Integration of R to VTK:

Adding Statistical Computation to a Visualization Toolkit

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Technical Leader

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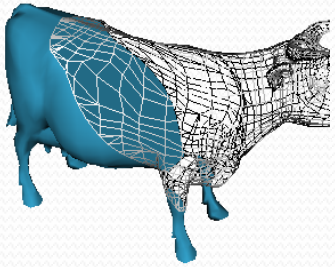
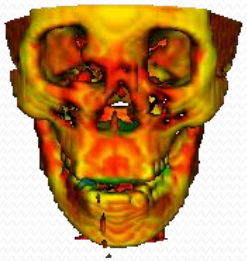
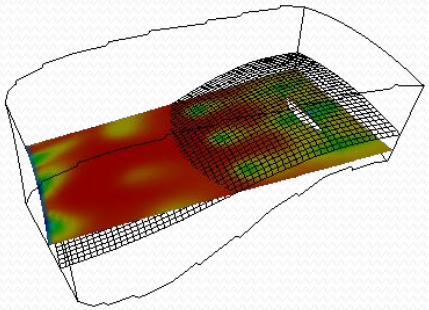
Basics – VTK

The **Visualization Toolkit (VTK)** is an open-source, freely available software system for 3D computer graphics, image processing and visualization.

- Scalar, vector, tensor, texture, and volumetric methods
- Advanced modeling techniques such as:
  - Implicit modeling,
  - Polygon reduction,
  - Mesh smoothing,
  - Cutting,
  - Contouring,
  - Delaunay triangulation.
- VTK:
  - Has an extensive information visualization framework,
  - Has a suite of 3D interaction widgets,
  - Supports parallel processing, and
  - Integrates with various databases on GUI toolkits such as Qt and Tk.
  - Cross-platform and runs on Linux, Windows, Mac and Unix platforms.





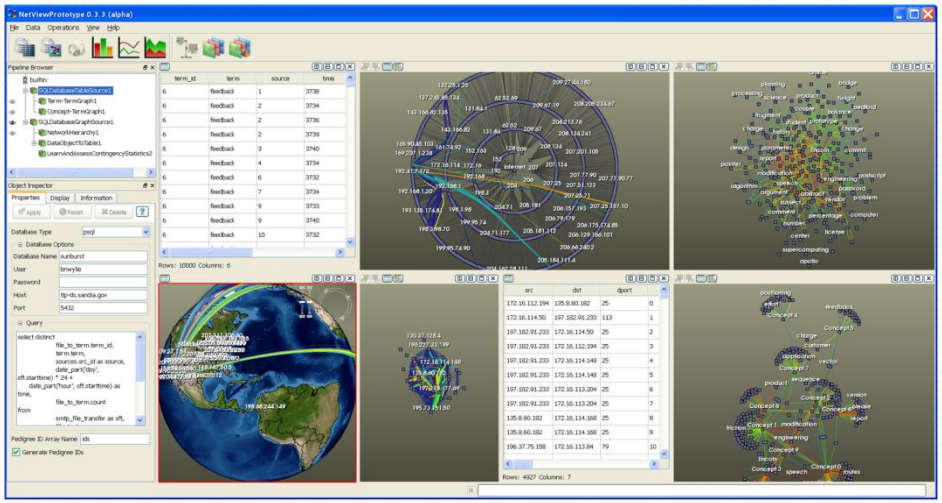


Basics – Titan

The **Titan Informatics Toolkit** is a collaborative effort between Sandia National Laboratories and Kitware Inc. It represents a significant expansion of the Visualization ToolKit (VTK) to support the ingestion, processing, and display of informatics data. By leveraging the VTK engine, Titan provides a flexible, component based, pipeline architecture for the integration and deployment of algorithms in the fields of intelligence, semantic graph and information analysis. Scalar, vector, tensor, texture, and volumetric methods

Titan Provides a set of data structures and algorithms for:

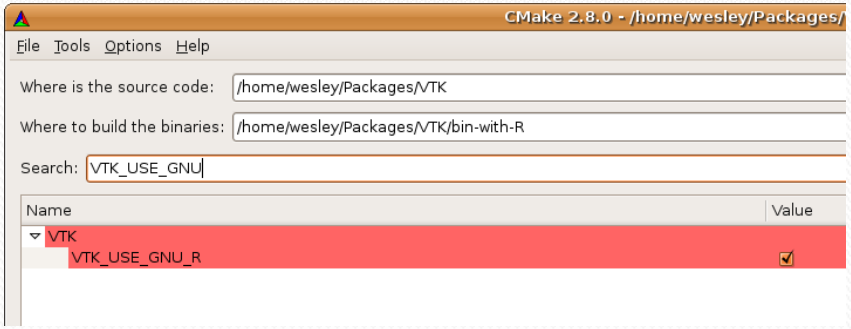
- Translation between VTK data structures and Graph/Tree data structures
- Access to databases
- Graph and Tree Layouts
- Graph and Tree Analysis

