SciFlo™: Scientific Knowledge Creation on the Grid Using a Semantically-Enabled Dataflow Execution Environment

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Do multi-instrument science by *authoring* a dataflow doc. for a *reusable* operator tree. Access scientific data by *naming* it.

SciFlo Engine

- iEarth Vision will be enabled by the open-source SciFlo Engine.
- Automate large-scale, multi-instrument science processing by *authoring* a dataflow document that specifies a *tree* of *executable* operators.
  - iEarth Visual Authoring Tool
  - Distributed Dataflow Execution Engine
  - Move operators (executables) to the data.
  - Built-in reusable operators provided for many tasks such as subsetting, co-registration, regridding, data fusion, etc.
  - Custom operators easily plugged in by scientists.
  - Leverage convergence of Web Services (SOAP) with Grid Services (Globus v3.2).
- Hierarchical namespace of objects, types, & operators.
  - sciflo.data.EOS.AIRS.L2.atmosphericParameters
  - sciflo.operator.EOS.coregistration.PointToSwath

Outline

- Enabling Technologies
  - Web Services: SOAP
  - Grid Services: OGSI & Globus v3.2
  - Parallel dataflow engines
  - Semantic Web: OWL inference using metadata
- SciFlo Distributed Dataflow System
  - Loosely-coupled distributed computing using Web (SOAP) and Grid services
  - Specifying a processing stream as an XML document
  - Dataflow engine for automated execution and load balancing
- Multi-Instrument Earth Science
  - Motivating Example: Compare the temperature & water vapor profiles retrieved from AIRS (Atmospheric Infrared Sounder) swaths and GPS limb soundings.

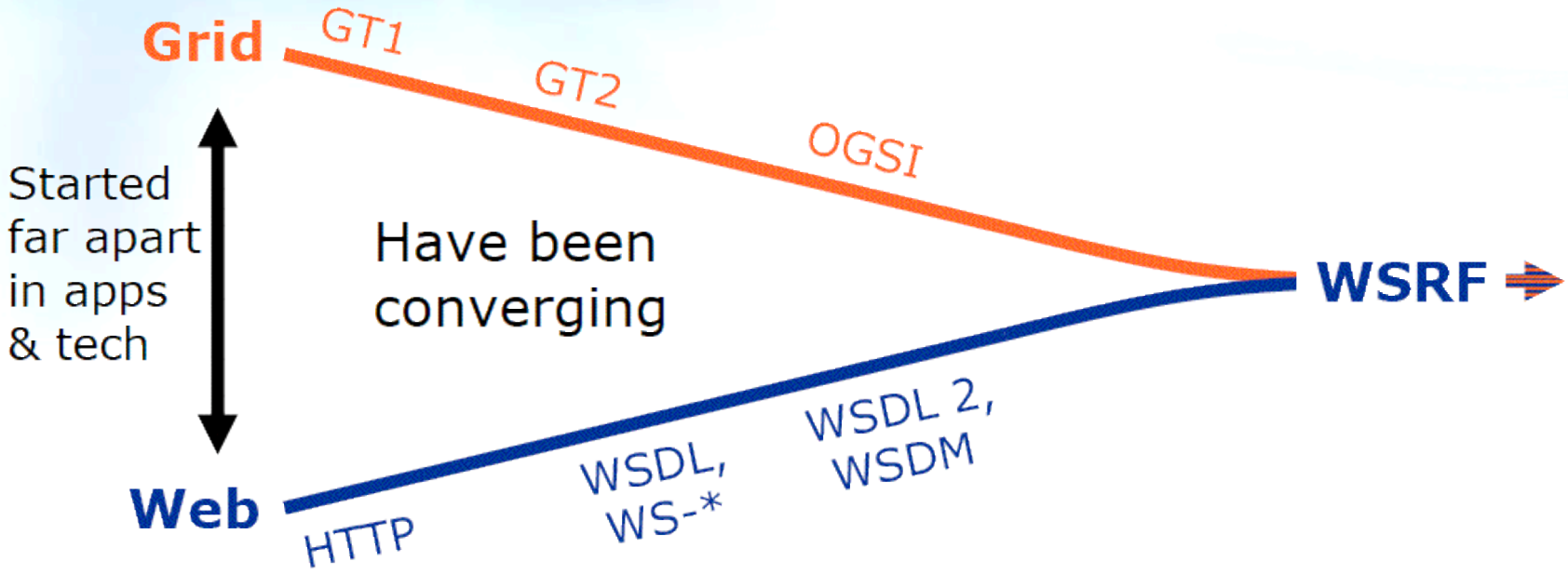
Third Generation of the Web

- SOAP-based Web Computing & Semantic Web
  - Exchange structured data in XML format (not HTML)
  - Semantics or “meaning” kept with the data
  - Emphasize programmatic interfaces
  - Web (Grid) Services
  - Leverage WS-Security and other WS-* standards
- Simple Object Access Protocol (SOAP)
  - Distributed Computing by Exchange of XML Messages
  - Lightweight, Loosely-Coupled API
  - Programming language independent
  - Multiple Transport Protocols Possible (HTTP, P2P)
  - Web Services Description Language (WSDL)
  - Publish Services in catalogs for automated discovery

Evolving Grid Computing Standards (I)

- History of Scientific Computing as a Utility
  - The Grid began as effort to tightly couple multiple super- or cluster computers together (e.g., Globus Toolkit v1 & v2).
  - Needed job scheduling, submission, monitoring, steering, etc.
  - SETI@HOME success
- OGSI: Open Grid Services Infrastructure
  - WS-Resource Framework (WSRF): Capabilities treated as storage or computing resources exposed on the web.
  - Globus v3.2 is open-source implementation using Java/C.
  - A service is Grid-enabled by inheriting from Java class.
  - Standard is complex and growing.
  - Challenge: Ease of installation & use.
- SciFlo is a lighter weight peer-to-peer (P2P) approach.

