The Uintah – VisIt coupled workflow

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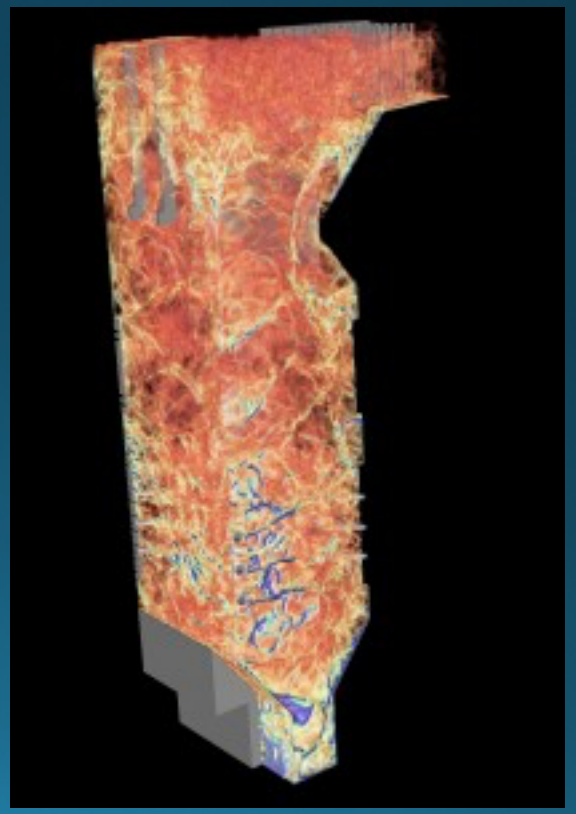
Uintah

- The Uintah software suite is a set of libraries and applications for simulating and analyzing complex chemical and physical reactions.
- http://www.uintah.utah.edu/projects.html



- **The Carbon-Capture Multidisciplinary Simulation Center –** exa-scale computing with V&V/UQ to more rapidly deploy a new technology for providing low cost, low emission electric power generation.

Uintah

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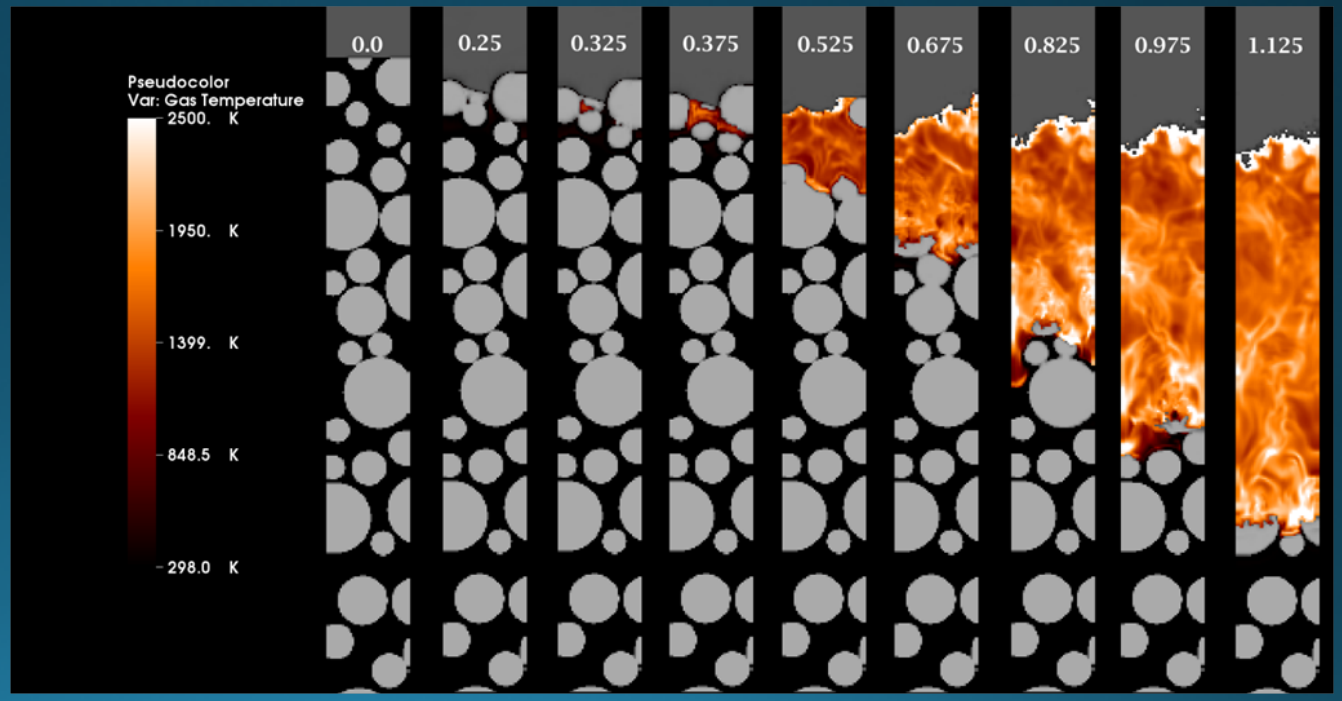
- **Multiscale Multidisciplinary Modeling of Electronic Materials Collaborative Research Alliance**



