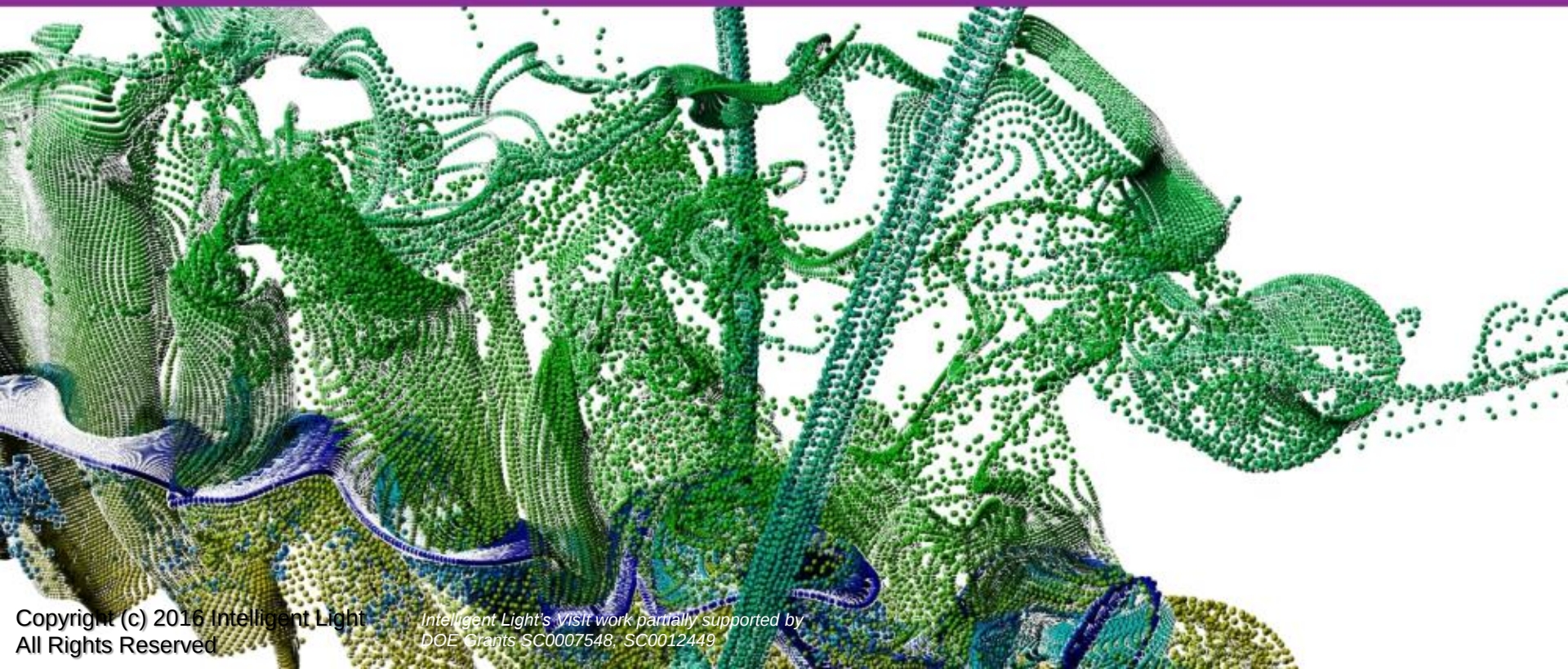
Applied Research Group

Seeking Answers, Deploying Solutions

Intelligent Light



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IN SITU PRODUCTION OF EXTRACT DATABASES FOR VISUALIZATION

WOIV 2016

Brad Whitlock & Earl P. N. Duque

Intelligent Light

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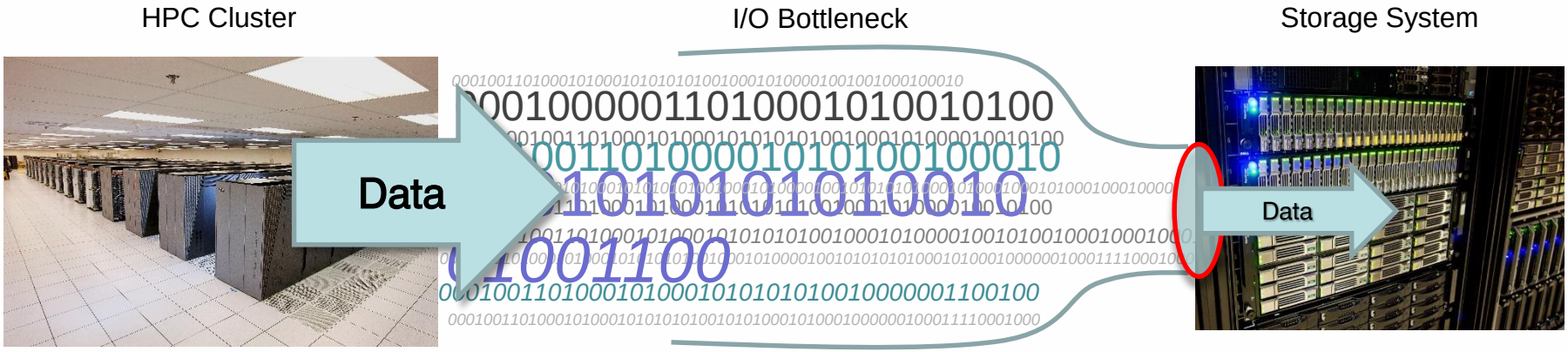
Problems of Running at Large Scale

- Simulations generate volumes of data that are impractical to write due to time and storage constraints
- A common workaround is to save data less frequently
  - Low temporal resolution
  - Possibly difficult to interpret
  - Possibly lost science
- Post-processing is also I/O intensive and slow



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Libsim puts VisIt in situ

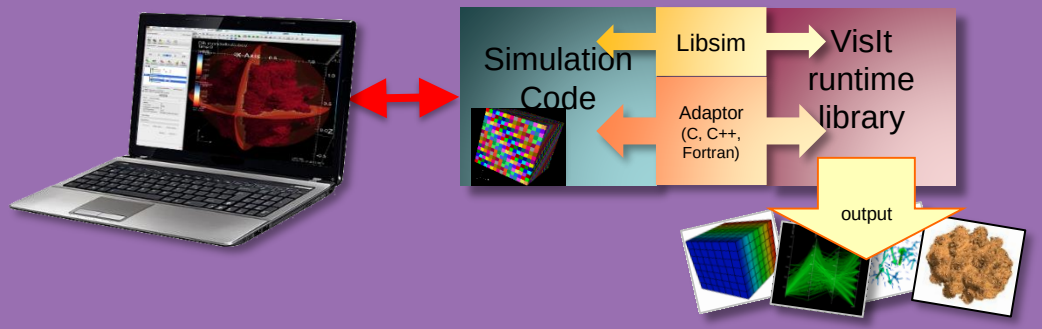
- VisIt provides Libsim, a library that simulations may use to let VisIt connect and access their data