Evolving Grid Computing Standards (II)



[From Globus Toolkit "Ecosystem" presentation at GGF11 by Lee Liming]

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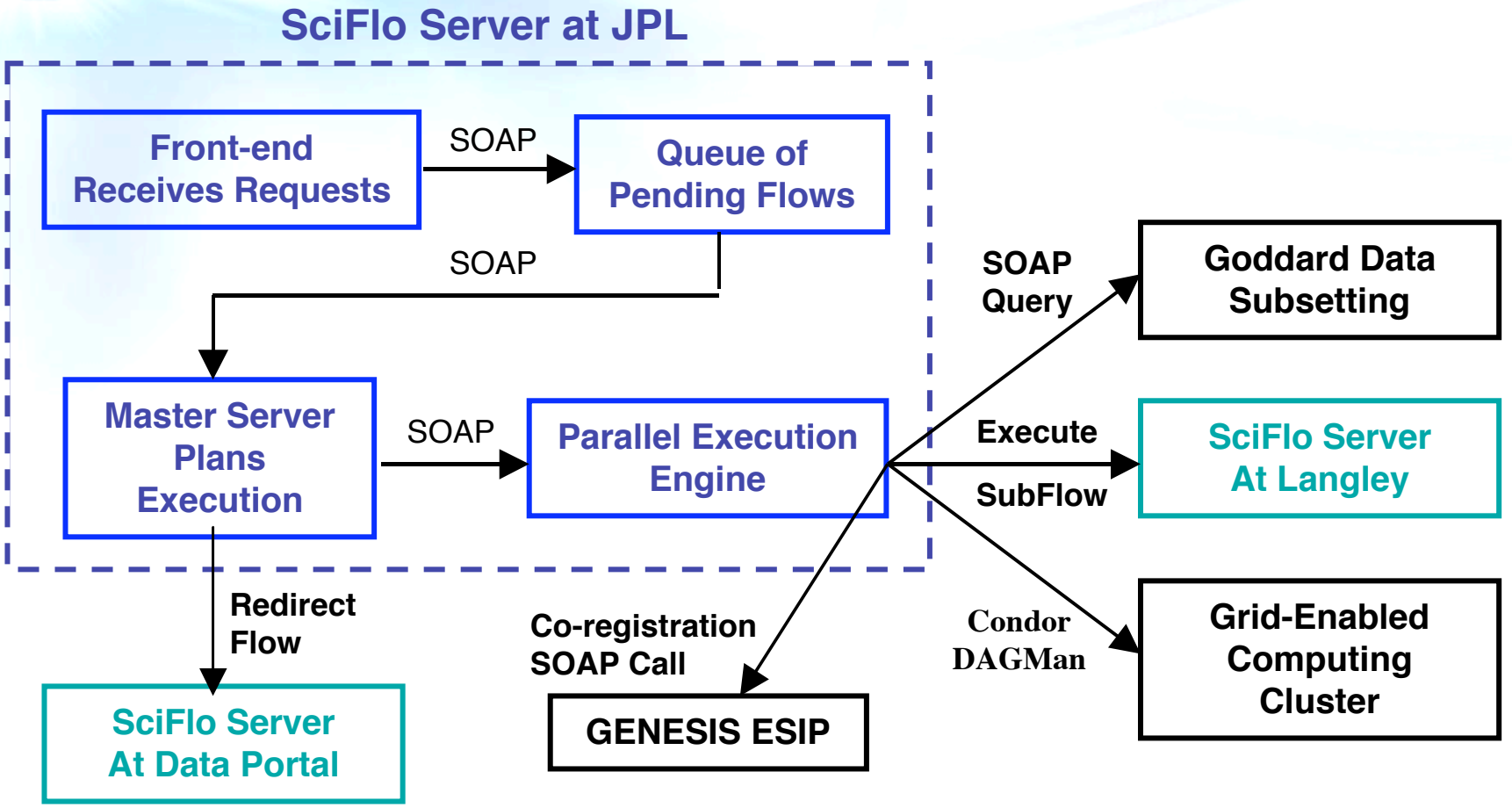
Distributed Computing Using SciFlo



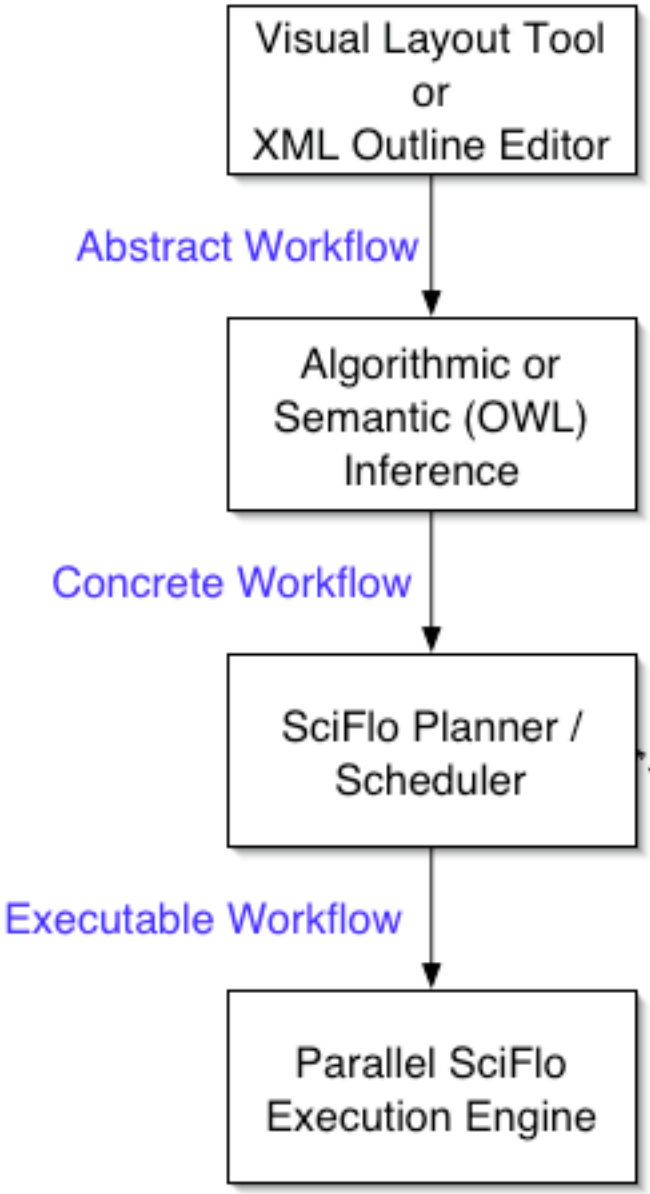
Inject data query or flow execution request into SciFlo network from any node.

Dataflow / Workflow Engines

- Grid:
  - Schedule & submit cluster computing jobs
  - Operator tree is a Directed Acyclic Graph (DAG)
  - CONDOR, CONDOR-G, DAGMan
  - Globus Alliance Standards: GSI, GRAM, MDS, RLS, XIO, etc.
  - Chimera -> Pegasus -> DAGMan -> Executing Grid Job
- Web:
  - Several web choreography standards
  - IBM's Business Process Execution Language (BPEL4WS)
- Less convergence here than in OGSI/WSRF
  - Marketplace winners?
  - 10 workflow groups spoke at Global Grid Forum (GGF) meeting
  - Sciflo will use some Globus capabilities via python bindings (pyGlobus).