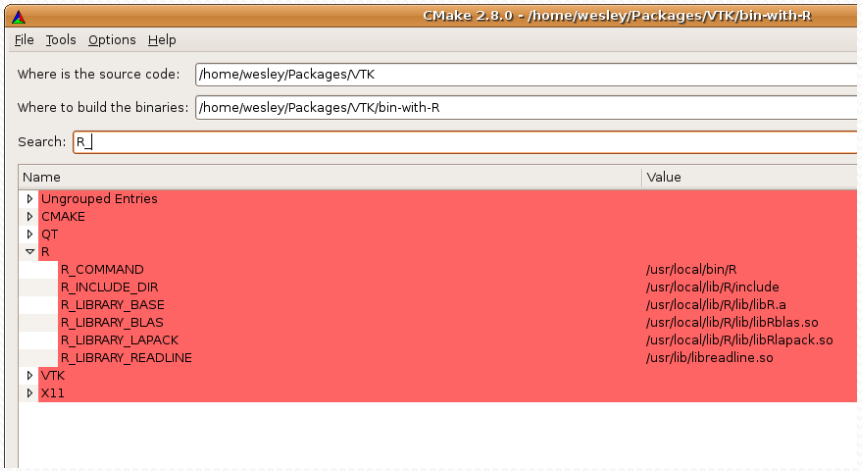


An application based on the Titan Informatics Toolkit is shown here displaying multiple views including table, graph and geospatial all semantically linked.

Enabling R in a VTK Build

- Obtain R Source
  - Build
  - Install
- VTK Uses CMake
  - Download VTK
  - During VTK configuration
    - cmake-gui <VTK-source>
    - Set VTK_USE_GNU_R On
    - Hit <Configure>
  - VTK uses the “R RHOME” command to determine the R configuration
    - Verify the R environment
    - Complete the VTK configuration
    - Build VTK as normal





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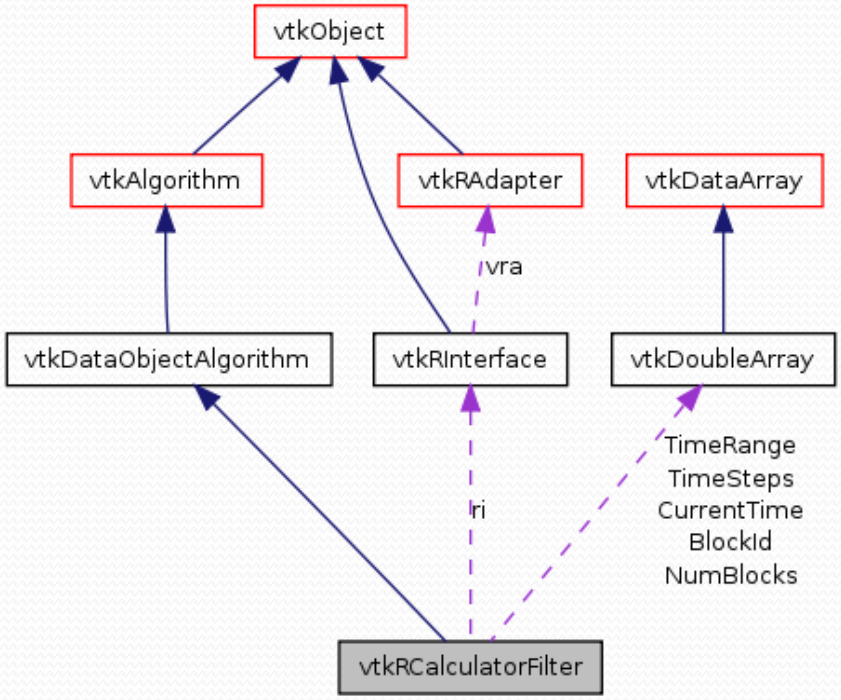
Interface to R

- vtkRCalculatorFilter
  - VTK filter API
- vtkRInterface
  - VTK Interface to embedded R Interpreter
  - Creates/Manages R Interpreter Instance
- vtkRAdapter
  - Lowest level of interface
  - Converts VTK Data to R SEXP
  - Converts R SEXP to VTK Data

