

SC22
Dallas, hpc
TX accelerates.

Enabling Catalyst Adoption in SPARC

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Outline

- Introduction
- Methodology
- Technical analysis
- Content analysis
- Conclusions and future work

Introduction

Catalyst:

- The in situ version of ParaView
- Has been accessible from several Sandia host codes for years
- Has demonstrated performance and scaling
- Has very few users at Sandia

Not the focus today:

- Performance and scaling
- Generalization to other user communities, other in situ approaches, or other in situ software

The objective of this work is to increase the adoption of Catalyst by SPARC analysts

pvpython workflow

Current ParaView scripting workflow:

- 1) Develop pipeline in Paraview, postprocessing results from a “nearby” simulation
- 2) Export python script
- 3) Modify script as needed for actual simulation

Exporting a script from the GUI will always be useful:

- Basic structure, starting point
- Snippets of code
- Tool to learn pvpython

- This workflow essentially leverages the GUI to address the usability of the scripting interface.
- If you have results from a nearby simulation, it might be the preferred approach.

How easy is it to modify the script for your simulation with Catalyst?

With confidence that it will work?



Methodology: Use Cases

This is a “bottom-up” approach

- Use Cases are **concrete** examples of **analyst** tasks that are used to identify **specific** issues
- **Recurring** specific issues indicate **general** issues

Some use cases will be adapted to provide Catalyst training on the SPARC Analysts

We interviewed 8 analysts across 8 walkthroughs

We very much appreciate the analysts' participation and feedback!

Use Cases

Image Generation

- Flowfield images (1)
- LES images (4)

Data Extraction

- LES diagnostics (5)
- Lineouts (6)

Data Manipulation

- Sectional Loads (2)
- Base pressure correlations (3)

In this presentation we only consider the Image Generation use cases

Use Case Walkthroughs (Think-Aloud Protocol)

1. Development

- SME Greg Weirs developed the Paraview steps to produce the desired output
- SME developed Analyst Instructions
- SME identified bugs and usability issues while determining the steps

2. Walkthrough Interview

- Analyst works through the instructions during the walkthrough interview with SME
- Analysts identify bugs and usability issues, provide feedback, and ask questions

3. UUA Content Analysis

- Project team reviews video and transcript of interview
- Identifies analyst statements and applies coding
- Analysis of coded data



Technical Analysis:
Specific Catalyst and
pvpython bugs and usability
issues

Content Analysis:
Factors enhancing or limiting
Catalyst adoption

UX Objectives and Approach

OBJECTIVES:

- 1) identify usability barriers in Catalyst and its Python scripting interface
- 2) develop recommendations to incentivize adoption