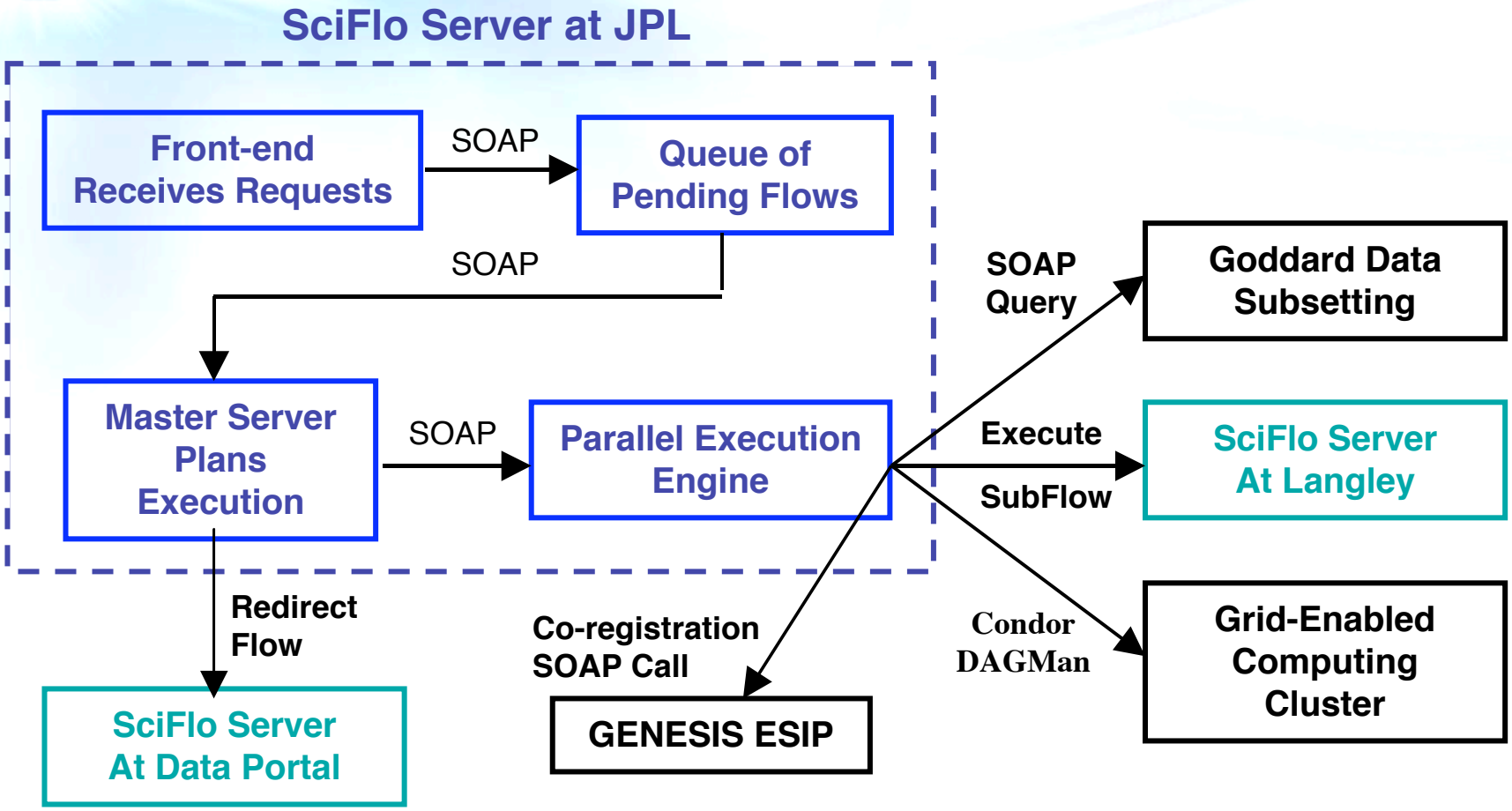
SciFlo: Scientific Knowledge Flow

Elaborating Workflow Documents



- Abstract (skeleton) Workflow is more easily authored.
  - Trivial data format & unit conversions auto-inserted.
  - As toolbox of known & reliable operators grows, even complex ops like regridding become trivial.
- Could use other backends if desired (BPEL, DAGMan).

Distributed Computing Using SciFlo



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Semantic Web

- History
  - DAML: DARPA Agent Markup Language
  - OWL: Ontology Web Language (from DAML+OIL)
  - Numerous inference engines & ontologies being developed
- Semantics for Web Services
  - OWL-S: OWL-based Web service ontology
  - Describe properties & capabilities in computer-interpretable form (beyond WSDL).
- SciFlo Semantics & Inference
  - Use WSDL+ & OWL-S to describe local operators (executables), remote services, & grid computing jobs.
  - Discover & select operators to fill in missing steps in a dataflow.

SciFlo: Scientific Knowledge Flow

- SciFlo's Strength Lies in Combining Many Elements into a Single Open-Source System
  - Abstract XML dataflow documents translated to concrete flows.
  - Parallel dataflow execution engine
  - Semantic inference using XML metadata
  - Move operators to the data.
  - SOAP architecture, but also P2P functionality.
  - Every node is both client & server; easy node replication.
  - One-click installation onto server or desktop nodes.
  - Initiate grid computations from your desktop.
- Access data objects by naming them!
  - P2P Distributed Namespace of data sources & operators
- Server architecture
  - Group of interacting SOAP services (replaceable modules)
  - Implementation in XML, python, & C/C++ (not Java)
- Strength in Numbers: Let a million nodes bloom!