- Avoids I/O and data movement
- Supports automated data product generation
- Also supports user-driven exploration of simulation data

VisIt

- Versatile open source software for visualizing and analyzing petascale simulation datasets

Libsim

- Enables simulations to perform data analysis and visualization in situ by applying VisIt algorithms to data.



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In Situ Extracts Workflow

- Use Libsim to instrument simulation so it produces surface extracts in FieldView

Extracts overcome in situ's greatest perceived weakness
– *that you need to have some idea of what you want to see in the end*

- Permits interactive exploration using post-processing methods
- Cheap enough to save frequently

In situ extracts produced | In situ extracts | In situ extracts visualized

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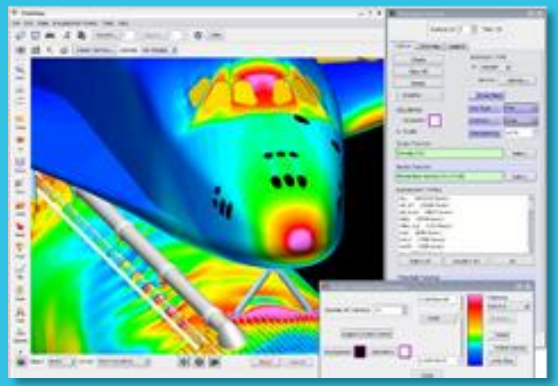
Extract Generation is Decoupled from Visualization