APPROACH

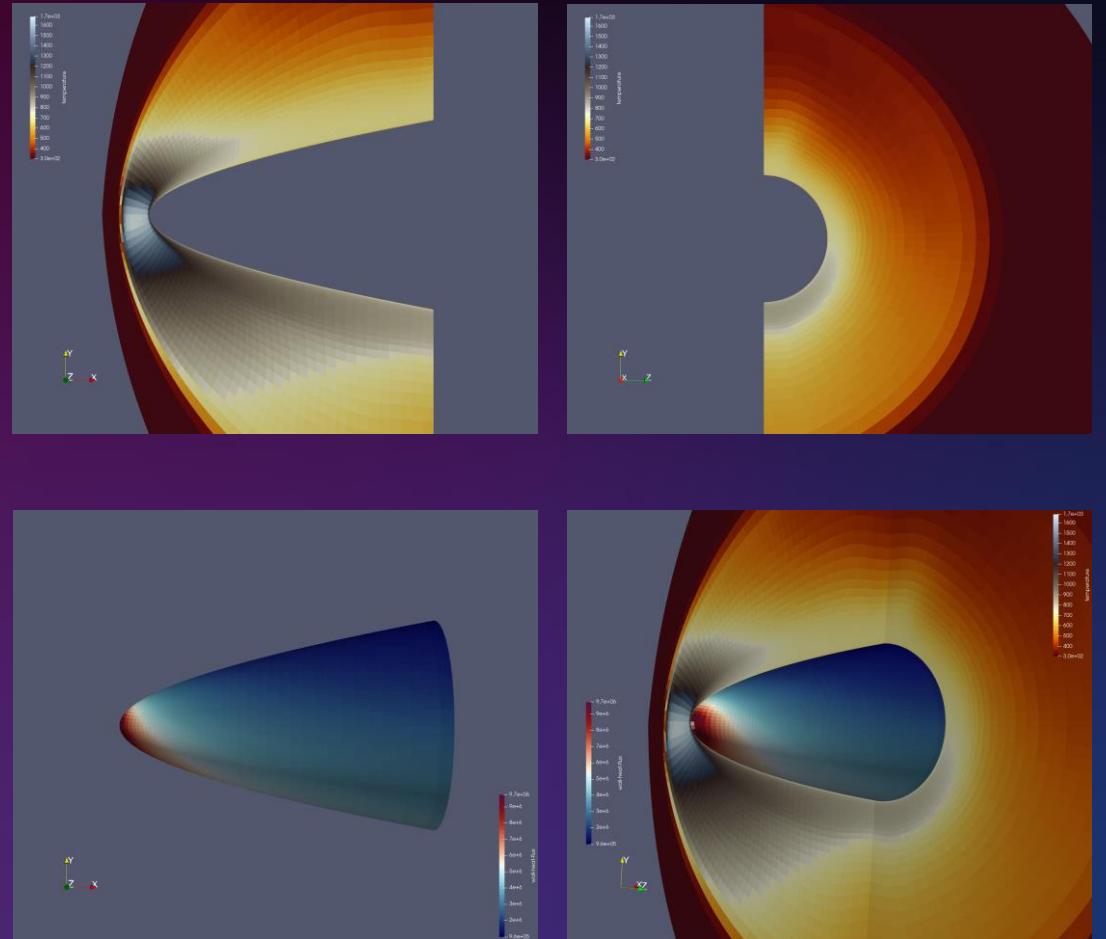
- Corroborate and/or identify UUA barriers via data manipulation requirements of 4-5 case studies (scenarios)
- Apply *discount usability engineering* (IEEE Software, 12,1,98-100; Nielsen, 1995)
- Conduct 4-5 *think aloud verbal protocol* with analysts/developers (Lewis, 1982)
- Capture audio/screen recording and transcription of Catalyst/Paraview workflow while user performs think aloud protocol, follow-up as needed with *task walkthrough* (Greenberg, 2003)
- Document observations and use case workflow
- Perform *content analysis* methodology for further data set exploration

Example Dataset: SPARC Test Vehicle

- Flow conditions:
 - Mach 5, sea level
 - 10° angle of attack
 - Perfect gas model, RANS
- Provides:
 - Flowfield Data (Volume)
 - Wall Data (Surface)
- SPARC simulation
 - 18 cores on 1 node of CTS-1
 - About an hour (near separation on lee side)