More SciFlo Details

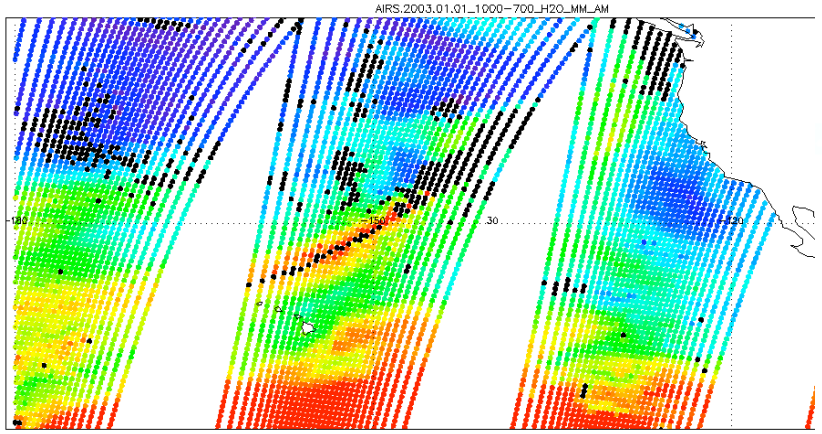
- Hardware Paradigm – Clusters of Linux & Windows PC's
- Each SciFlo node is both a client & server
- Stream data through an operator tree using SOAP calls
- Move operators to large data sources
- One-click installation onto server or desktop
- SciFlo client waits for results from queued flows.
- "Smart" Visual Programming Tool to author flow
- Distributed P2P catalogs of data sources and operators
- Server Execution Steps:
  - Validate, TypeCheck, Embellish, Schedule, Execute, Freeze/Thaw, DeliverResults
- Server architecture is a group of interacting SOAP services (replaceable modules)
- Implementation in XML, python, & C/C++ (not Java)

SciFlo: Scientific Knowledge Flow

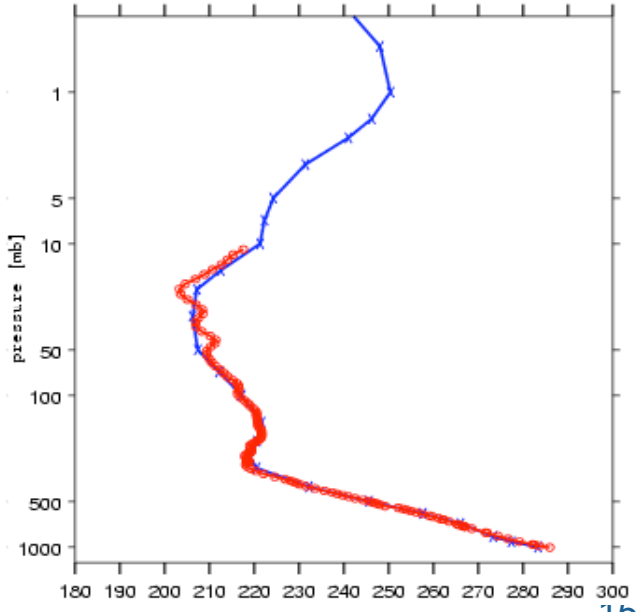
Motivating Examples

- **Data Discovery & Access**
  - What atmospheric temperature data (from all EOS instruments) is available in the tropical Pacific on Jan. 3, 2004? Retrieve it.

AIRS Swaths



- **Multi-Instrument Science Questions**
  - Compare the AIRS temperature profiles to the GPS temperature profiles and to the ECMWF model grid over the oceans.

