value, longitude
Latitude range: -36.2 to 37.5
Longitude range: -23 to 53.4
Year range: 1960 to 2000
Number of stations: 68
Download Job XML
Download Job Results

Storage

- All your work is stored in a secure file system
  - Accessible through your account
  - Only you manage your jobs, you manage only your jobs
  - Retrieve or reuse results at any time
  - Job ‘package’ downloadable
    - Metadata
    - Input data
    - Raw and processed results

IsoMAP isoscapes modeling, analysis and prediction

Logout

Welcome, Gabriel Bowen

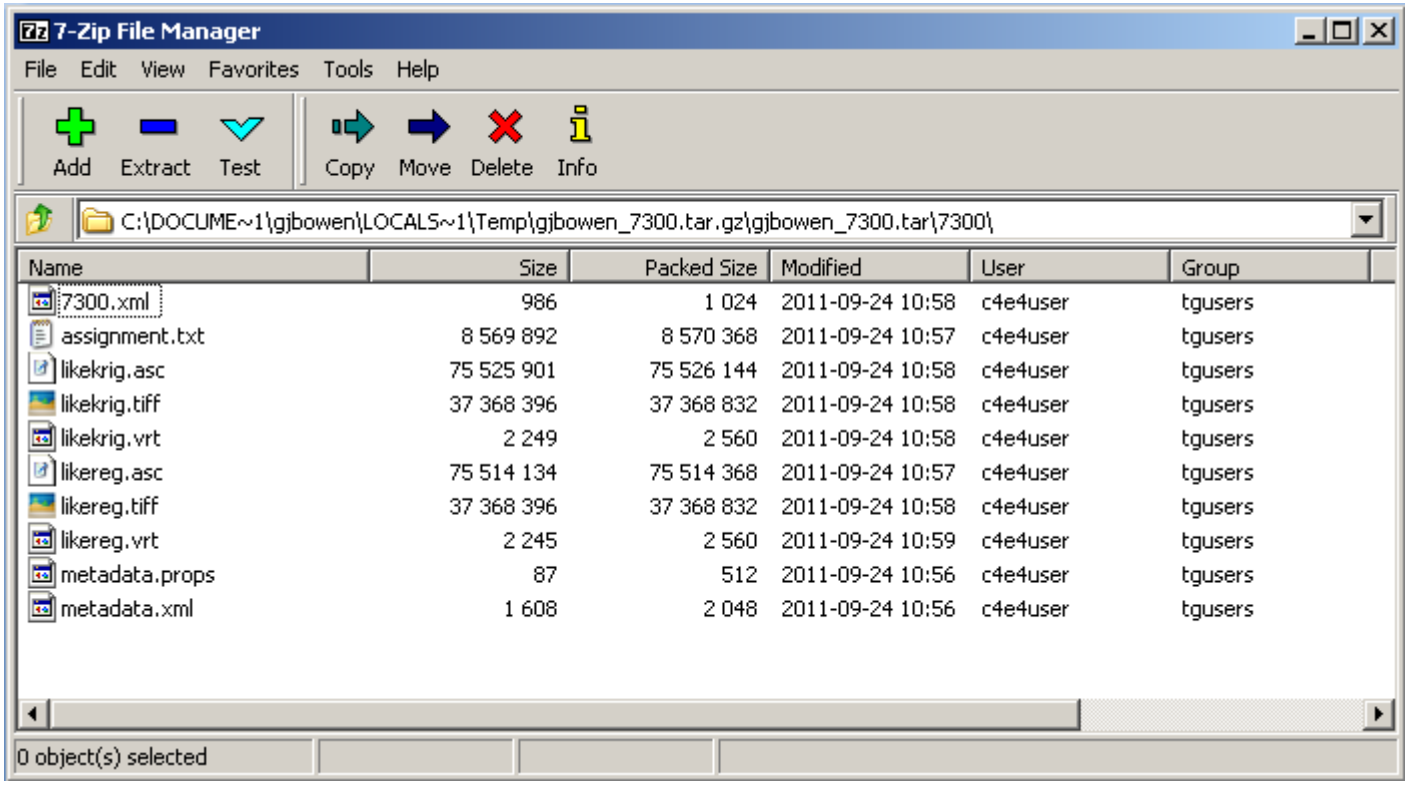
Administration | Manage Feedbacks | About IsoMAP | Precipitation Model | **My Jobs**