- Extract visualization can run on separate compute resources
- Fewer cores can be allocated
- Users can leverage their preferred visualization software

FieldView

- Sold for CFD post-processing since 1991
- Over 3000 licenses of FieldView in use today throughout the world
- Industries ranging from aerospace and automotive to nuclear engineering, turbomachinery, wind energy and food processing



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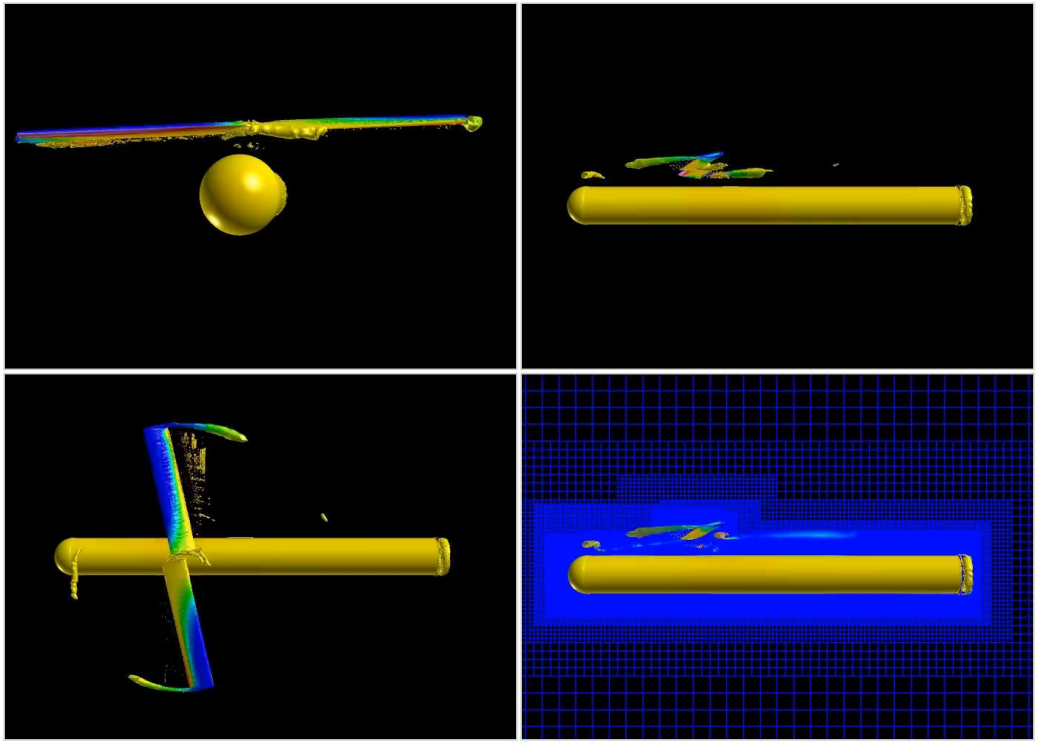
CREATE-AV Kestrel

- Fixed-wing air vehicle simulation suite
- Unstructured and AMR geometries
- Extract overhead 2-3% of solver runtime to output isosurface and slice extracts to classic XDB format on 1024 cores
  - Writing volume data at same frequency would take 30% of runtime
- Extracts 21x smaller (427Mb vs 9.1Gb)



B. Whitlock, J.R. Forsythe, S. M. Legensky *"In Situ Infrastructure Enhancements for Data Extract Generation"*, AIAA SciTech, January 2016, San Diego, CA