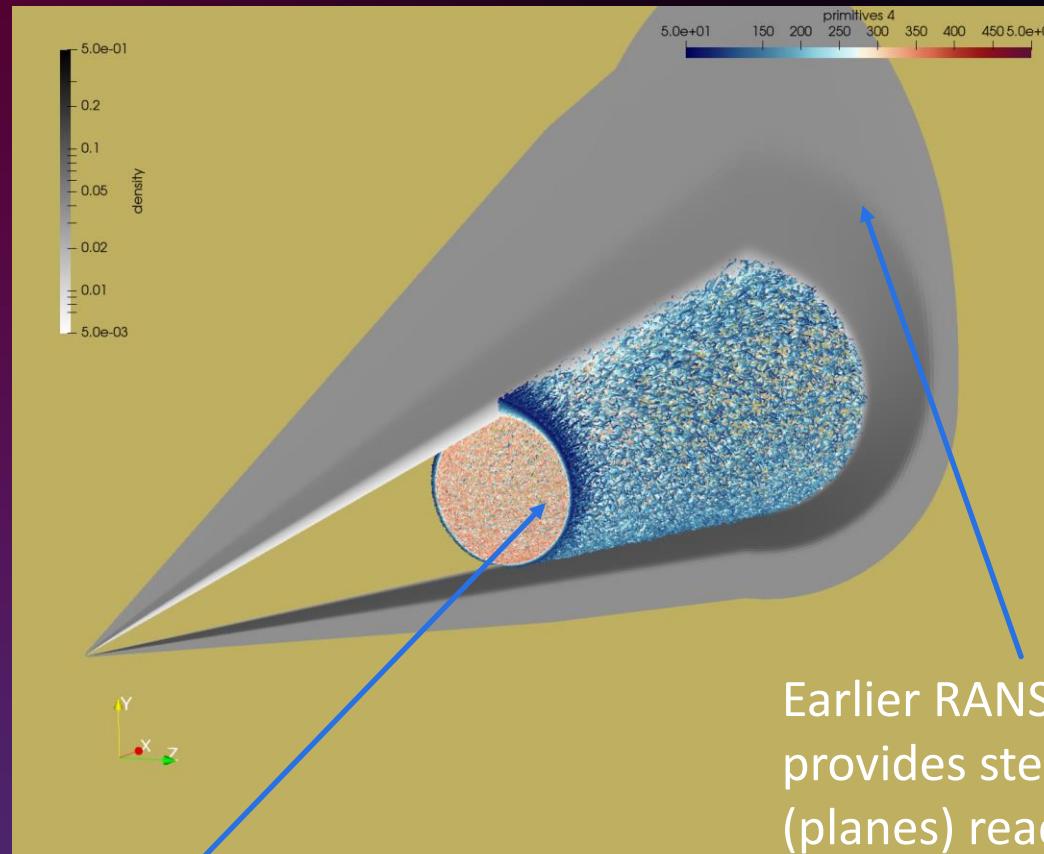
This dataset is used for all Use Cases
except the LES cases

Images generated by Catalyst



Example Dataset: LES of Flow Over a Cone

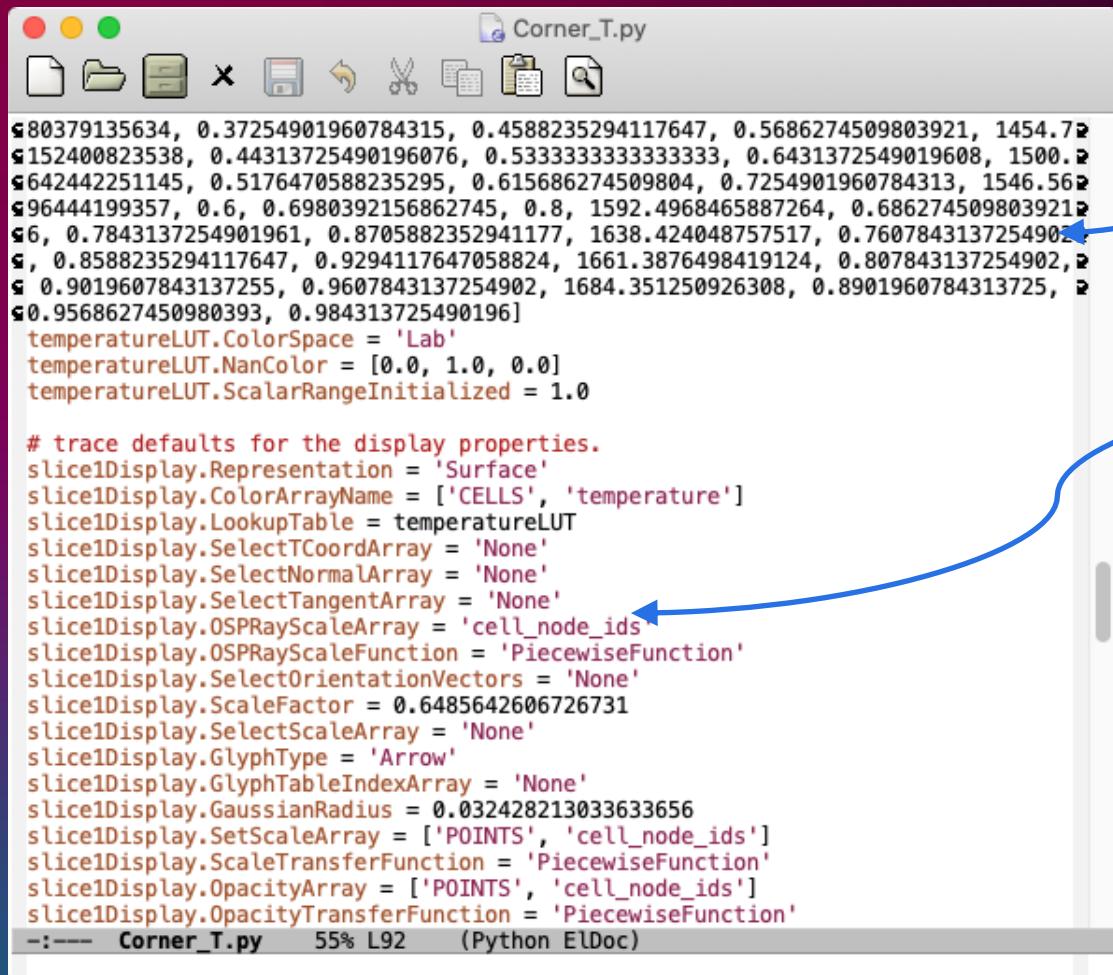
- Flow conditions:
 - Mach 8, 5000ft altitude
 - 6° angle of attack
 - Perfect gas model, LES
- LES provides, in situ:
 - Transient flowfield
 - data
- RANS provides, from files:
 - Steady state flowfield data
- SPARC simulation
 - 3600 cores on 100 nodes of CTS-1
 - About 24hrs to go through startup transient, significantly less to take turbulence statistics