Uintah

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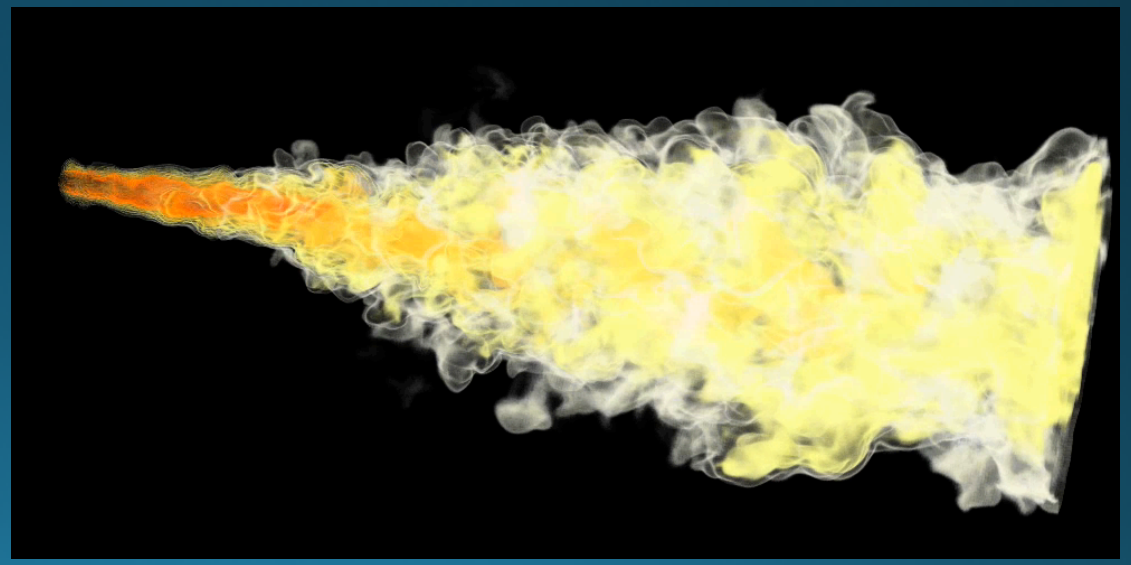
- **Clean Energy from Fossil Fuels –** model various energy technologies from traditional air-fired coal, oxy-fired coal/natural gas, fluidized bed coal combustion and coal gasification to more exotic coal technologies such as chemical looping and under ground thermal treatment.



VisIt – libsim

- Allows a connection between the application and VisIt via sockets.
  - Dynamically loads VisIt's runtime libraries that allows the simulation to act as VisIt's compute engine.
  - Uses a middle layer to move application data to VisIt.

- Using VisIt's libsim as part of the work flow for the:
  - **Runtime layer** where computer scientists develop and maintain infrastructure – i.e. memory, mpi scheduling.
  - **Application layer** where domain scientists develop and maintain the meshing and physics.
  - **User layer** where scientists visualization and analyze the simulation results.

VisIt – libsim

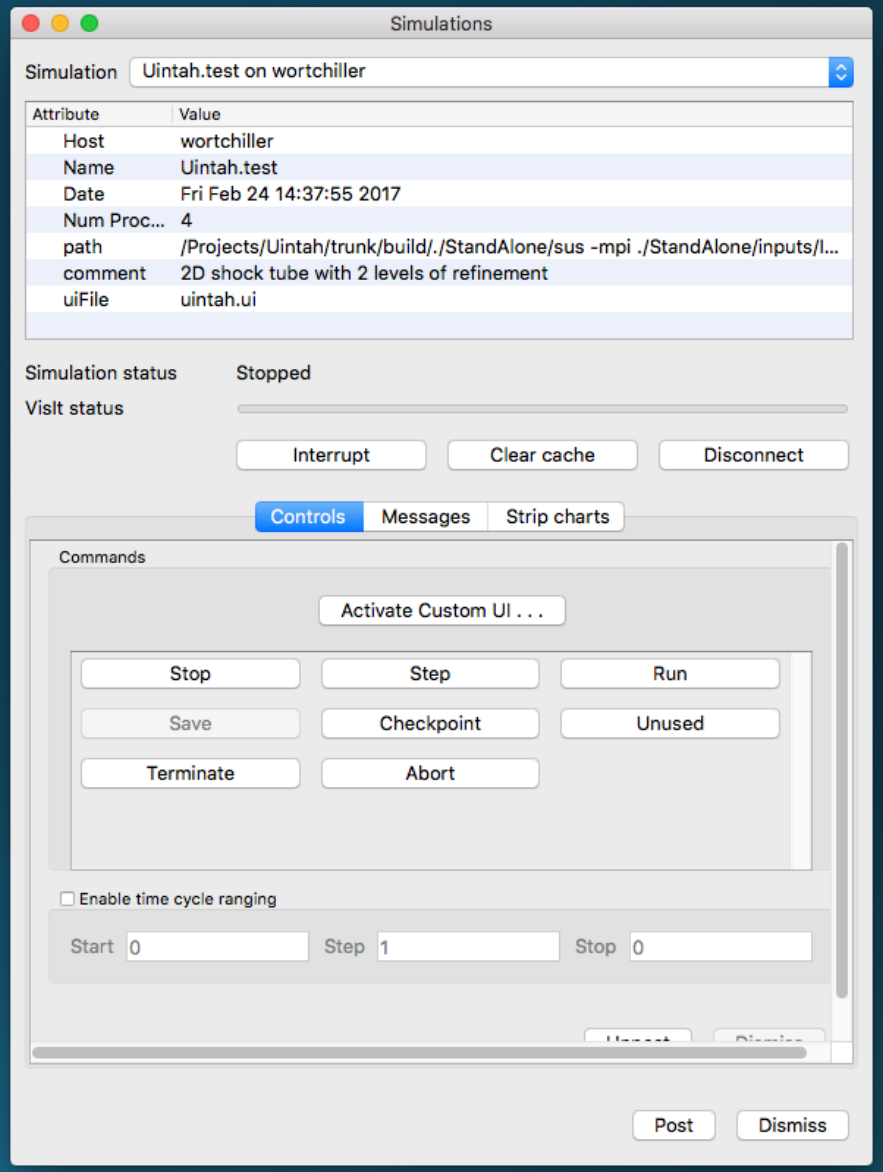
- VisIt's libsim provides for a custom UI
  - Qt based UI
    - Any Qt widgets may be used but VisIt must be able to handle the Signals and Slots.
      - Line Edits, Checkbox, Combobox, etc.
  - Custom UI becomes an application specific dashboard.
  - Setup by the application at runtime – can have different dashboards for different simulation types (though the application must support each dashboard).