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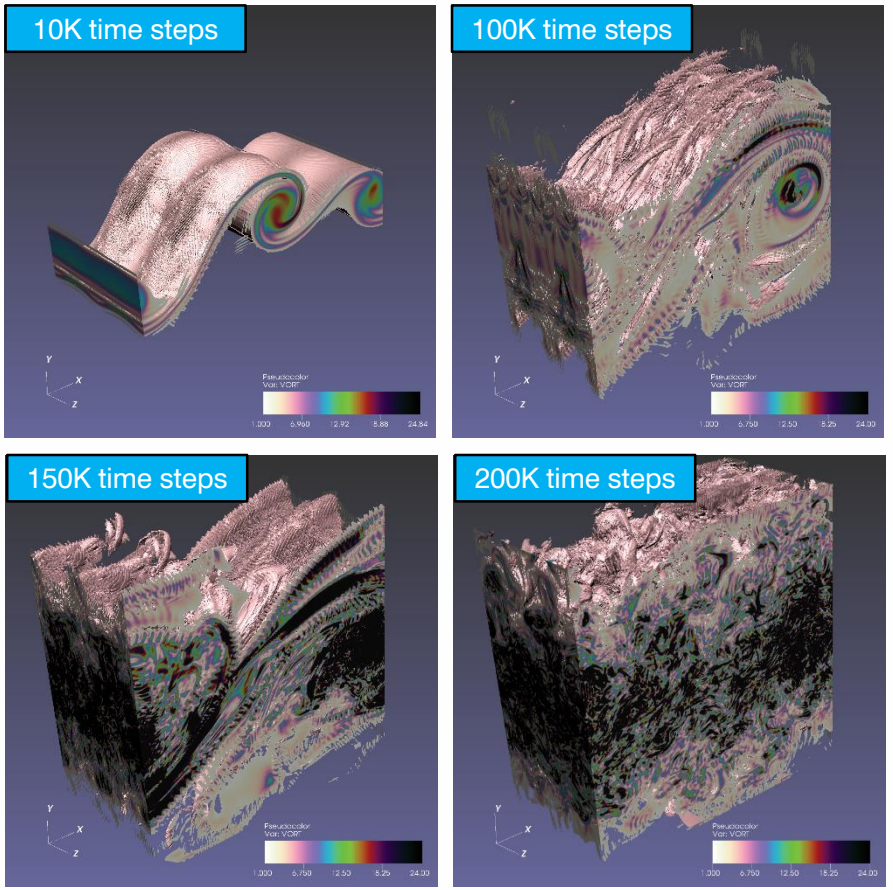
AVF-LESLIE

- Reacting flow code for DNS/LES investigation of canonical reactive flows
  - Simulated turbulent mixing layer mimics the dynamics encountered when two fluid layers slide past one another
    - Found in ocean and atmospheric fluid dynamics
    - Found in combustion and chemical processing
    - 2 sliding fluid layers are subject to instabilities and can evolve from largely 2-d laminar flow 3-d homogenous turbulent flow
  - Written in Fortran 90 with MPI



Isosurfaces and slices of vorticity magnitude showing progression of vortex braiding and breakdown