Fri Sep 23 11:15:18 EDT 2011

Owner of Jobs: **gjbowen**

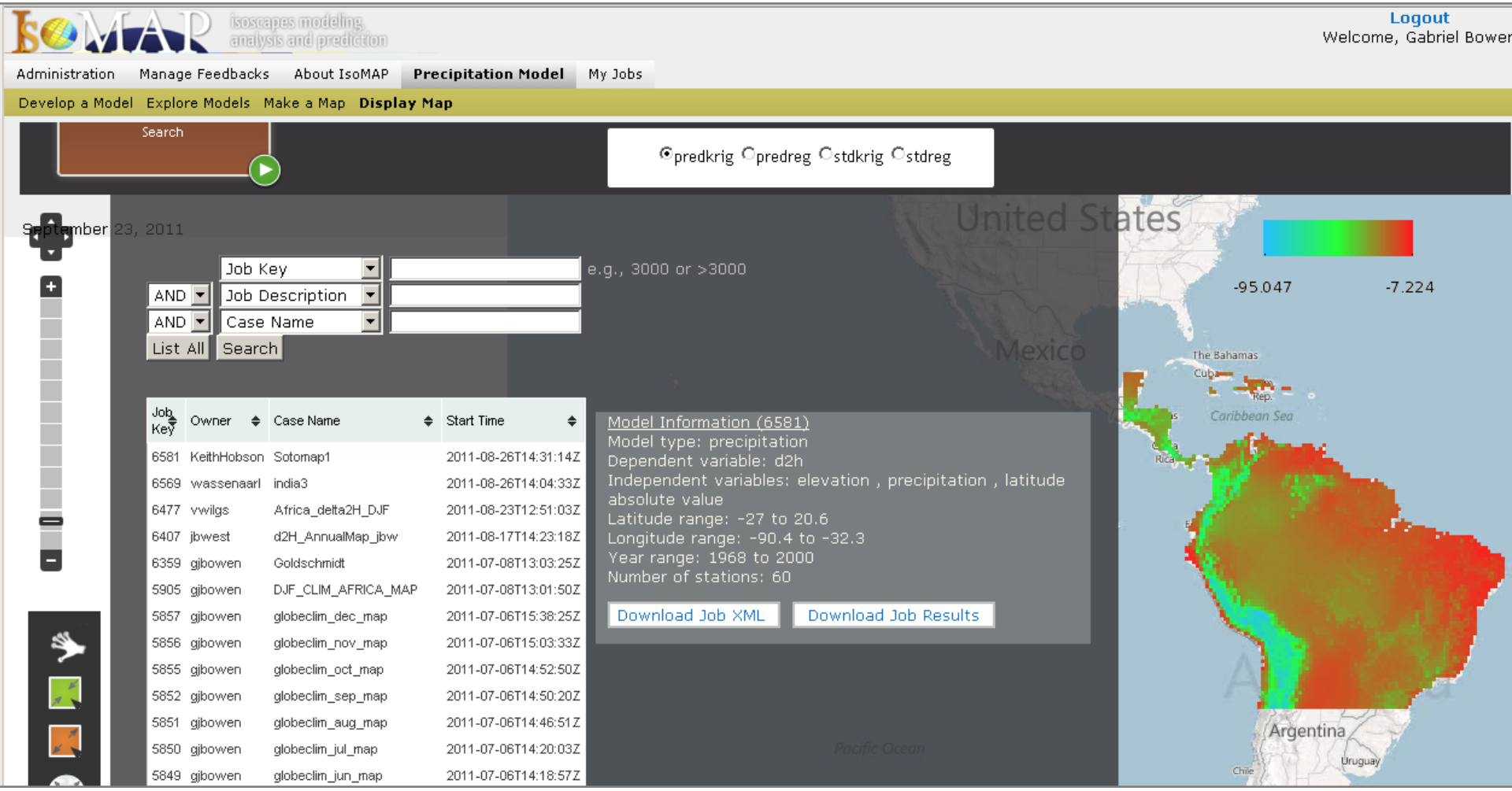
Refresh Jobs !