VisIt – libsim

- Missing bits
  - Better connection to the simulation variables and the runtime performance values.
  - Simulation variables are global to the simulation and can be of the following:
    - Time based (time step)
    - Mesh based (AMR)
    - Problem spec (initial values, solution order)
    - Operational (output and dump file frequency)
    - Runtime analysis variables
  - Runtime performance values (memory, I/O, task time, mpi timimg)

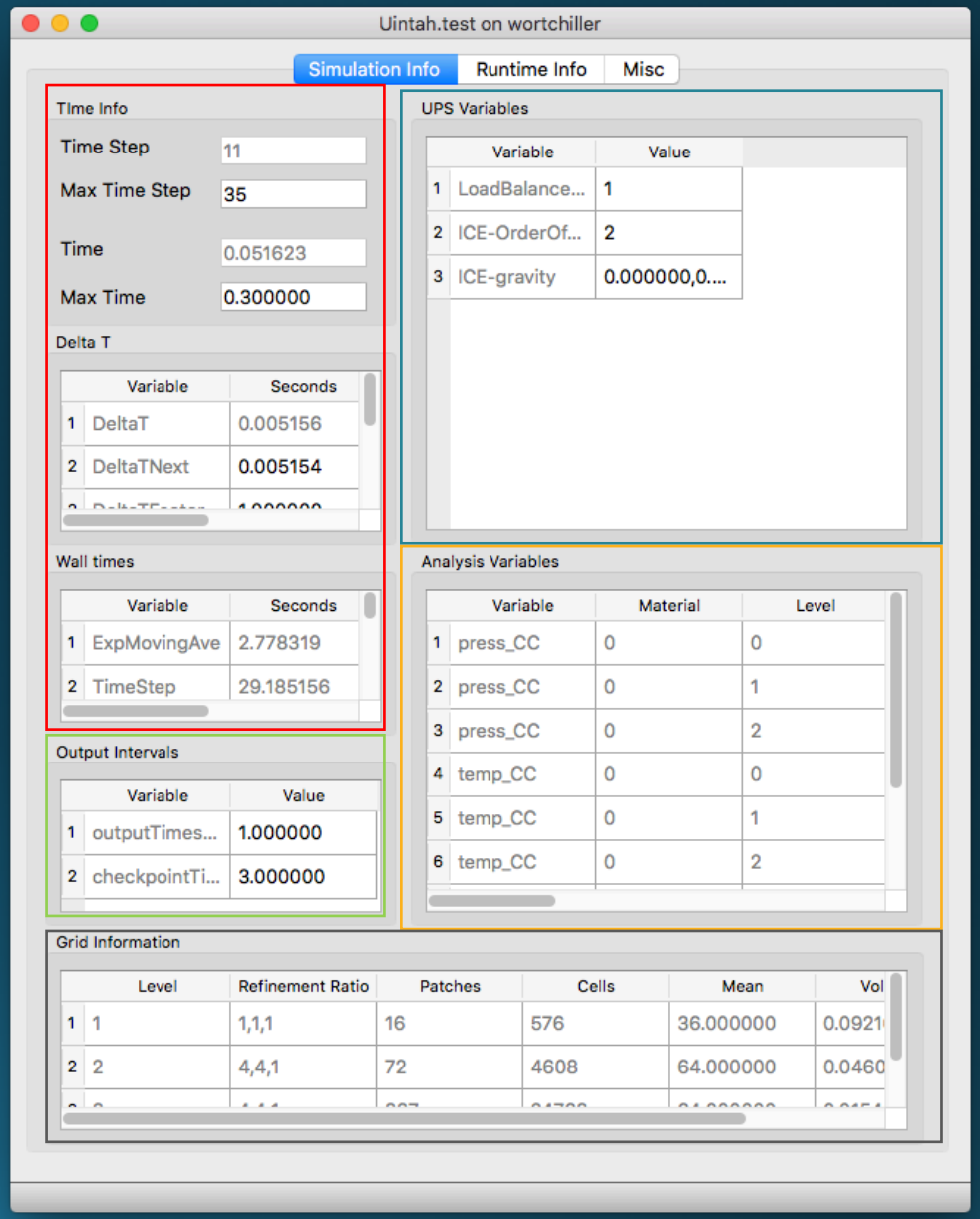
VisIt – libsim

- Simulation Window
  - Tabs are common to all simulations
    - Controls Tab
      - Commands are a unique to the application
      - Time cycle ranging now enabled.
    - Message Tab –
      - Reporting messages that might otherwise go application or error log files.
    - Strip Charts –
      - Global values over time.



Vislt – Custom UI

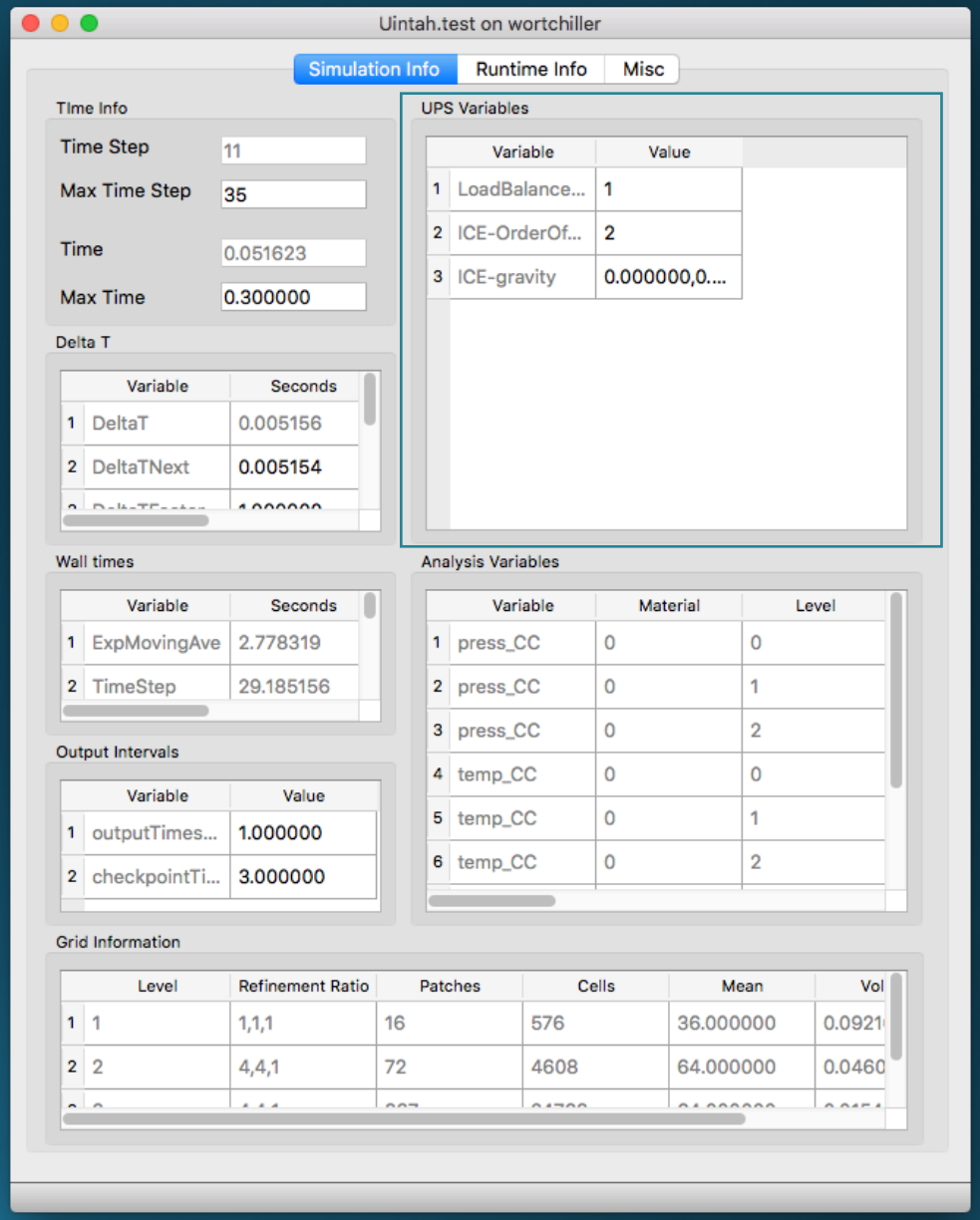
- Simulation dashboard
  - Time info
  - Output parameters
  - Grid information
  - UPS Variables
    - (Uintah Problem Specification)
  - User defined analysis