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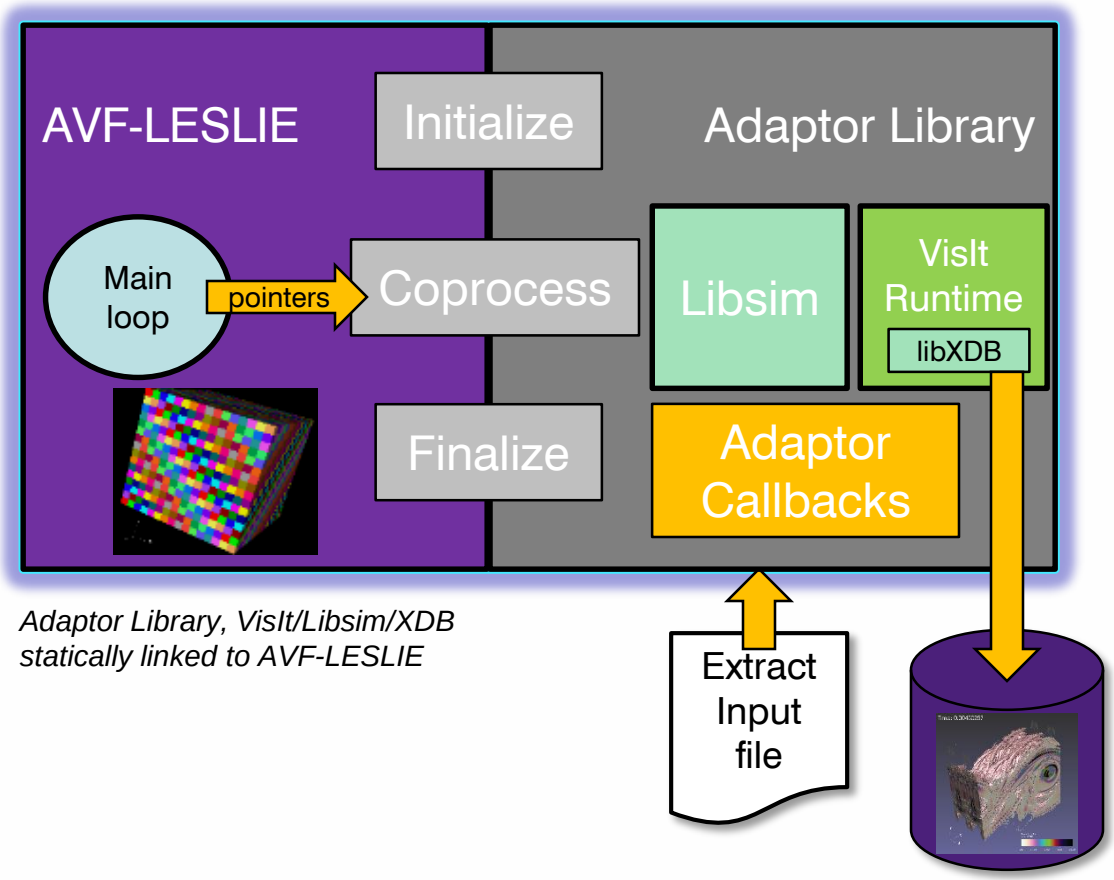
Instrumenting AVF-LESLIE

- Created adaptor library for AVF-LESLIE
- Reads list of extracts from input file
- Calls “coprocess” function when we want to generate extracts
- Pass pointers to mesh and field data to be exposed to VisIt via Libsim inside adaptor callbacks
- Extracts are generated and saved to XDB format



Adaptor Library, VisIt/Libsim/XDB statically linked to AVF-LESLIE

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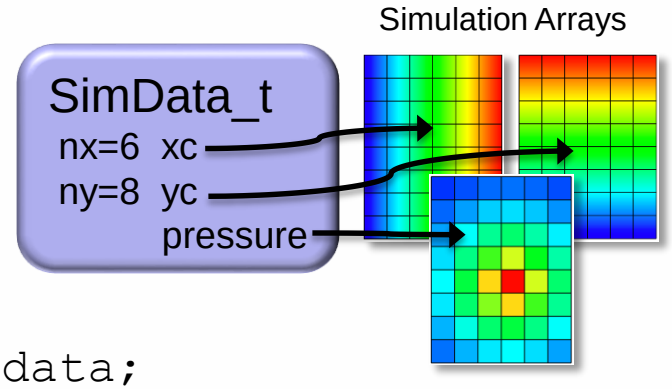
Example GetVariable Function

```
// Example
visit_handle
GetVariable(int domain, char *name,
    void *cbdata)
{
    visit_handle h;
    SimData_t *sim = (SimData_t *)cbdata;

    return h;
}
```



Allocate VariableData object, save information about simulation array

Indicates owner of the

Indicates number of array

The array being shared

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AVF-LESLIE In Situ Setup

- AVF-LESLIE runs on Titan
  - Turbulent mixing layer problem
  - 1025^3 grid points
  - Strong scaling study *(same grid size used as number of cores increases, decreasing work per core)*
  - In Situ Rendering workflow from 8K-131K cores
  - In Situ Extracts workflow from 8K-32K cores
    - Generate 1 isosurface of vorticity (computed by adaptor) and save extract to FieldView XDB
    - XDB files rendered on local workstation
  - Enhanced version of VisIt 2.10 with some bug fixes