Classes originally authored by Thomas Otahal at Sandia National Labs




```
vtkSmartPointer<vtkRCalculatorFilter> calc =
        vtkSmartPointer<vtkRCalculatorFilter>::New();
 calc->SetRoutput(0);
 calc->SetInputConnection(tab->GetOutputPort());
 calc->PutArray("0", "metabData");
 calc->GetArray("correl","correl");
 calc->SetRscript("correl<-cor(metabData)");
 calc->Update();
 calc->GetOutput()->Print(std::cout);
```

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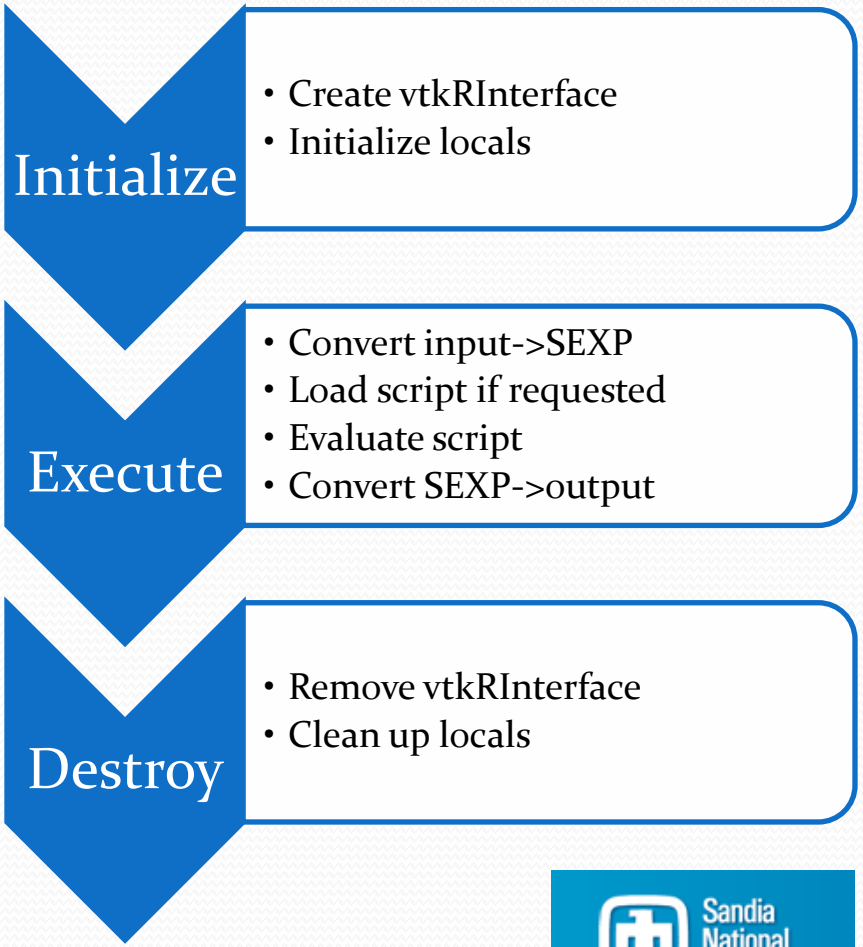
vtkCalculatorFilter Flow

- **Public Member Functions**
  - virtual const char * GetClassName ()
  - virtual int IsA (const char *type)
  - void PrintSelf (ostream &os, vtkIndent indent)
  - void PutArray (const char *NameOfVTKArray, const char *NameOfRvar)
  - void GetArray (const char *NameOfVTKArray, const char *NameOfRvar)
  - void RemoveAllPutVariables ()
  - void RemoveAllGetVariables ()
  - void PutTable (const char *NameOfRvar)
  - void GetTable (const char *NameOfRvar)
  - virtual void SetRscript (const char *)
  - virtual char * GetRscript ()
  - virtual void SetScriptFname (const char *)
  - virtual char * GetScriptFname ()
  - virtual void SetRoutput (int)
  - virtual int GetRoutput ()
  - virtual void SetTimeOutput (int)
  - virtual int GetTimeOutput ()
  - virtual void SetBlockInfoOutput (int)
  - virtual int GetBlockInfoOutput ()
  - virtual int ProcessRequest (vtkInformation *request, vtkInformationVector **inputVector, vtkInformationVector *outputVector)
- **Static Public Member Functions**
  - static vtkRCalculatorFilter * New ()
  - static int IsTypeOf (const char *type)
  - static vtkRCalculatorFilter * SafeDownCast (vtkObject *o)