Key	Case Name	Model Run Type	Application Type	Job Status	StartTime	TimeTaken	Job Queue	Download	Action
6359	Goldschmidt	Prediction	Precipitation	DONE	2011-08-12 13:57:25	4 m 59 s	ccsm	Metadata | Results	Publish Delete
6105	newtest	Model Fitting	Precipitation	DONE	2011-07-27 06:11:54	3 m 2 s	ccsm	Metadata | Results	Publish Delete
5905	DJF_CLIM_AFRICA_MAP	Prediction	Precipitation	DONE	2011-07-08 13:08:06	0 m 40 s	ccsm	Metadata | Results	Unpublish Delete
5903	DJF_CLIM_AFRICA_4	Model Fitting	Precipitation	DONE	2011-07-08 13:03:25	2 m 1 s	ccsm	Metadata | Results	Publish Delete
5902	DJF_CLIM_AFRICA_3	Model Fitting	Precipitation	DONE	2011-07-08 13:01:50	3 m 22 s	ccsm	Metadata | Results	Unpublish Delete
5900	DJF_CLIM_AFRICA_2	Model Fitting	Precipitation	DONE	2011-07-08 12:58:21	0 m 21 s	ccsm	Metadata | Results	Publish Delete
5898	DJF_CLIM_AFRICA_1	Model Fitting	Precipitation	DONE	2011-07-08 12:55:03	0 m 17 s	ccsm	Metadata | Results	Publish Delete
5857	globeclim_dec_map	Prediction	Precipitation	DONE	2011-07-06 21:15:45	5 hr 42 m	ccsm	Metadata | Results	Publish Delete
5856	globeclim_nov_map	Prediction	Precipitation	DONE	2011-07-06 21:14:54	5 hr 21 m	ccsm	Metadata | Results	Publish Delete
5855	globeclim_oct_map	Prediction	Precipitation	DONE	2011-07-06 21:13:55	5 hr 19 m	ccsm	Metadata | Results	Publish Delete
5852	globeclim_sep_map	Prediction	Precipitation	DONE	2011-07-06 21:05:13	5 hr 6 m	ccsm	Metadata | Results	Publish Delete
5851	globeclim_aug_map	Prediction	Precipitation	DONE	2011-07-06 21:01:18	4 hr 48 m	ccsm	Metadata | Results	Publish Delete
5850	globeclim_jul_map	Prediction	Precipitation	DONE	2011-07-06 20:59:42	4 hr 52 m	ccsm	Metadata | Results	Publish Delete
5849	globeclim_jun_map	Prediction	Precipitation	DONE	2011-07-06 20:58:04	4 hr 38 m	ccsm	Metadata | Results	Publish Delete
5848	globeclim_may_map	Prediction	Precipitation	DONE	2011-07-06 20:56:07	5 hr 4 m	ccsm	Metadata | Results	Publish Delete
5833	globeclim_dec	Model Fitting	Precipitation	DONE	2011-07-06 15:38:25	28 m 1 s	ccsm	Metadata | Results	Publish Delete
5832	globeclim_nov	Model Fitting	Precipitation	DONE	2011-07-06 15:03:33	27 m 47 s	ccsm	Metadata | Results	Publish Delete
5831	globeclim_oct	Model Fitting	Precipitation	DONE	2011-07-06 14:52:50	24 m 0 s	ccsm	Metadata | Results	Publish Delete
5829	globeclim_sep	Model Fitting	Precipitation	DONE	2011-07-06 14:50:20	23 m 37 s	ccsm	Metadata | Results	Publish Delete