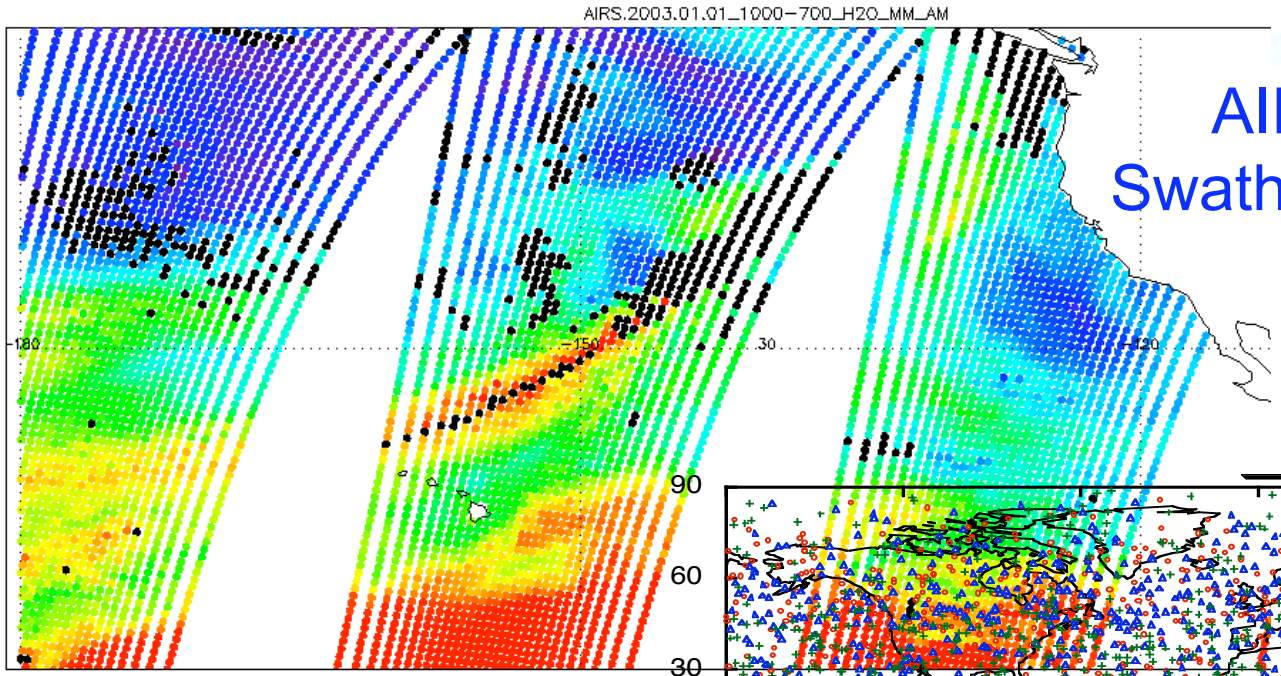


Data Access by Naming

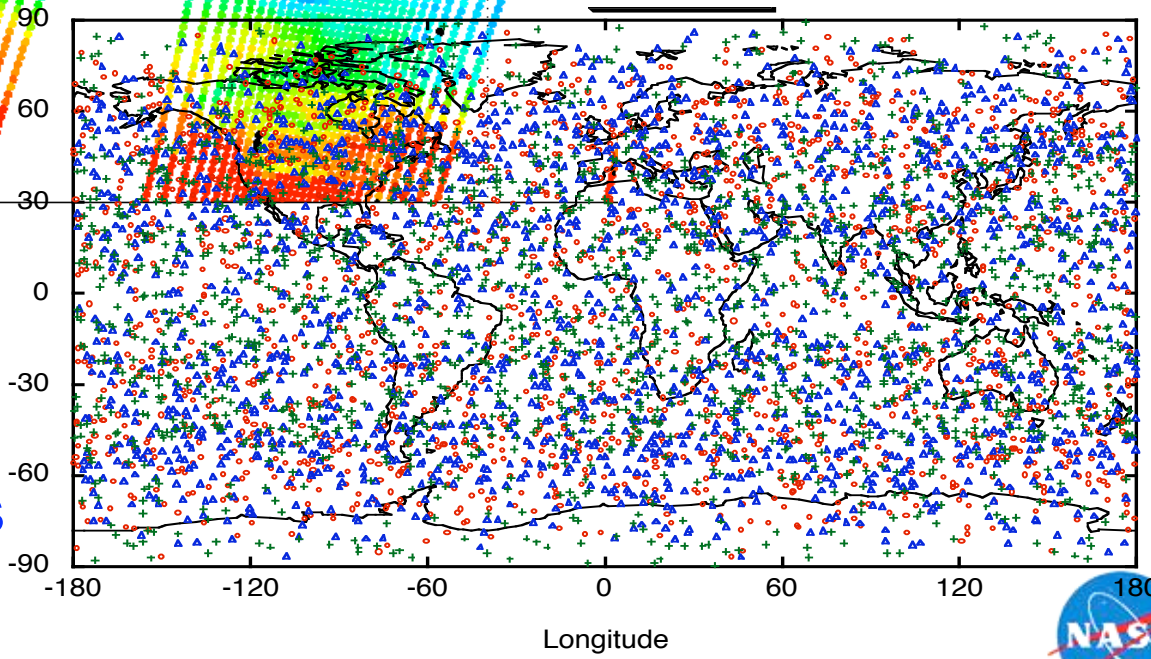
- Permanent Hierarchical Names ("Holy Grail")
  - Naming Authority assigned at each namespace level
  - Distributed P2P namespace (P2P catalog lookup)
- Proper Names
  - AIRS Level2 Parameter Retrieval Dataset (granules):
    sciflo.data.EOS.AIRS.L2.atmosphericParameters (or metadata)
  - Generic Point-To-Swath Co-registration Operator:
    sciflo.operator.EOS.coregistration.PointToSwath
- Generic Names
  - Atmospheric Temperature Data:
    sciflo.data.atmosphere.temperature.profile (or .grid)
  - Name resolves to list of EOS datasets
  - Semantics attached (3DGeoParameterGrid of temperature)

SciFlo: Scientific Knowledge Flow

AIRS/GPS Co-registration: Swath to Point



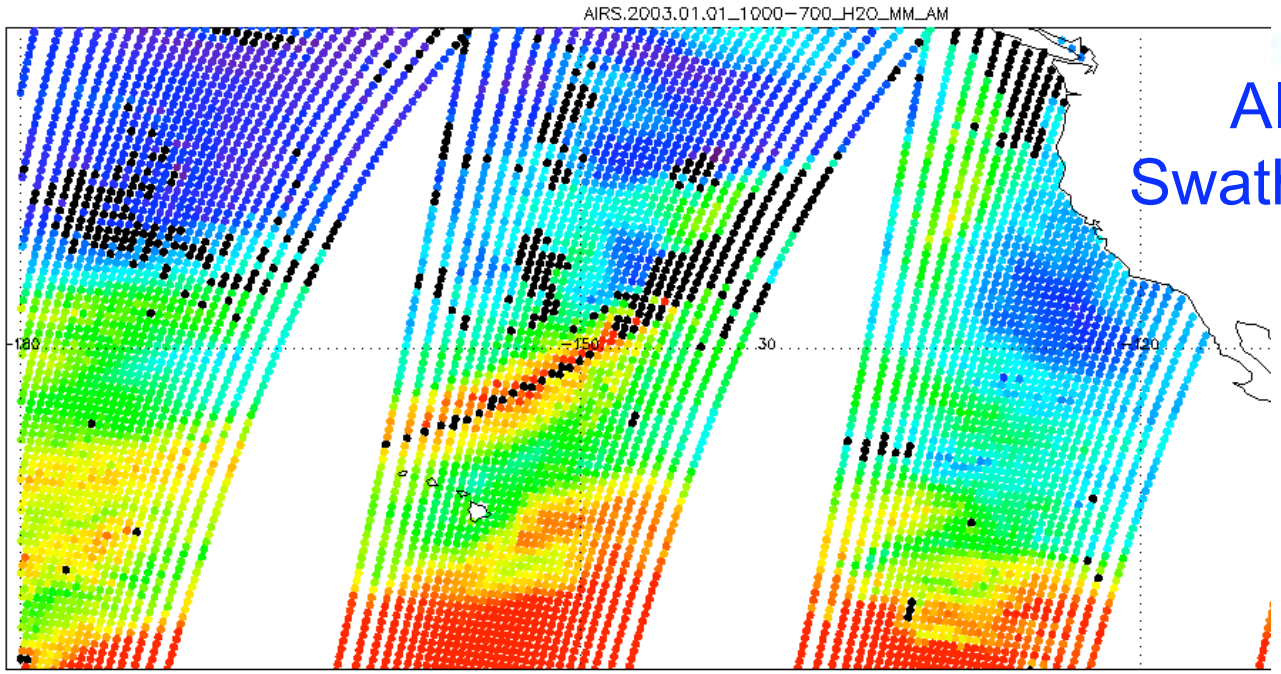
AIRS Level2
Swaths over Pacific



GPS Level2
Profile Locations

SciFlo: Scientific Knowledge Flow

AIRS/GPS Co-registration: Point to Swath



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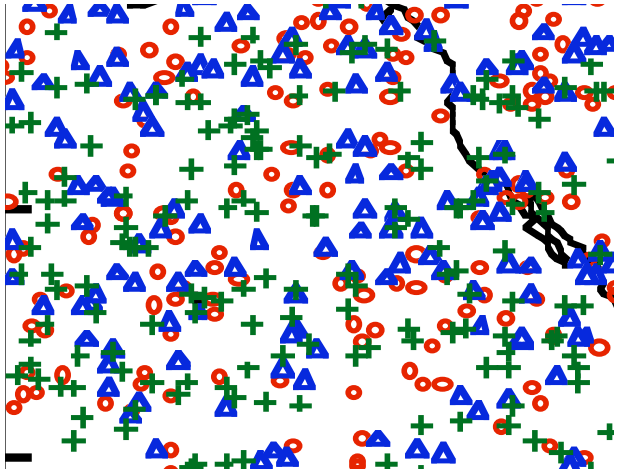