VisIt – Custom UI

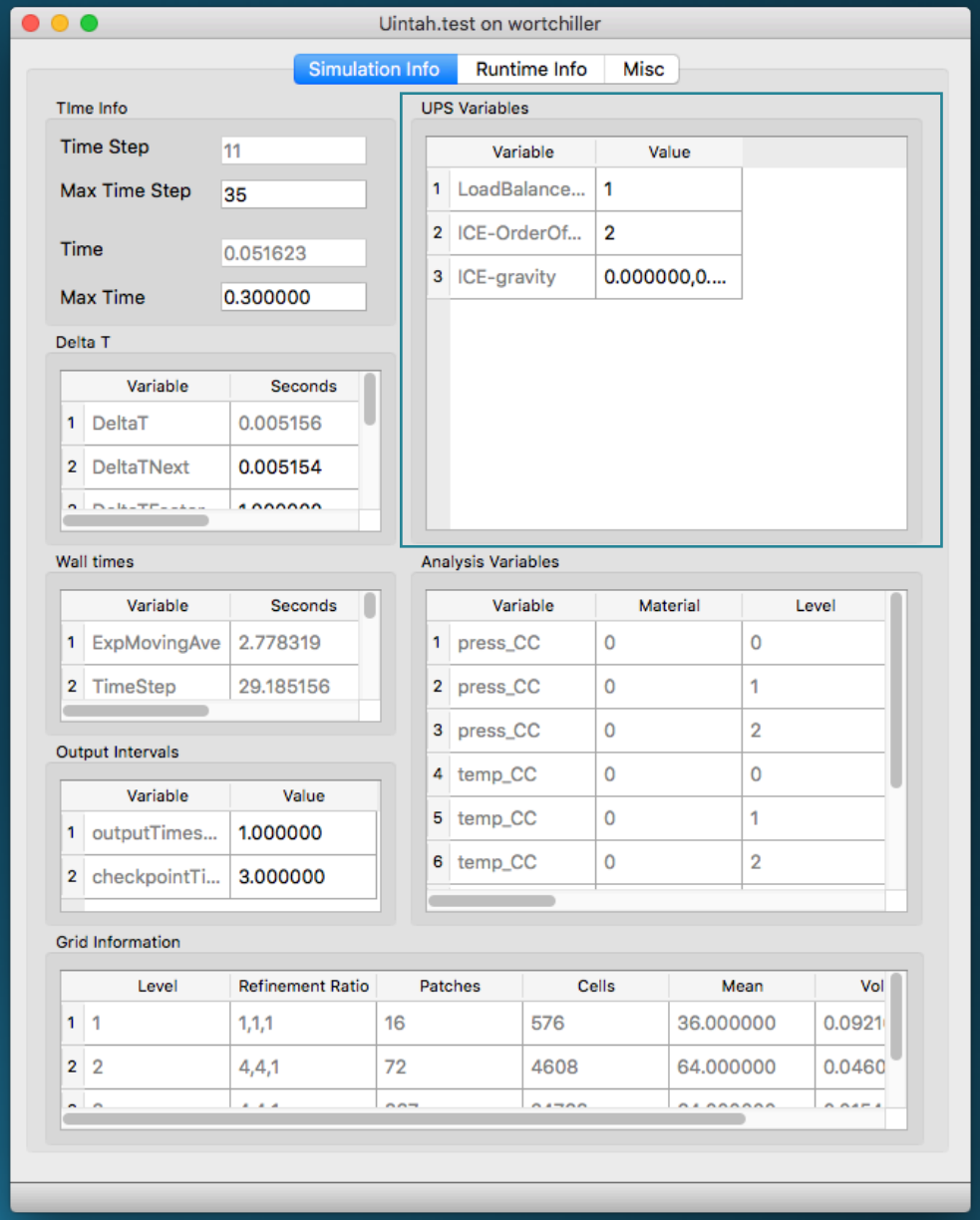
- Tables with generic variables uses a very lightweight structure to communicate between the application and libsim:

```
struct interactiveVar {
        std::string name;
        TypeDescription::Type type;
        int*    Ivalue;
        double* Dvalue;
        Vector* Vvalue;
        bool    modifiable; // If true the user may modify the value,
                            // otherwise it is read-only.
        bool    modified;   // If true the variable was modified by the
                            // user.
        bool    recompile;  // If true and the variable was modified force
                            // the task graph to be recompiled.
};
```



Vislt – Custom UI

- Application developer setups the structure at startup and inspects the structure before each time step execution.
  - Variable may require the task graph to be recompiled.
- Libsim callback is responsible updating pointer and modified flag.
- UPS Variables are generic across the application components.