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vtkCalculatorFilter Flow

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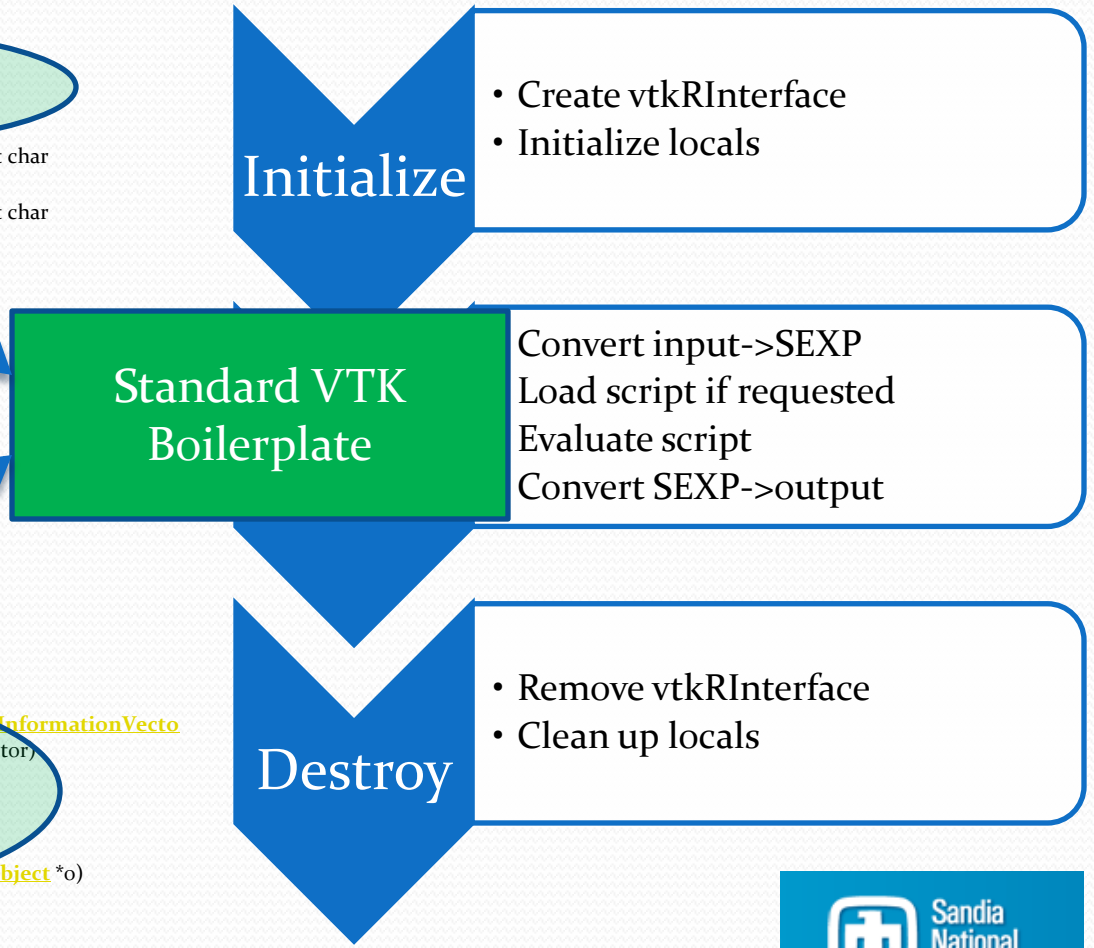