7-Zip File Manager
File Edit View Favorites Tools Help
Add Extract Test Copy Move Delete Info
C:\DOCUME~1\gjbowen\LOCALS~1\Temp\gjbowen_7300.tar.gz\gjbowen_7300.tar\7300\
Name Size Packed Size Modified User Group
7300.xml 986 1 024 2011-09-24 10:58 c4e4user tgusers
assignment.txt 8 569 892 8 570 368 2011-09-24 10:57 c4e4user tgusers
likekrig.asc 75 525 901 75 526 144 2011-09-24 10:58 c4e4user tgusers
likekrig.tiff 37 368 396 37 368 832 2011-09-24 10:58 c4e4user tgusers
likekrig.vrt 2 249 2 560 2011-09-24 10:58 c4e4user tgusers
likereg.asc 75 514 134 75 514 368 2011-09-24 10:57 c4e4user tgusers
likereg.tiff 37 368 396 37 368 832 2011-09-24 10:58 c4e4user tgusers
likereg.vrt 2 245 2 560 2011-09-24 10:59 c4e4user tgusers
metadata.props 87 512 2011-09-24 10:56 c4e4user tgusers
metadata.xml 1 608 2 048 2011-09-24 10:56 c4e4user tgusers
0 object(s) selected

Sharing

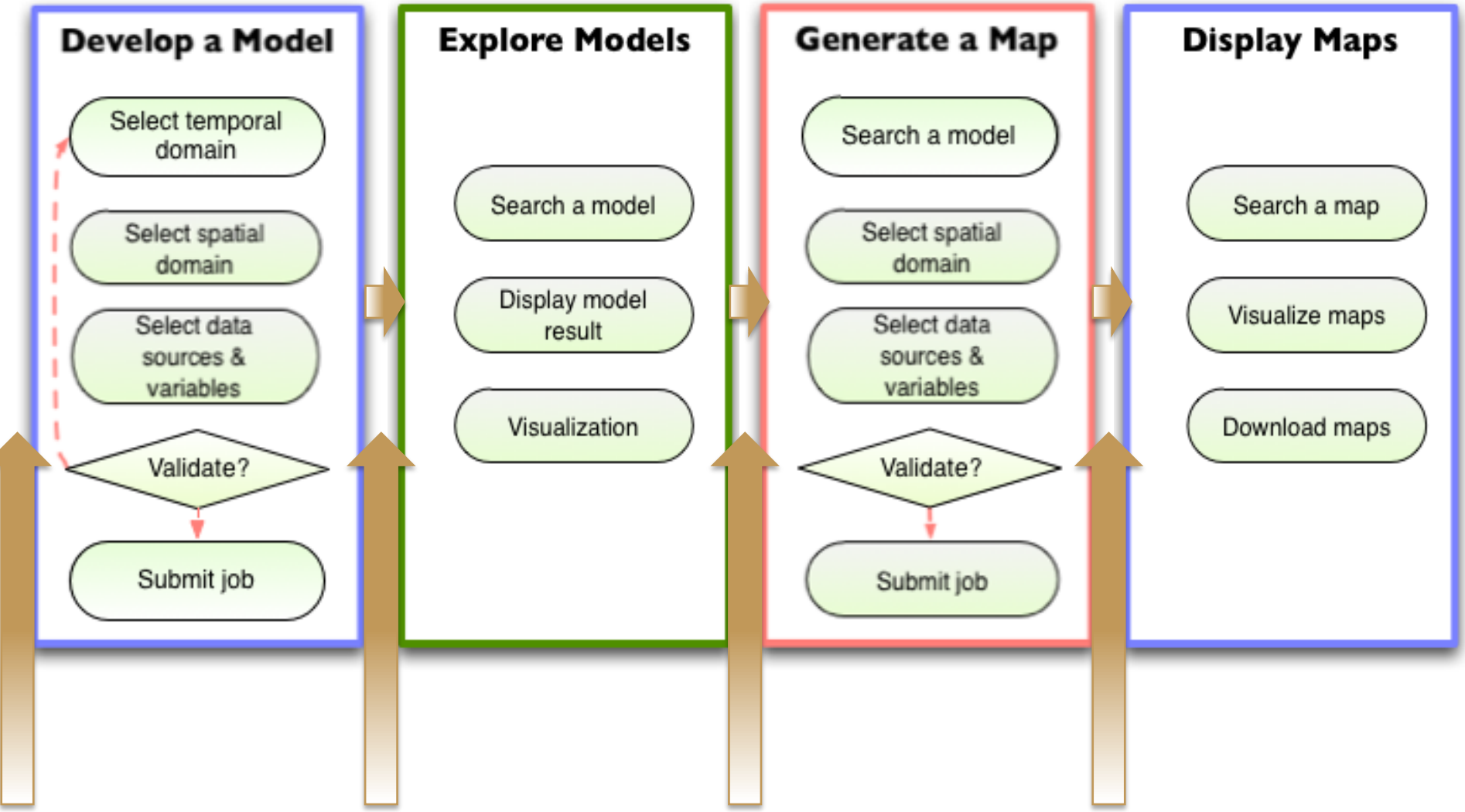
- IsoMAP lets you publish your work, making it:
  - Visible to others
  - Downloadable by others
  - Usable by others
- Current mechanism primitive
  - All-or-none
  - Local only
- Long-term vision includes groups, external discovery