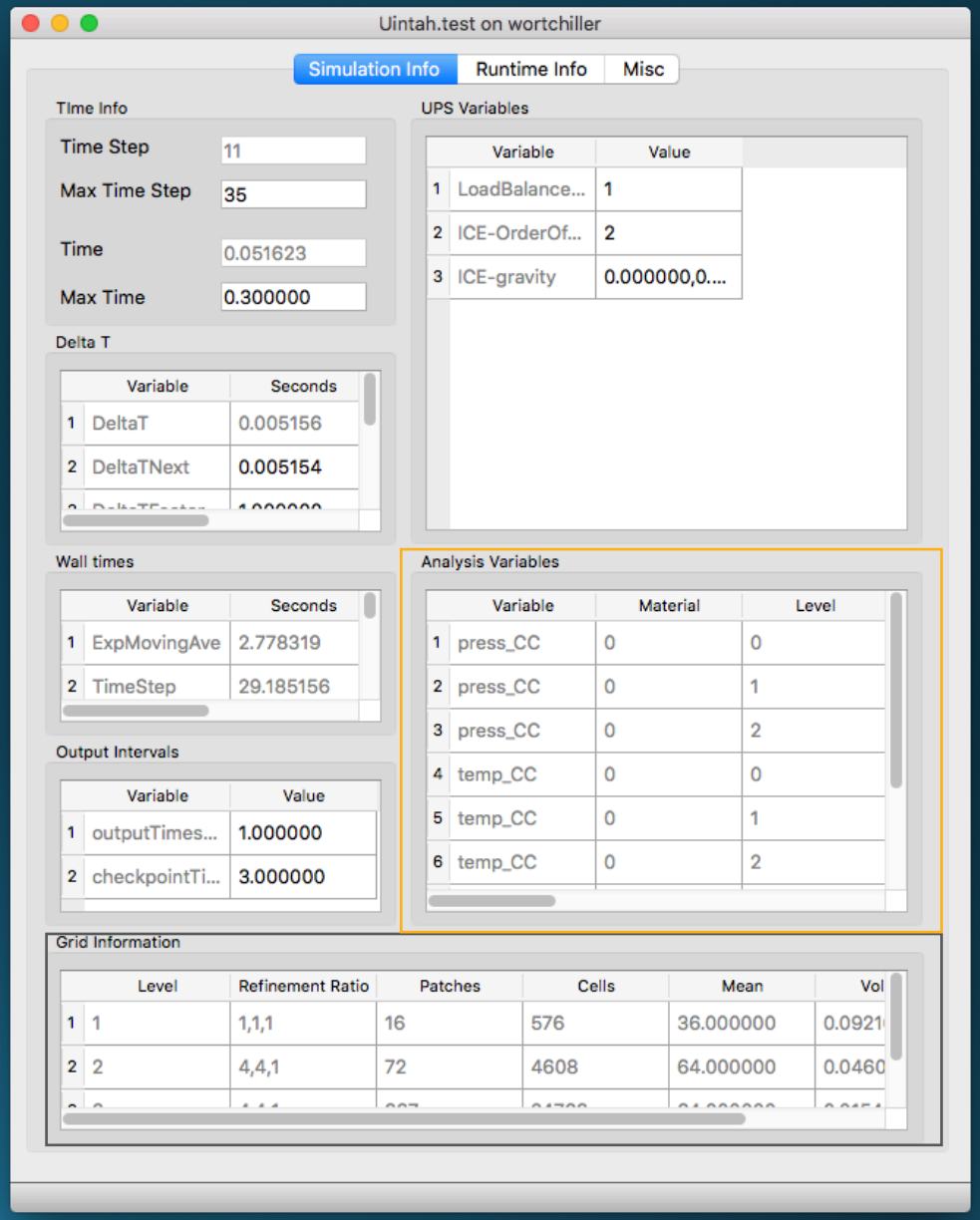


VisIt – Custom UI

- Tables with analysis variables uses a very lightweight structure to communicate between the application data archive and libsim:

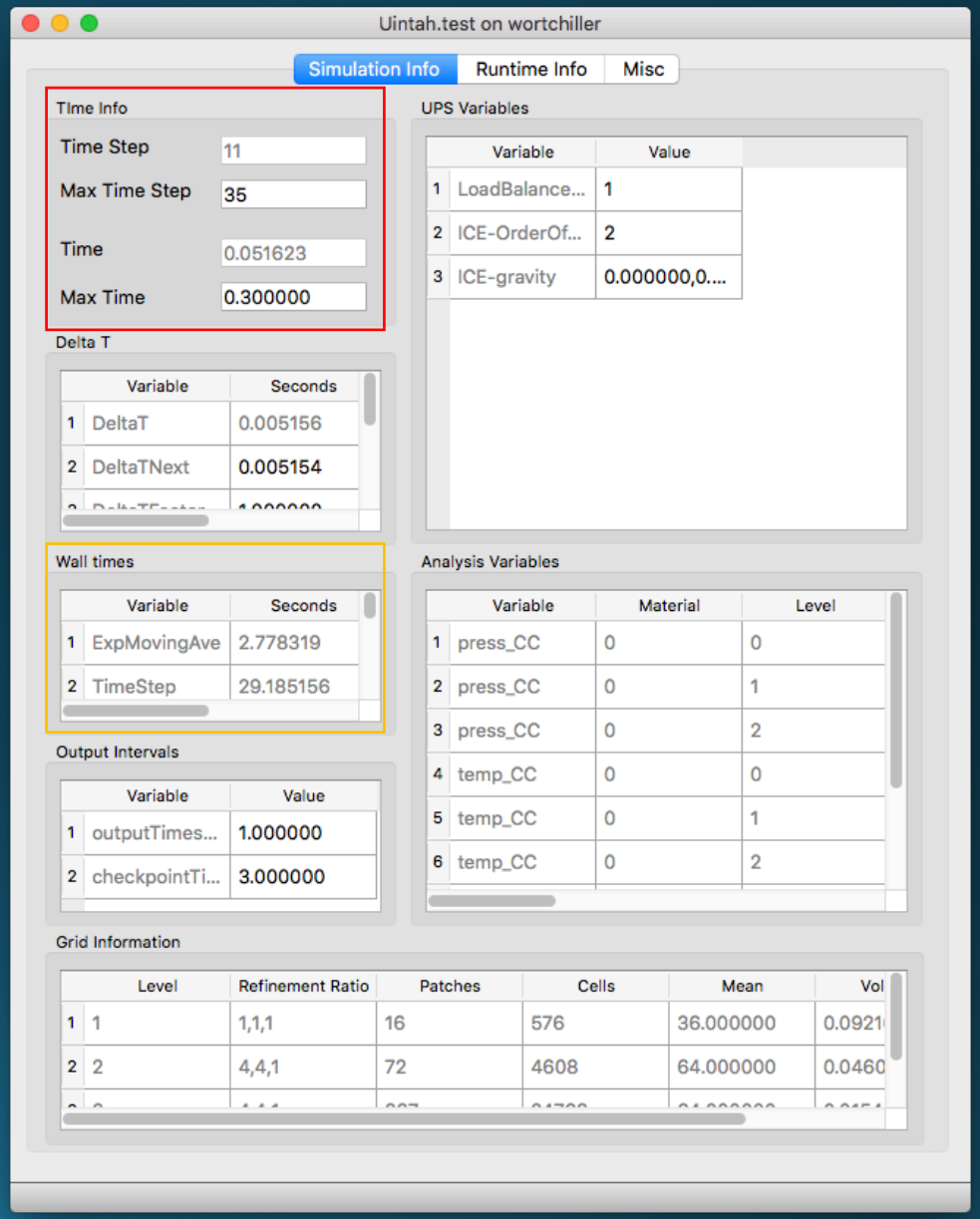
```
struct analysisVar {
        AnalysisType analysisType;
        VarLabel* label;
        VarLabel * reductionMinLabel;
        VarLabel * reductionMaxLabel;
        };
```