LES simulation provides fine-scale data near cone surface

Earlier RANS simulation provides steady state data (planes) read from files

Exported scripts are verbose



```
Corner_T.py
80379135634, 0.37254901960784315, 0.4588235294117647, 0.5686274509803921, 1454.72
152400823538, 0.44313725490196076, 0.5333333333333333, 0.6431372549019608, 1500.0
642442251145, 0.5176470588235295, 0.615686274509804, 0.7254901960784313, 1546.56
96444199357, 0.6, 0.6980392156862745, 0.8, 1592.4968465887264, 0.686274509803921
6, 0.7843137254901961, 0.8705882352941177, 1638.424048757517, 0.7607843137254902
, 0.8588235294117647, 0.9294117647058824, 1661.3876498419124, 0.807843137254902,
0.9019607843137255, 0.9607843137254902, 1684.351250926308, 0.8901960784313725,
0.9568627450980393, 0.984313725490196]
temperatureLUT.ColorSpace = 'Lab'
temperatureLUT.NanColor = [0.0, 1.0, 0.0]
temperatureLUT.ScalarRangeInitialized = 1.0

# trace defaults for the display properties.
slice1Display.Representation = 'Surface'
slice1Display.ColorArrayName = ['CELLS', 'temperature']
slice1Display.LookupTable = temperatureLUT
slice1Display.SelectTCoordArray = 'None'
slice1Display.SelectNormalArray = 'None'
slice1Display.SelectTangentArray = 'None'
slice1Display.OSPRayScaleArray = 'cell_node_ids'
slice1Display.OSPRayScaleFunction = 'PiecewiseFunction'
slice1Display.SelectOrientationVectors = 'None'
slice1Display.ScaleFactor = 0.6485642606726731
slice1Display.SelectScaleArray = 'None'
slice1Display.GlyphType = 'Arrow'
slice1Display.GlyphTableIndexArray = 'None'
slice1Display.GaussianRadius = 0.032428213033633656
slice1Display.SetScaleArray = ['POINTS', 'cell_node_ids']
slice1Display.ScaleTransferFunction = 'PiecewiseFunction'
slice1Display.OpacityArray = ['POINTS', 'cell_node_ids']
slice1Display.OpacityTransferFunction = 'PiecewiseFunction'
-:--- Corner_T.py 55% L92 (Python ElDoc)
```

Last entries of the the table
mapping temperature
values to colors

Representation
properties never set or
modified by the user

Verbosity is a barrier to usability
because the user cannot find the the
sections of the script to focus on