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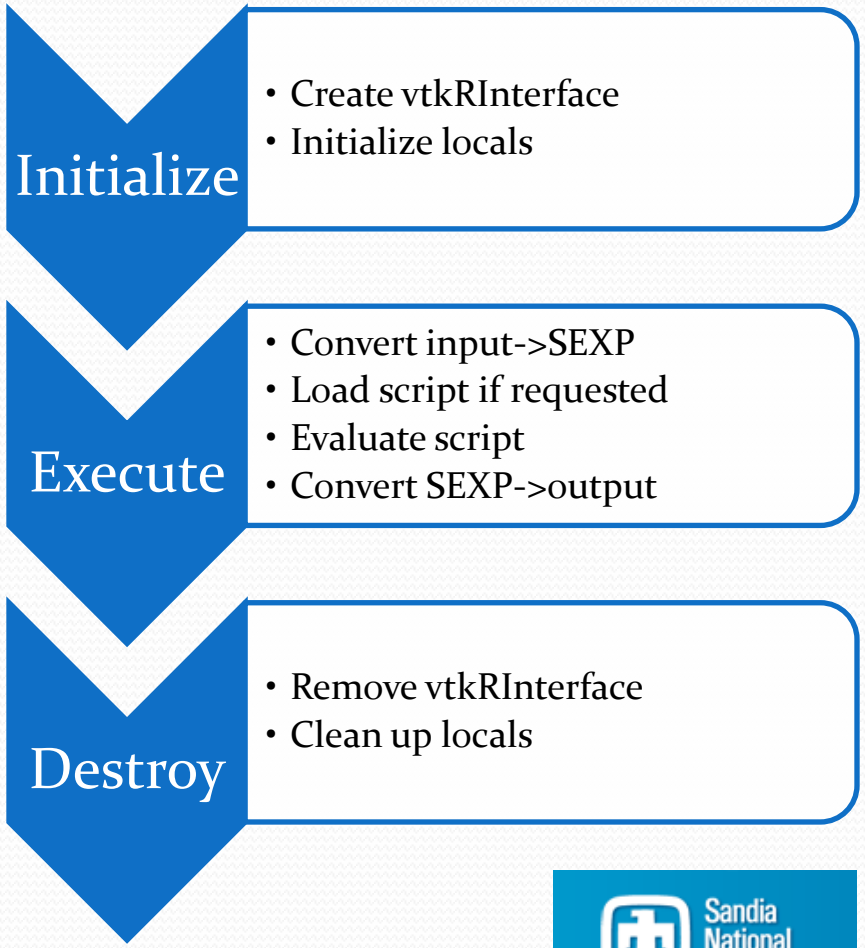
vtkCalculatorFilter Flow

Inputs:

- void PutArray (const char *NameOfVTKArray, const char *NameOfRvar)
- void PutTable (const char *NameOfRvar)
- void RemoveAllPutVariables ()

Outputs:

- void GetArray (const char *NameOfVTKArray, const char *NameOfRvar)
- void RemoveAllGetVariables ()
- void GetTable (const char *NameOfRvar)



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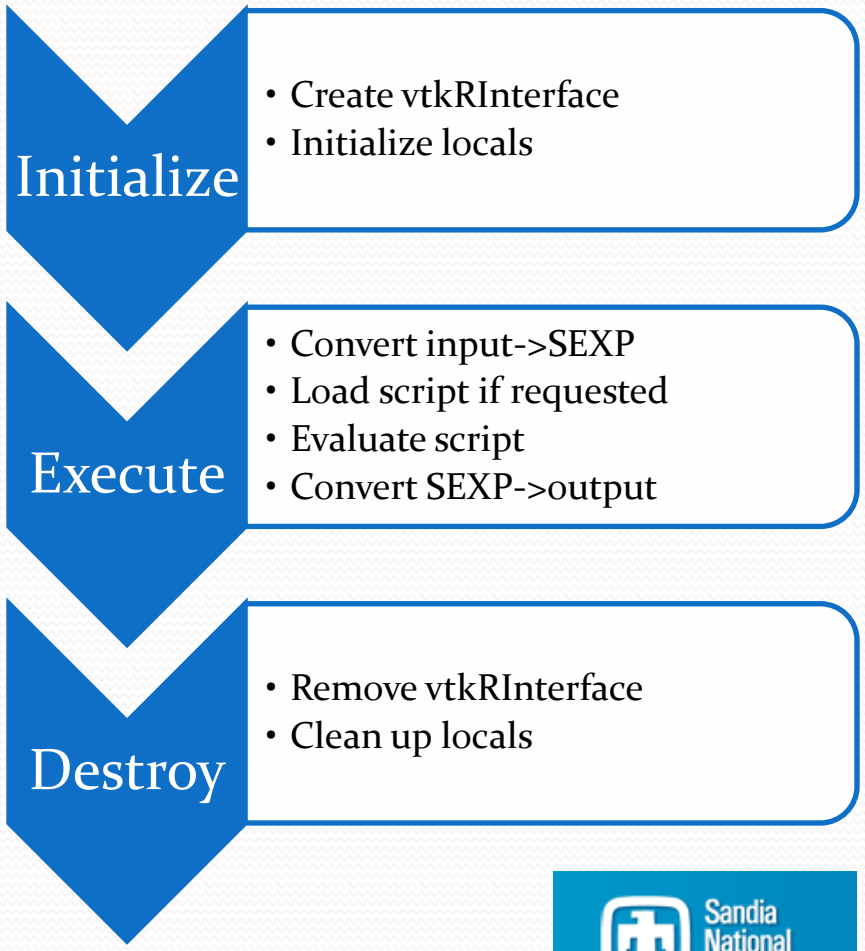
vtkCalculatorFilter Flow