- Not yet generic to all analysis tools.
- Grid information – uses application grid information directly. AMR data is shared.



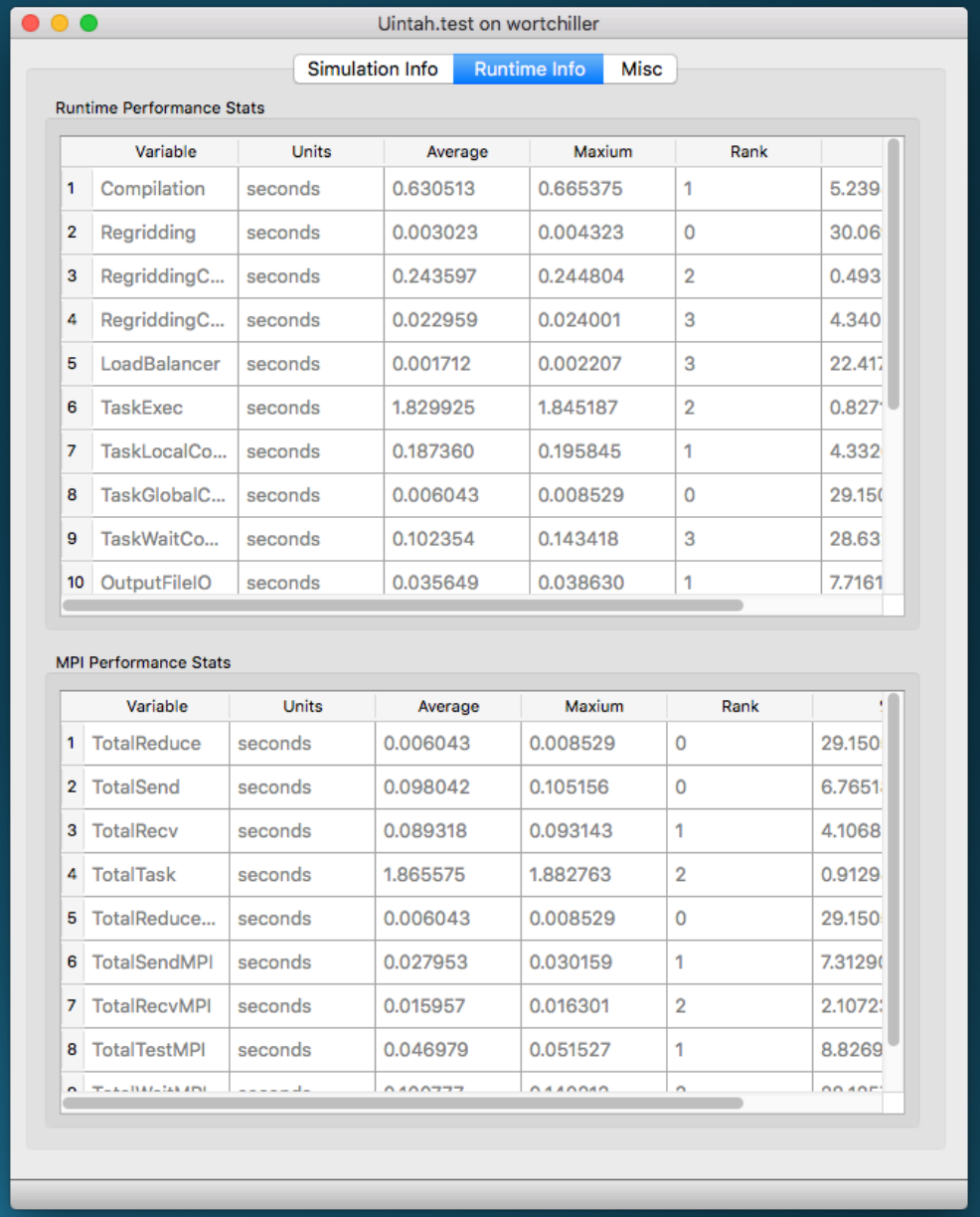
Vislt – Custom UI

- Simulation dashboard
  - Individual vs table variables.
    - Individual variables require their own callback methods.
    - Tables can be modified on the fly (i.e. as the simulation runs variables can be added or removed)
  - Variables are directly linked to the application or via access methods.
    - Can do computational steering



VisIt – Custom UI

- Runtime performance variables.
  - Uses a lightweight templated mapper class that holds:
    - The variable (a enumerated key value).
    - The value.
    - The variable name.
    - The variable units.
  - Application developer sees a std::map
    - Insert method is over ridden.
  - Derived type allows reductions for average value and maximal value with rank.
  - Mapper is shared with libsim.