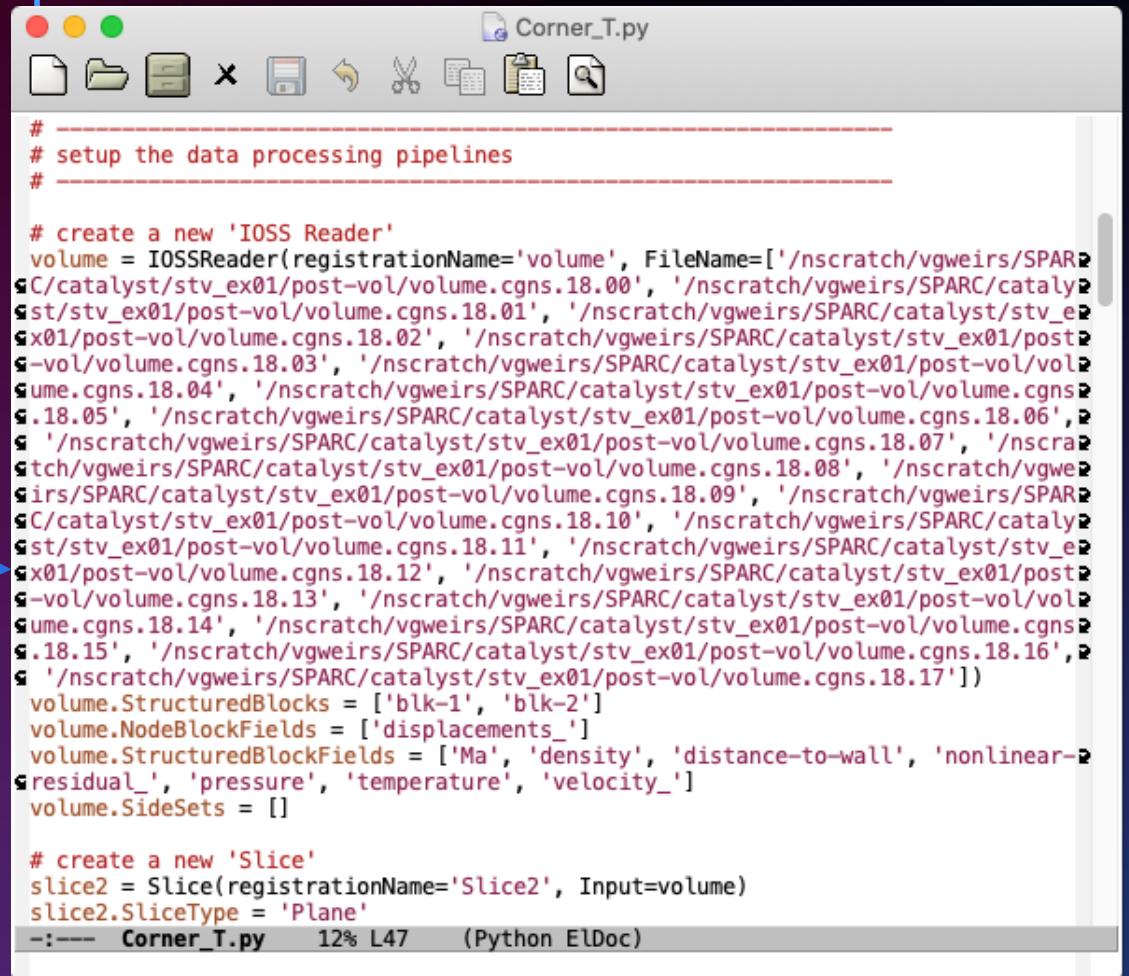
Exported scripts are dataset specific

Information was not explicitly entered;
most was determined automatically

- Filenames
- Blocks
- Variables

(This is a file reader that Catalyst would ignore, but the interactive and batch python clients use file readers.)

Specificity is a barrier to usability
when the intent is to modify the
script for a different dataset.