R Scripts Control:

- virtual void SetRscript (const char *)
- virtual char * GetRscript ()
- virtual void SetScriptFname (const char *)
- virtual char * GetScriptFname ()
- virtual void SetRoutput (int)
- virtual int GetRoutput ()

Execution Control:

- virtual void SetTimeOutput (int)
- virtual int GetTimeOutput ()
- virtual void SetBlockInfoOutput (int)
- virtual int GetBlockInfoOutput ()



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Auto-Generation

- Now consider a specific set of R functionality
- Filter needs to:
  - Identify inputs
  - Identify the R operations
  - Identify R outputs
- Why not automate this?

- Automation is an interaction between:
  - A R filter template
    - vtkRGenericInterface.h.in
    - vtkRGenericInterface.cxx.in
  - A GUI/Interaction module
    - E.g. vtkWebModuleHandler.h
    - E.g. vtkWebModuleHandler.cxx
  - A CMake macro to connect the two and define the inputs

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Auto-Generation

- **Macro:**

```
Visomics_CREATE_MODULE(
  MODULE_NAME                 "voXCorrelHandler"
  ANALYSIS                    "xcorrel"
  VISUALIZATION_BASE          "voWebModuleHandler"
  MODULE_INPUTS               "metabData"
  MODULE_OUTPUTS              "correl"
  R_COMMAND                   "correl<-cor(metabData)"
  VISOMICS_SHOW_CORRELATION
                              "1"
  VISOMICS_SHOW_ROTATED_COORDINATES
                              "0"
  VISOMICS_SHOW_ROTATION_MATRIX
                              "0"
  VISOMICS_SHOW_STANDARD_DEVIATION
                              "0"
  VISOMICS_SHOW_GENERIC_ARRAY
                              "0"
)
```

- Currently Available:
  - "voHierarchicalClusterHandler"
  - "voFoldChangeHandler"
  - "voTTestHandler"
  - "voPLSHandler"
  - "voXCorrelHandler"
  - "voPCAHandler"

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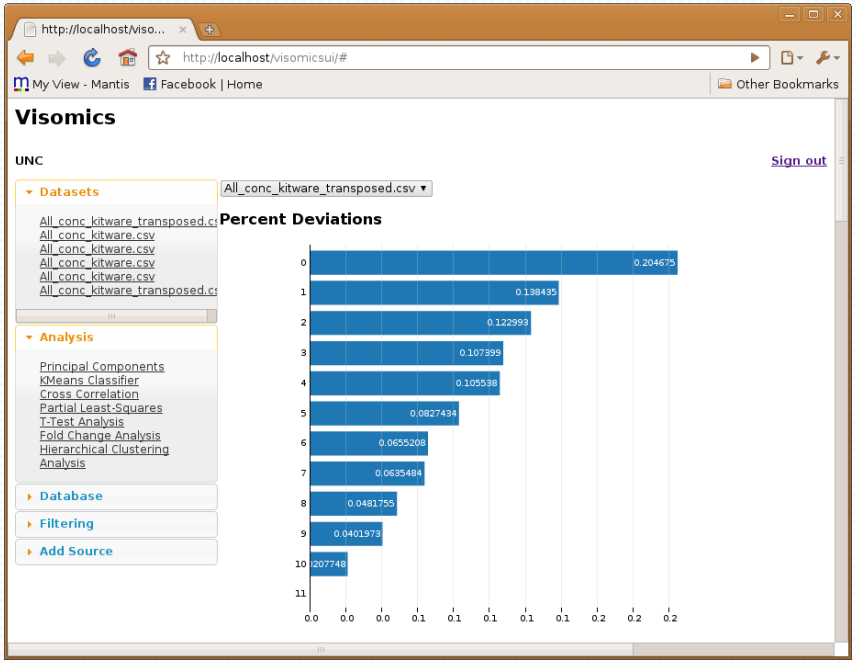
‘Omics Application

- One application is a research vehicle for ‘omics efforts
- Input is measured gene expression/metabolite concentrations
  - Multiple experiments
  - Cases and Controls
- Output is relationships
  - Correlations
  - Significance