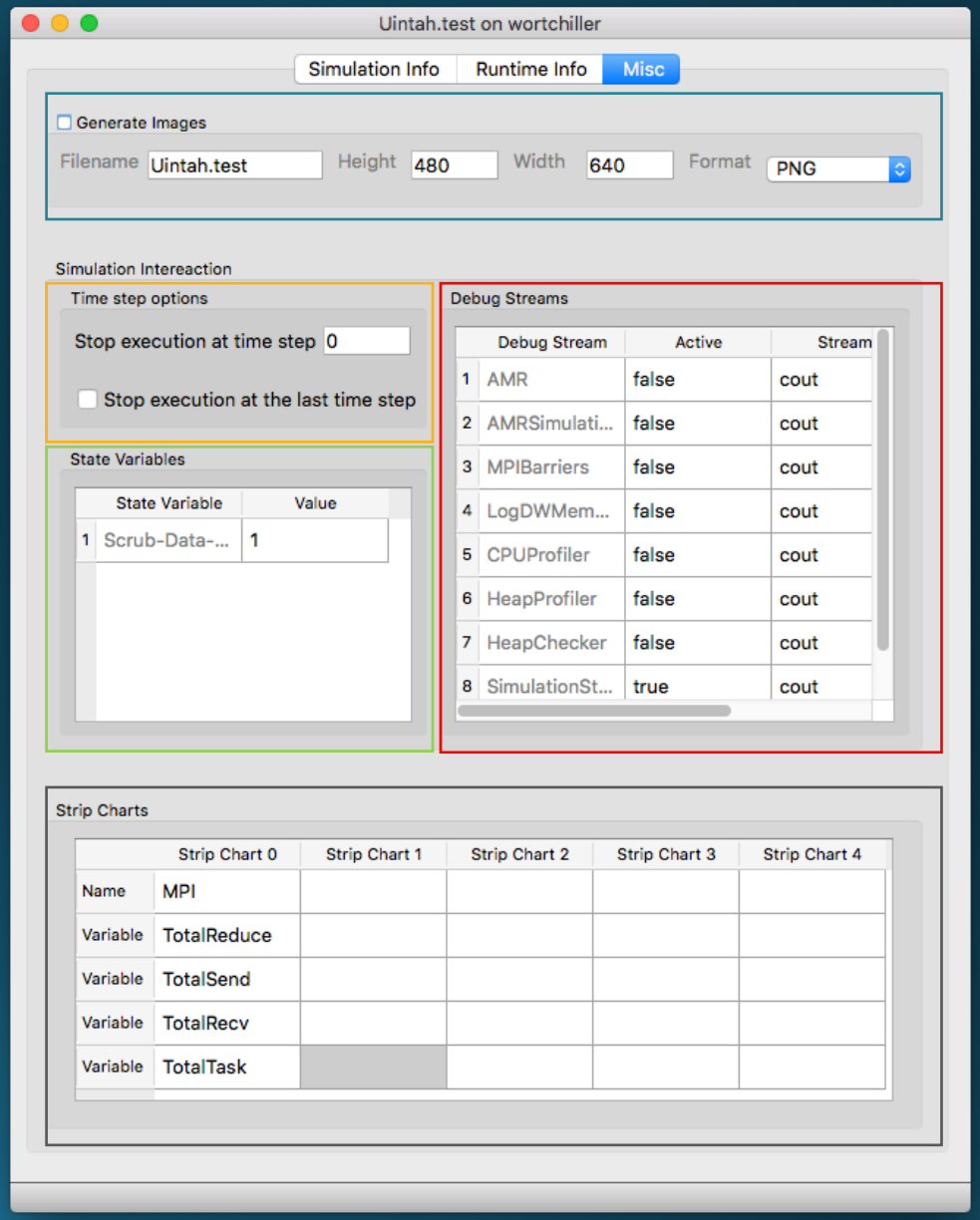


	Variable	Units	Average	Maxium	Rank	
1	Compilation	seconds	0.630513	0.665375	1	5.239
2	Regridding	seconds	0.003023	0.004323	0	30.06
3	RegriddingC...	seconds	0.243597	0.244804	2	0.493
4	RegriddingC...	seconds	0.022959	0.024001	3	4.340
5	LoadBalancer	seconds	0.001712	0.002207	3	22.41
6	TaskExec	seconds	1.829925	1.845187	2	0.827
7	TaskLocalCo...	seconds	0.187360	0.195845	1	4.332
8	TaskGlobalC...	seconds	0.006043	0.008529	0	29.15
9	TaskWaitCo...	seconds	0.102354	0.143418	3	28.63
10	OutputFileIO	seconds	0.035649	0.038630	1	7.7161

	Variable	Units	Average	Maxium	Rank	
1	TotalReduce	seconds	0.006043	0.008529	0	29.150
2	TotalSend	seconds	0.098042	0.105156	0	6.7651
3	TotalRecv	seconds	0.089318	0.093143	1	4.1068
4	TotalTask	seconds	1.865575	1.882763	2	0.9129
5	TotalReduce...	seconds	0.006043	0.008529	0	29.150
6	TotalSendMPI	seconds	0.027953	0.030159	1	7.3129
7	TotalRecvMPI	seconds	0.015957	0.016301	2	2.1072
8	TotalTestMPI	seconds	0.046979	0.051527	1	8.8269

VisIt – Custom UI

- Nice to have features.
  - Generate image frames automatically
    - Used when data is too large to dump to disk.
  - Stopping the execution at specific time steps.
    - Useful for debugging
  - Global state variables
    - Controlling Data Warehouse intermediate variables – used for visual debugging.
  - Controlling debug streams.
    - Direct pointer link is shared with libsim.
  - Strips Charts
    - Allows for the monitoring of global values over the life time of the simulation.