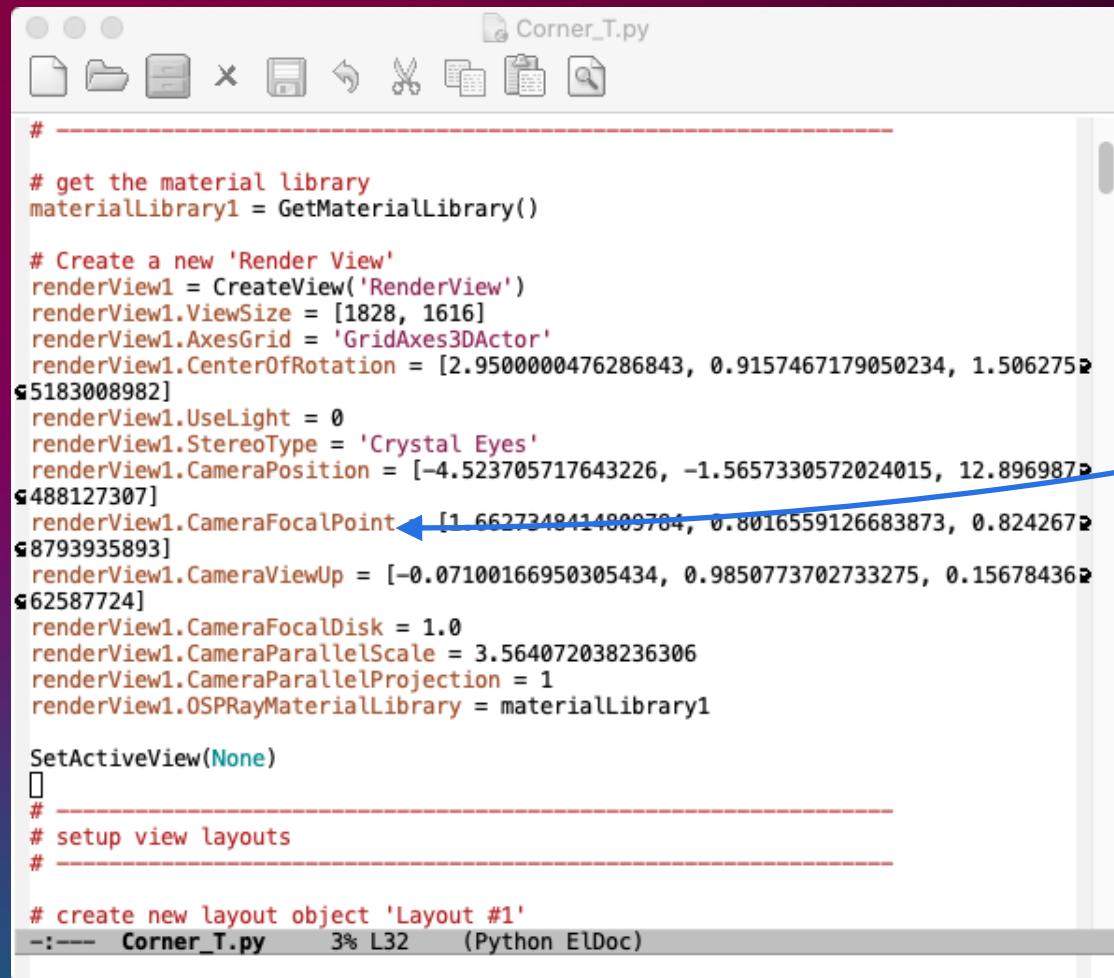
The screenshot shows a Python code editor window with the file 'Corner_T.py' open. The code is a script for data processing, specifically for a 'IOSS Reader'. It defines a 'volume' object with various properties and methods. The code is highly specific to the dataset 'volume.cgns.18.00' and its structure. A blue arrow points from the 'Variables' list in the text above to the 'volume' object in the code editor. The code editor interface includes a toolbar with icons for file operations, a status bar showing 'Corner_T.py 12% L47 (Python ElDoc)', and a vertical scroll bar on the right.

```
# -----
# setup the data processing pipelines
# -----

# create a new 'IOSS Reader'
volume = IOSSReader(registrationName='volume', FileName=['/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.00', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.01', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.02', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.03', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.04', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.05', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.06', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.07', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.08', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.09', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.10', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.11', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.12', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.13', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.14', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.15', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.16', '/nscratch/vgweirs/SPARC/catalyst/stv_ex01/post-vol/volume.cgns.18.17'])
volume.StructuredBlocks = ['blk-1', 'blk-2']
volume.NodeBlockFields = ['displacements_']
volume.StructuredBlockFields = ['Ma', 'density', 'distance-to-wall', 'nonlinear-residual_', 'pressure', 'temperature', 'velocity_']
volume.SideSets = []

# create a new 'Slice'
slice2 = Slice(registrationName='Slice2', Input=volume)
slice2.SliceType = 'Plane'
```