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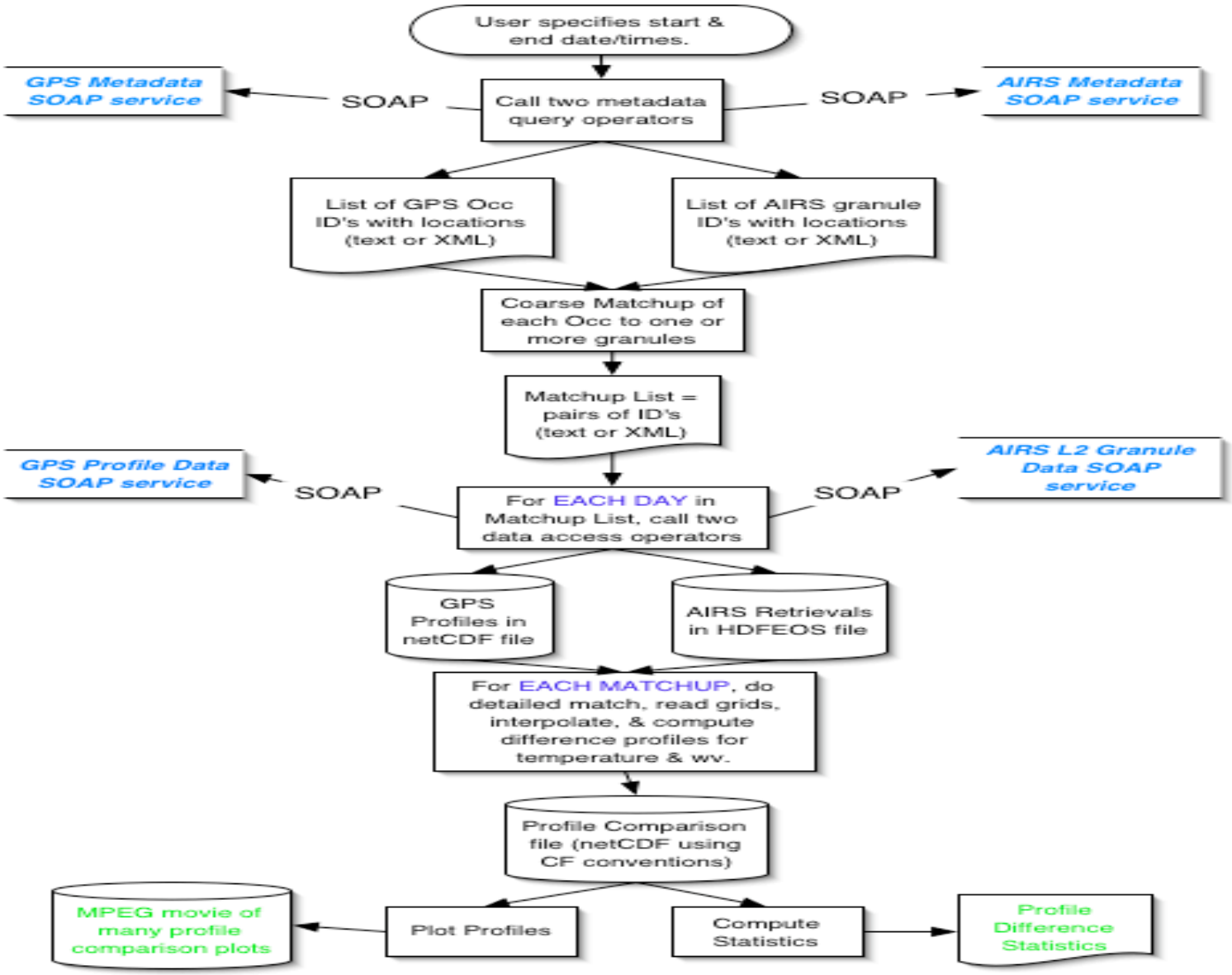
AIRS versus GPS Flowchart



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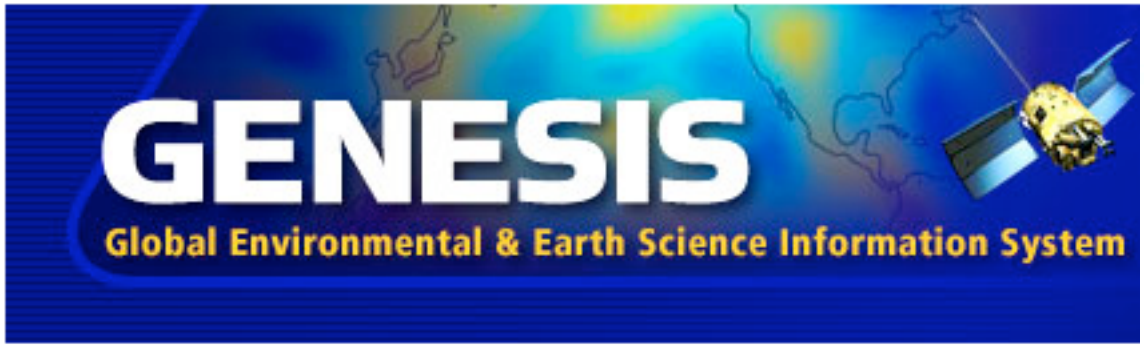
AIRS & GPS Temperature Matchup Demo



you are at: home » Registered User's Area » GPS-AIRS Matchup Demo

Starting Date/Time	2003 / 01 / 03 00 : 00
Ending Date/Time	2003 / 01 / 03 23 : 59
Time Tolerance (seconds)	60
Location Tolerance (km)	1000
Priority	1
Retrieval Type Max (between 0 and 100)	10
Land Fraction Min	0
Land Fraction Max	.1
Output whole swath?	☐

OK

- **Interface:** HTML web form auto-generated from XML dataflow doc.
- **Input:** User enters start/end time & other co-registration criteria.
- **Flow Execution:** Calls 2 SOAP data query services & total of 8 operators on 4 computers.

SciFlo: Scientific Knowledge Flow

AIRS & GPS Temperature Matchup Demo

you are at: home » Registered User's Area » GPS-AIRS Matchup Demo

Start Date/Time:	2003-01-03 00:00
End Date/Time:	2003-01-03 23:59
Time Tolerance (seconds):	60
Location Tolerance (km):	1000.0
Priority:	1
Retrieval Type Max (between 0 and 100):	10
Land Fraction Min:	0.0
Land Fraction Max:	0.1
Output whole swaths:	False

Checking GPS-AIRS matchup session...done (matchup file already exists and is current).
Number of matches found: 4
Getting matchup plots...done.
Getting swf movie of plots...done.