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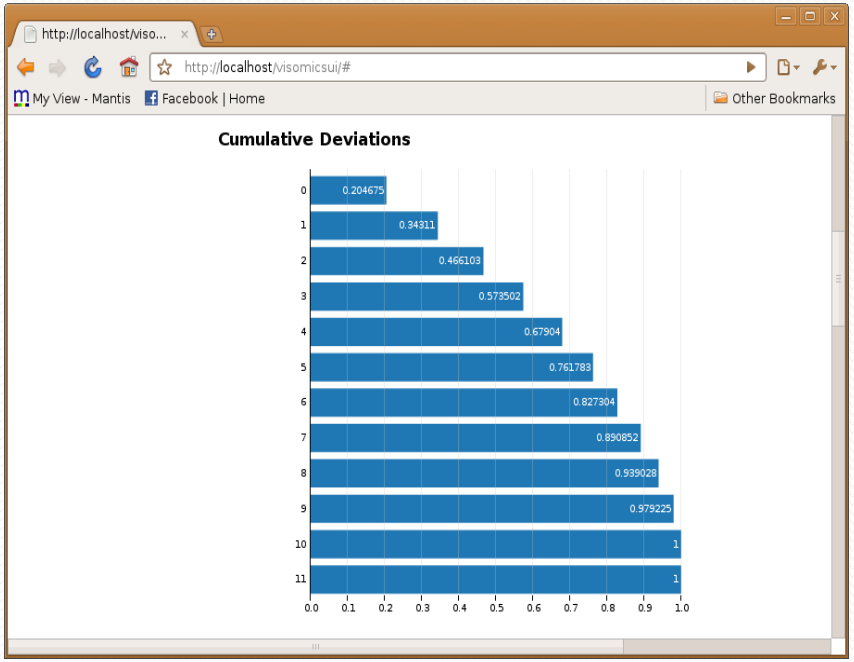

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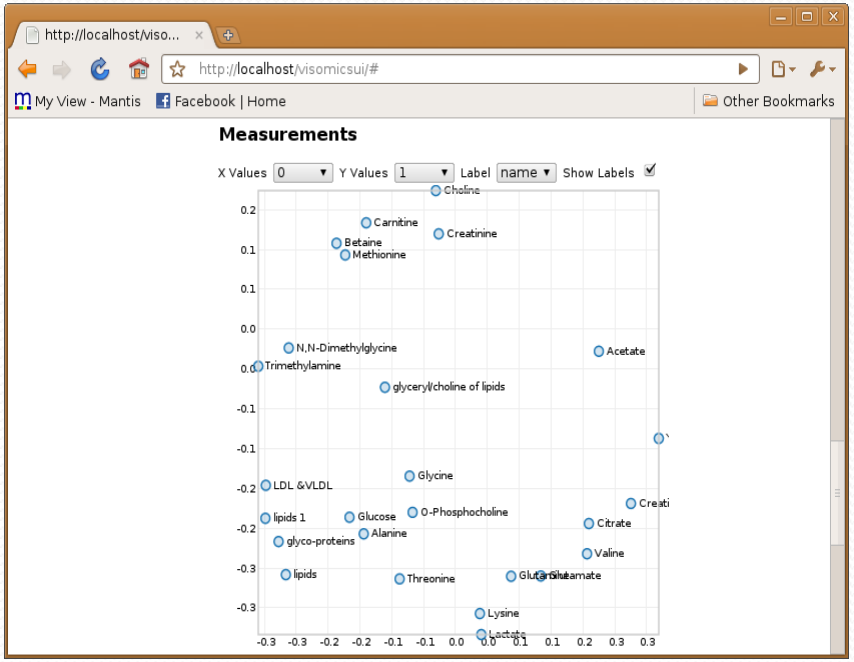

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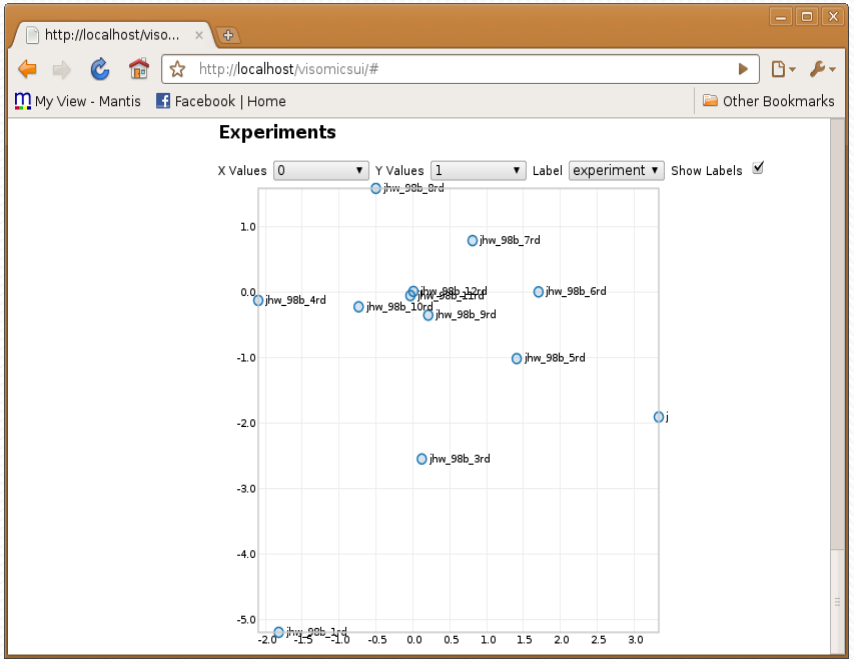