VisIt – Libsim UI

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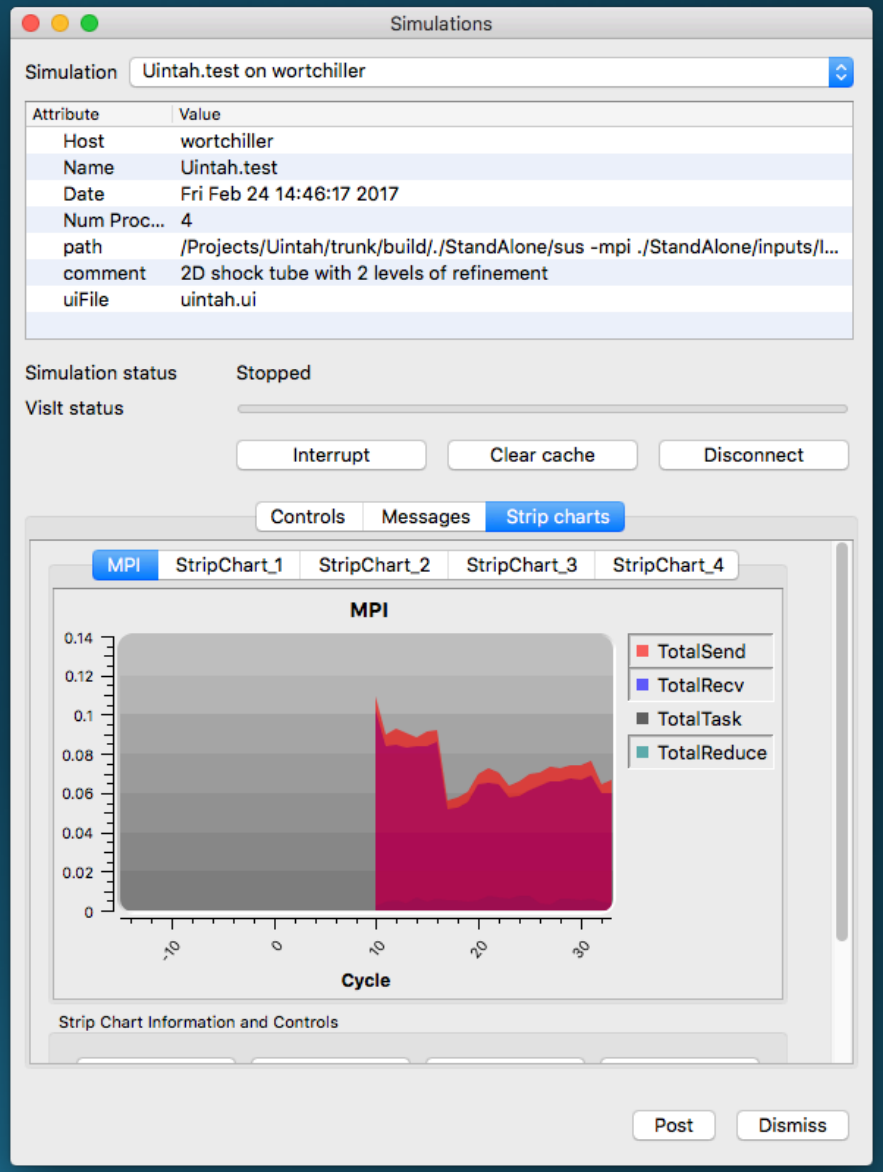
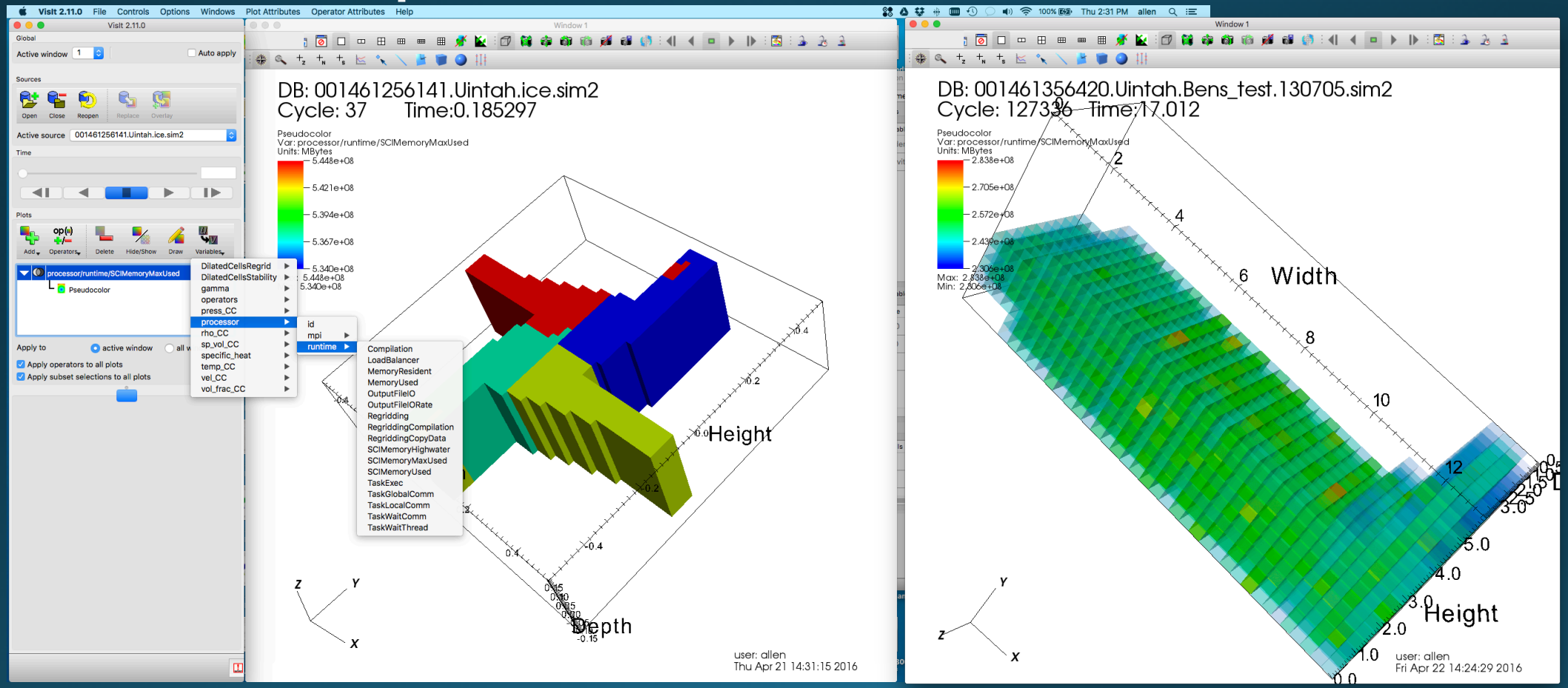


Uintah – VisIt coupled workflow

- Lightweight wrappers are key
  - Structures and methods that are on the application side and used by the application are preferred.
  - Qt Table very generic but not exactly the nicest UI.

- Wrappers are used by both the infrastructure and application scientists as part of development workflow.

Visualization of runtime performance values – processor based.



The Uintah – VisIt coupled workflow

- Documentation for developers and users:
  - http://uintah-build.sci.utah.edu/trac/wiki/VisitUintahInSitu

- Acknowledgements
  - Our many colleagues on the VisIt and Uintah teams.
  - This material is based upon work supported by the Department of Energy, National Nuclear Security Administration, under Award Number(s) DE-NA0002375.