Finished processing.

Click here to download the NetCDF file.

Click here to download tgz of postscript plots.

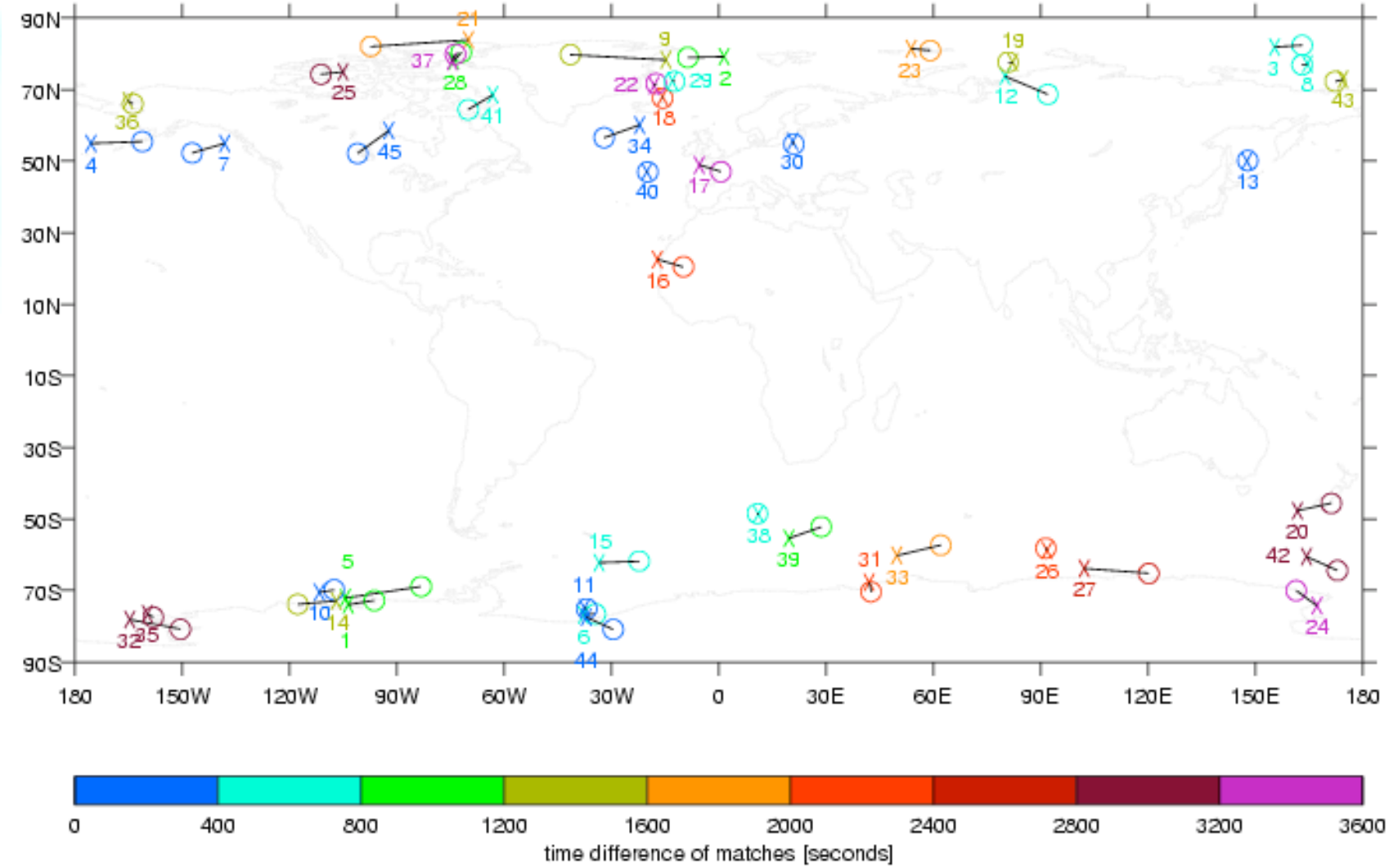
Click here to create and download mpeg movie (may take a while).

Flash movie:

- **Results Page:** Shows status updates during execution and then final results.
- **Caching:** Reuse intermediate data products or force recompute.
- **Results:** Merged data in netCDF file & plots as Flash movie.