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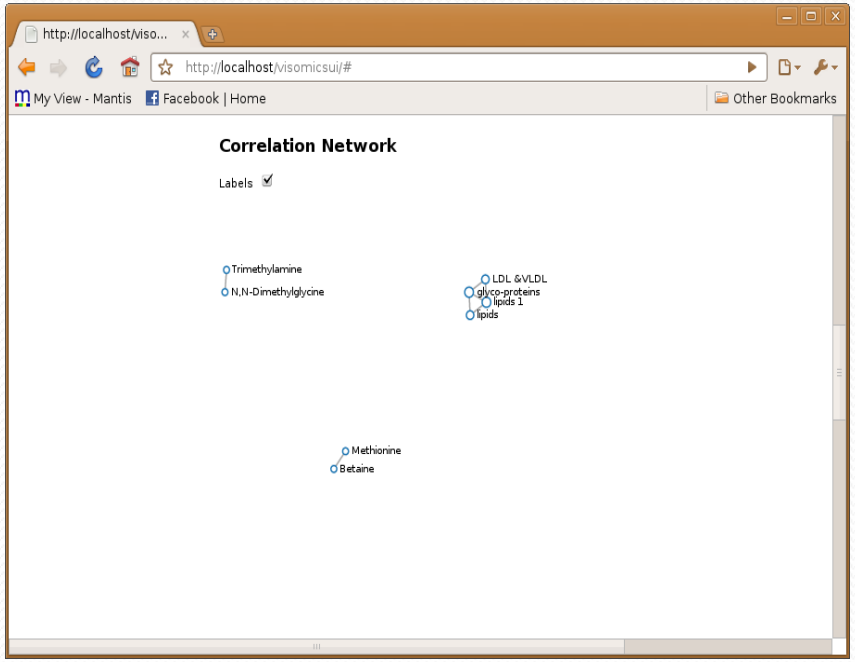

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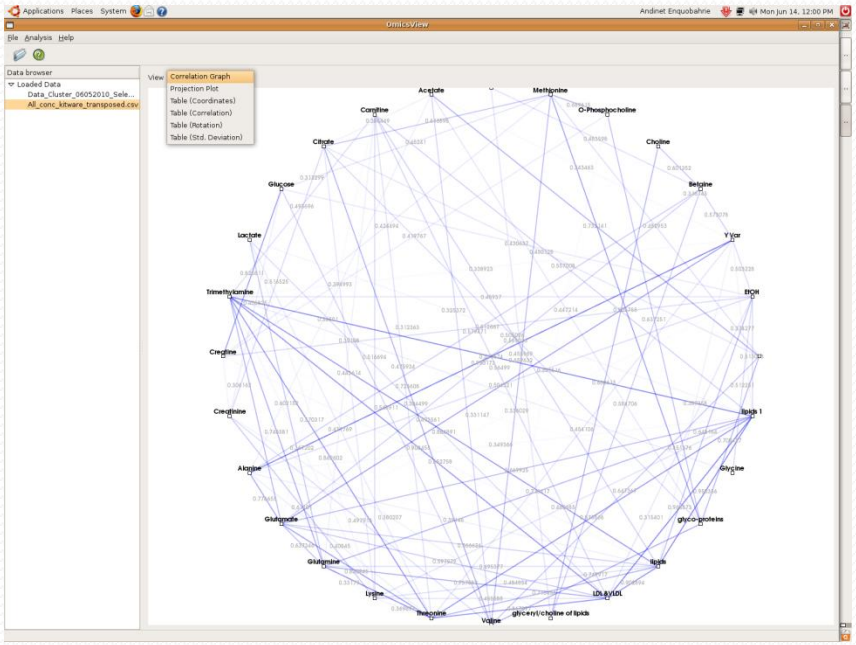
Desktop Version

- Still working on the hooks and automation.
  - R
  - QT
  - VTK
  - Titan



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