View (camera) properties are not intuitive



```
# get the material library
materialLibrary1 = GetMaterialLibrary()

# Create a new 'Render View'
renderView1 = CreateView('RenderView')
renderView1.ViewSize = [1828, 1616]
renderView1.AxesGrid = 'GridAxes3DActor'
renderView1.CenterOfRotation = [2.9500000476286843, 0.9157467179050234, 1.5062752
5183008982]
renderView1.UseLight = 0
renderView1.StereoType = 'Crystal Eyes'
renderView1.CameraPosition = [-4.523705717643226, -1.5657330572024015, 12.8969872
488127307]
renderView1.CameraFocalPoint = [1.6627348414809784, 0.8016559126683873, 0.8242672
8793935893]
renderView1.CameraViewUp = [-0.07100166950305434, 0.9850773702733275, 0.156784362
62587724]
renderView1.CameraFocalDisk = 1.0
renderView1.CameraParallelScale = 3.564072038236306
renderView1.CameraParallelProjection = 1
renderView1.OSPRayMaterialLibrary = materialLibrary1

SetActiveView(None)
()

# setup view layouts
()

# create new layout object 'Layout #1'

```

-:--- Corner_T.py 3% L32 (Python ElDoc)

A user could understand what these properties mean with a schematic

But they would still have a hard time adjusting the values without the GUI or a similar tool

Such properties reduce usability for any use besides archiving.

pypython Filters are concisely represented

While the Views and Representations (Displays) are not satisfactory, Filters and Extracts are clear and concise

- For quantitative analyses, Views and Representations are not needed
- If the GUI can generate clear code for Filters and Extracts, maybe its output for Views and Representations can be improved



```
# create a new 'Slice'
slice2 = Slice(registrationName='Slice2', Input=volume)
slice2.SliceType = 'Plane'
slice2.HyperTreeGridSlicer = 'Plane'
slice2.SliceOffsetValues = [0.0]

# init the 'Plane' selected for 'SliceType'
slice2.SliceType.Origin = [2.95, 0.0, 0.0]

# init the 'Plane' selected for 'HyperTreeGridSlicer'
slice2.HyperTreeGridSlicer.Origin = [1.4417453155408007, 0.916163029237911, 1.512
16143433093596]

# create a new 'Slice'
slice1 = Slice(registrationName='Slice1', Input=volume)
slice1.SliceType = 'Plane'
slice1.HyperTreeGridSlicer = 'Plane'
slice1.SliceOffsetValues = [0.0]

# init the 'Plane' selected for 'SliceType'
slice1.SliceType.Origin = [0.0, 0.0, 1e-06]
slice1.SliceType.Normal = [0.0, 0.0, 1.0]

# init the 'Plane' selected for 'HyperTreeGridSlicer'
slice1.HyperTreeGridSlicer.Origin = [1.4417453155408007, 0.916163029237911, 1.512
16143433093596]

# -----
# setup the visualization in view 'renderView1'
# -----

# show data from slice1
slice1Display = Show(slice1, renderView1, 'GeometryRepresentation')

-:--- Corner_T.py 23% L84 (Python ElDoc)
```

Technical Findings for Image Generation

Representations and Views

- pypython scripts are verbose
- pypython scripts embed data-specific information

Auxiliary objects (e.g., color lookup tables)

- Explicitly specified when they could be referenced
- Embed dataset bounds
- Impractical to modify directly

Image extracts should be rethought:

- Appearance in the pipeline browser is misleading;
View state is saved, not pipeline state
- Likelihood of clobbering previous extracts is high
- No mechanism for multiple views in a single image

Image Generation Summary

- Analysts have started using Catalyst for image generation;
usability issues are inconveniences
- Generally, issues identified have straightforward solutions
- Required improvements are in the details, implementation, and testing, rather than conceptual

UUA Content Analysis

- For each walkthrough, each member of the project team reviewed the video and transcript
- Analyst statements relevant to usability and adoption were identified and coded
- Coding: interpreting analysts statements and assigning them to a single category

Characteristics of Innovations

E. M. Rogers, 1995, *Diffusion of Innovations*, pg. 15-17.

Relative Advantage

The degree to which an innovation is perceived as better than the idea it supersedes. The greater the perceived relative advantage of an innovation, the more rapid its rate of adoption will be.

Compatibility

The degree to which an innovation is perceived as being consistent with the existing values, past experiences, and needs of potential adopters.

Complexity

The degree to which an innovation is perceived as difficult to understand and use. New ideas that are simple to understand are adopted more rapidly than innovations that require the adopter to develop new skills and understandings.

Trialability

The degree to which an innovation may be experimented with on a limited basis. An innovation that is trialable represents less uncertainty to the individual who is considering it for adoption, as it is possible to learn by doing.

Observability

The degree to which the results of an innovation are visible to others. The easier it is for individuals to see the results of an innovation, the more likely they are to adopt it.



UUA Content Analysis - Results

Use Case	Relative Advantage	Compatibility	Complexity	Trialability	Observability
Image generation					
(1) Flowfield	26	62	48	49	14
(4) LES images	6	33	16	31	3

Data is coarse; don't try to draw fine distinctions

- 2 walkthroughs for use case (1), 1 for use case (4)
- Each analyst is unique
- Coders (analyzing transcripts) are also unique, with varied backgrounds

- Compatibility: analysts see how Catalyst fits in their existing workflow
- Trialability: analysts find it easy to experiment with Catalyst to learn how to use it
- Complexity: Following a Catalyst script is ok, but significant modification is more daunting
- Relative advantage: Catalyst offers something better than their existing solution
- Observability: Analysts have heard of or seen Catalyst being useful for others so they would pursue it

Data for Image Generation UUA Analysis

*Raw data from Teams's automated voice-to-text transcription of collegial, informal conversations – please don't judge our grammar too harshly!

- Some components of it, I -- I think you're right, where it would be more valuable to be able to dig into the Python script. But in term of, um, you know, setting -- **setting up a script, hooking it to SPARC and all that, it seems, uh, pretty well streamlined.** (trialability)
- Yeah, process-wise, I think it's, yeah, I think it's, uh, very -- very useful. (compatibility)
- So, if you just had the -- a catalyst input file, we could tack on to, um, example one or two in the SPARC examples. That would just be another place for people just to pull down an example that they can just hit "go" on, and it'll -- and Catalyst will work. (trialability)
- **My initial reaction is everything was relatively painless... .** The syntax changes are very straightforward in the input file. (complexity)
- In a lot of those instances...we want high frequency images, say, to make movies..but we might want to shed the data that is associated...we don't want terrabyte size files. (observability)

Conclusions

- For Visualization, we have identified a number of Catalyst and pypython usability issues but are confident they can be addressed
- Analysts are interested in adopting Catalyst for the capabilities it provides; several walkthrough analysts are already adopting Catalyst in their production workflows
- Direct engagement with end users takes time, but provides invaluable information for increasing software adoption

Next Steps

Grow Catalyst user base with Visualization and accessible Quantitative Analysis

- Remaining SPARC/Catalyst production readiness issues will be easier to identify with a user community
- Develop SPARC/Catalyst training – we have already discussed this with the SPARC team
- Extend Catalyst adoption to other host codes: SIERRA SM/SD (solid mechanics/solid dynamics)

With Kitware

- Catalyst API2.0 (leverages Conduit)
- Generate cleaner pvython scripts from ParaView
- Improve Image Extractors



Quantitative Analysis Path Forward

Different Solutions for Different Quantitative Tasks