SciFlo: Scientific Knowledge Flow

AIRS/GPS Matchups



Wilson et al., 07/20/04

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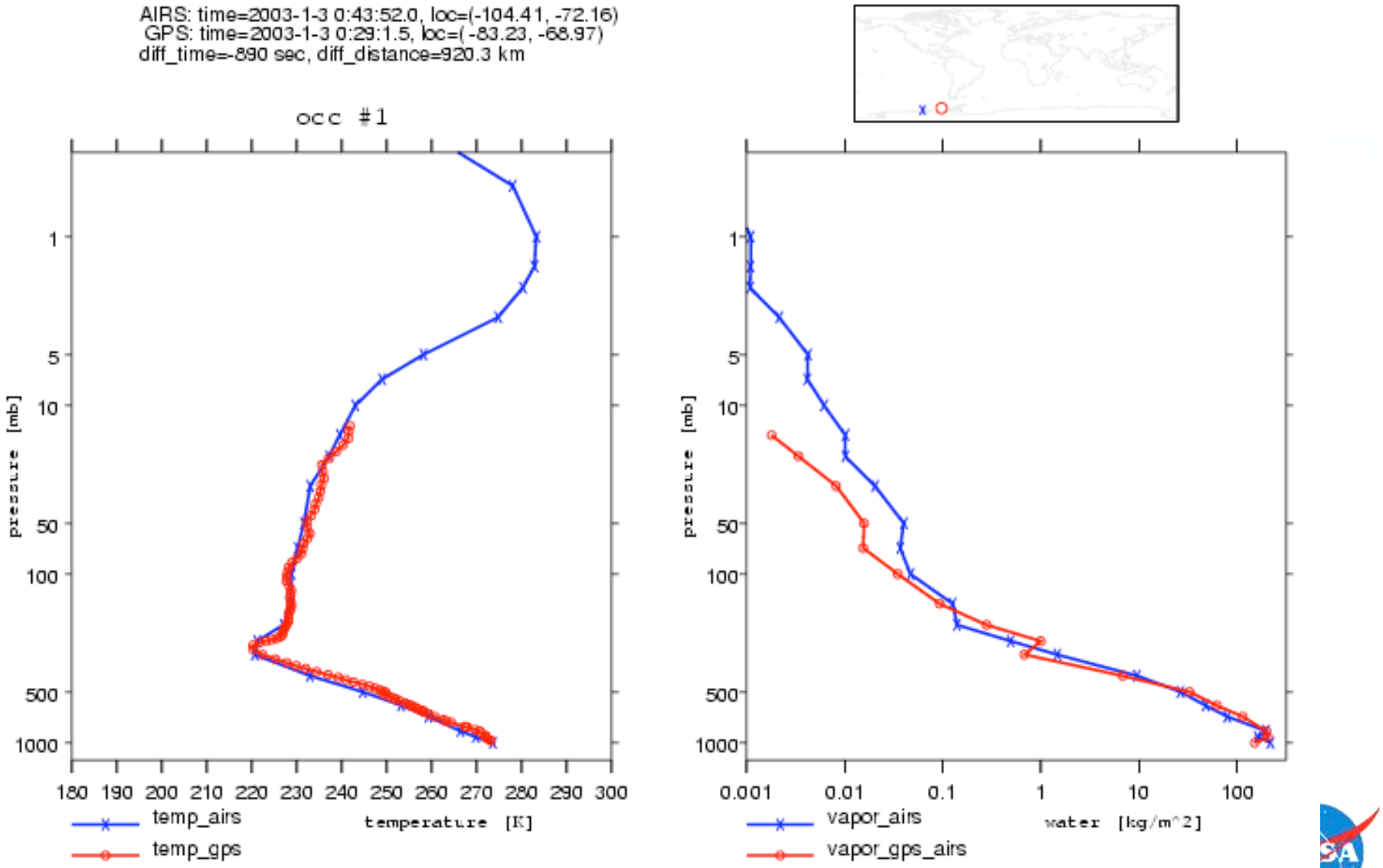
AIRS/GPS Temperature & Water Vapor Comparison Plots



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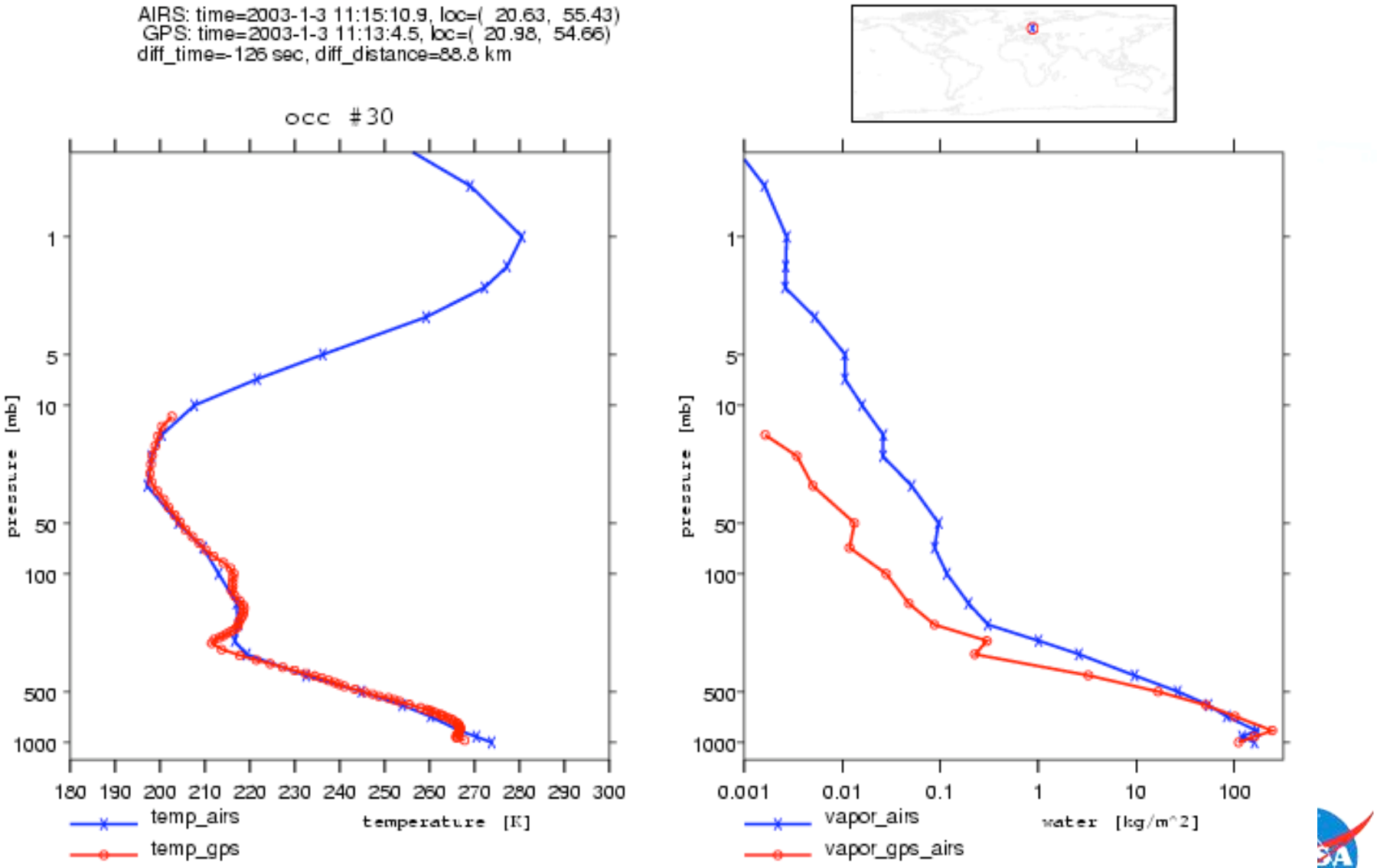

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Summary

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  - Abstract XML dataflow documents
  - Semantic inference using XML metadata
  - Parallel dataflow execution engine
  - Move operators to the data.
  - Every node is both client & server; easy node replication.
  - SOAP architecture, but also P2P functionality.
  - Initiate grid computations from your desktop.
- Goal: SciFlo nodes inside all Science Data Centers
- Multi-Instrument Earth Science
  - Instrument Cross-Comparisons
  - Multi-Instrument Science Portals
  - Large-scale multivariate statistical studies and verification of weather/climate models.