IsoMAP
isoscapes modeling, analysis and prediction
Logout
Welcome, Gabriel Bower
Administration
Manage Feedbacks
About IsoMAP
Precipitation Model
My Jobs
Develop a Model
Explore Models
Make a Map
Display Map
Search
predkrig
predreg
stdkrig
stdreg
September 23, 2011
Job Key
e.g., 3000 or >3000
AND
Job Description
AND
Case Name
List All
Search
Job Key
Owner
Case Name
Start Time
6581 KeithHobson Sotomap1 2011-08-26T14:31:14Z
6569 wassenaarl india3 2011-08-26T14:04:33Z
6477 vwilgs Africa_delta2H_DJF 2011-08-23T12:51:03Z
6407 jbwest d2H_AnnualMap_jbw 2011-08-17T14:23:18Z
6359 gjbowen Goldschmidt 2011-07-08T13:03:25Z
5905 gjbowen DJF_CLIM_AFRICA_MAP 2011-07-08T13:01:50Z
5857 gjbowen globeclim_dec_map 2011-07-06T15:38:25Z
5856 gjbowen globeclim_nov_map 2011-07-06T15:03:33Z
5855 gjbowen globeclim_oct_map 2011-07-06T14:52:50Z
5852 gjbowen globeclim_sep_map 2011-07-06T14:50:20Z
5851 gjbowen globeclim_aug_map 2011-07-06T14:46:51Z
5850 gjbowen globeclim_jul_map 2011-07-06T14:20:03Z
5849 gjbowen globeclim_jun_map 2011-07-06T14:18:57Z
Model Information (6581)
Model type: precipitation
Dependent variable: d2h
Independent variables: elevation , precipitation , latitude absolute value
Latitude range: -27 to 20.6
Longitude range: -90.4 to -32.3
Year range: 1968 to 2000
Number of stations: 60
Download Job XML
Download Job Results
United States
Mexico
Pacific Ocean
-95.047
-7.224
The Bahamas
Cuba
Caribbean Sea
Argentina
Uruguay
Chile

Hierarchical Analysis

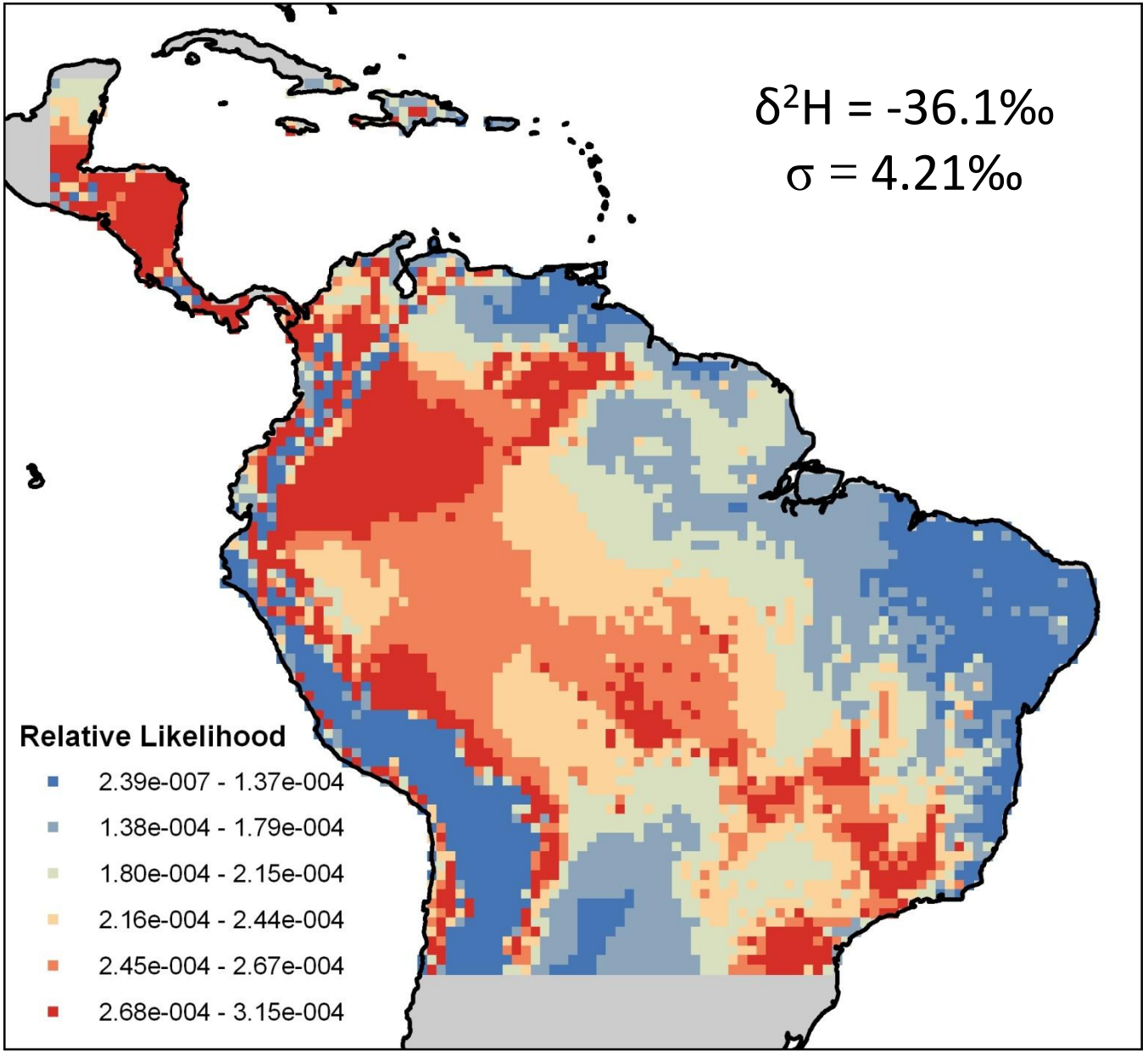
- IsoMAP is designed to let you build one analysis on top of another
  - Organize your analysis workflow as modular steps
  - Develop derived isoscapes and complex analyses using consistent, traceable methods
  - Store and document intermediate data products
  - Multiple entry points along the analysis workflow

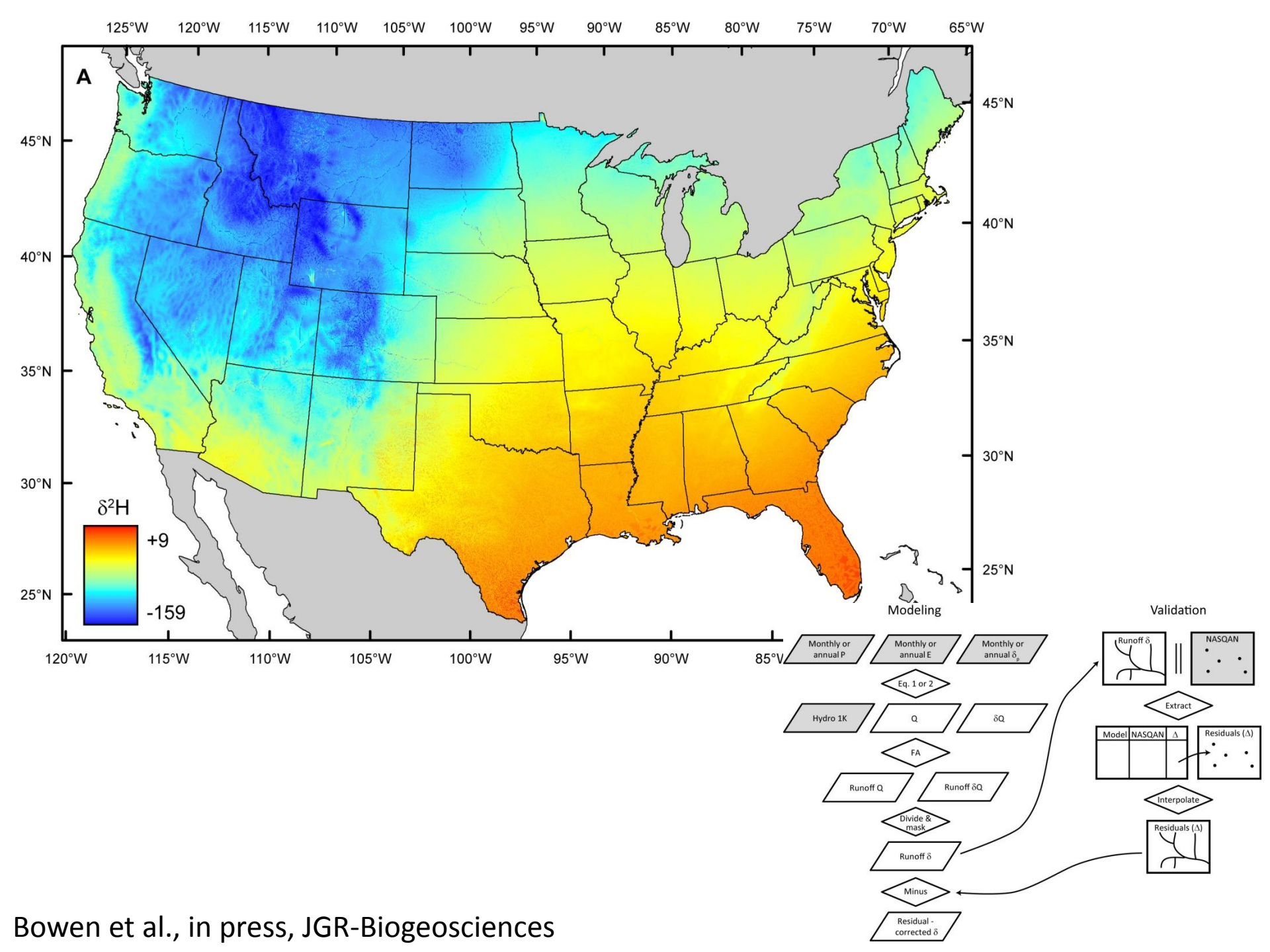
Precipitation Modeling Workflow



Hierarchical Analysis

- Geospatial assignment
  - Uses IsoMAP precipitation isoscapes as input
  - Basic version prototyped
  - Production-ready within 1-2 weeks
- Leaf water models
  - Uses IsoMAP precipitation isoscapes as input
  - Code ready, implementation to be started this fall
  - Anticipated release spring 2012


δ^2H = -36.1‰
σ = 4.21‰
Relative Likelihood
2.39e-007 - 1.37e-004
1.38e-004 - 1.79e-004
1.80e-004 - 2.15e-004
2.16e-004 - 2.44e-004
2.45e-004 - 2.67e-004
2.68e-004 - 3.15e-004



Bowen et al., in press, JGR-Biogeosciences

IsoMAP User Experience

- Design targets flexibility, accessibility, modularity
- That said, we've focused 1st on content, and quirks remain
  - IE compatibility
  - Shorthand notation
  - Inefficiency with respect to user input
  - Incomplete documentation
  - Bugs

IsoMAP User Experience

- We are working on these issues, and hopefully will accelerate our progress as content roll-out is completed
- Useful resources:
  - Documents (quick guide, statistics white paper, systems design paper…see flash drive)
  - Video tutorials (introductory video available now, more to follow)
  - Us (isomap@purdue.edu)

IsoMAP 2.0?

- We are seeking funding to extend on our work
- 3 major emphases
  - New analysis and modeling tools
  - Support user-supplied data
  - Link to distributed data resources
- The ultimate goal is to serve a broad research and education community by providing end-to-end data management and analysis tools
- To do this, we need your perspective, your input, and your vision