Titan

- Oak Ridge National Laboratory
- Cray XK7
- 27 Petaflops (theoretical peak)
- 18,688 nodes with 16 AMD cores
- 710 Terabytes memory
- 30 Petabytes storage

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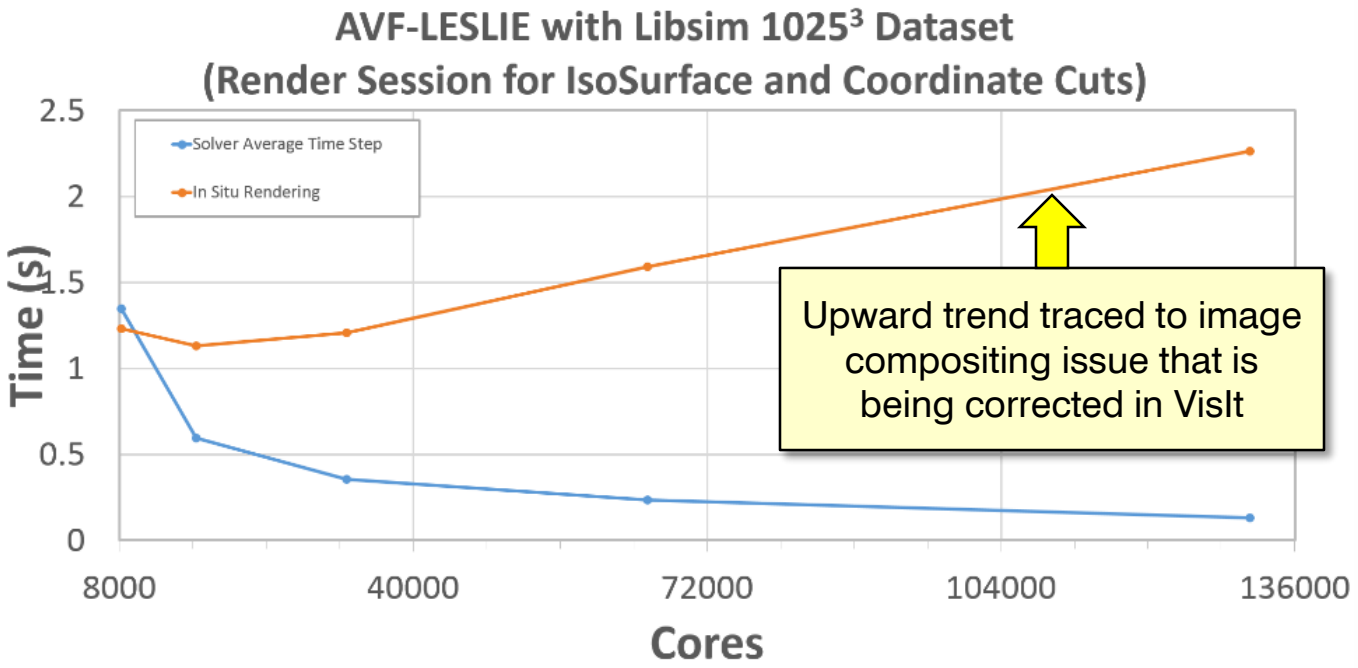
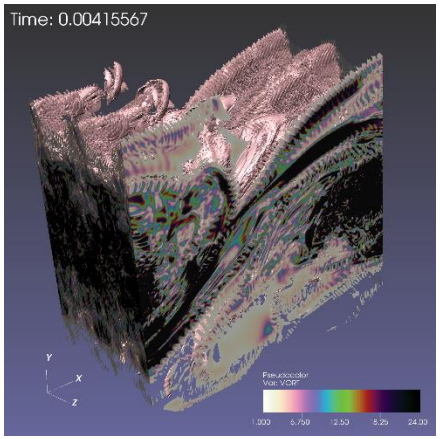
In Situ Rendering Workflow





- Calculate isosurfaces and slices of vorticity using VisIt session file for plot setup
- Save 1600^2 PNG image every 5^{th} iteration
- Run on Titan from 8K to 131K cores
- More work for visualization than for the solver in this case!

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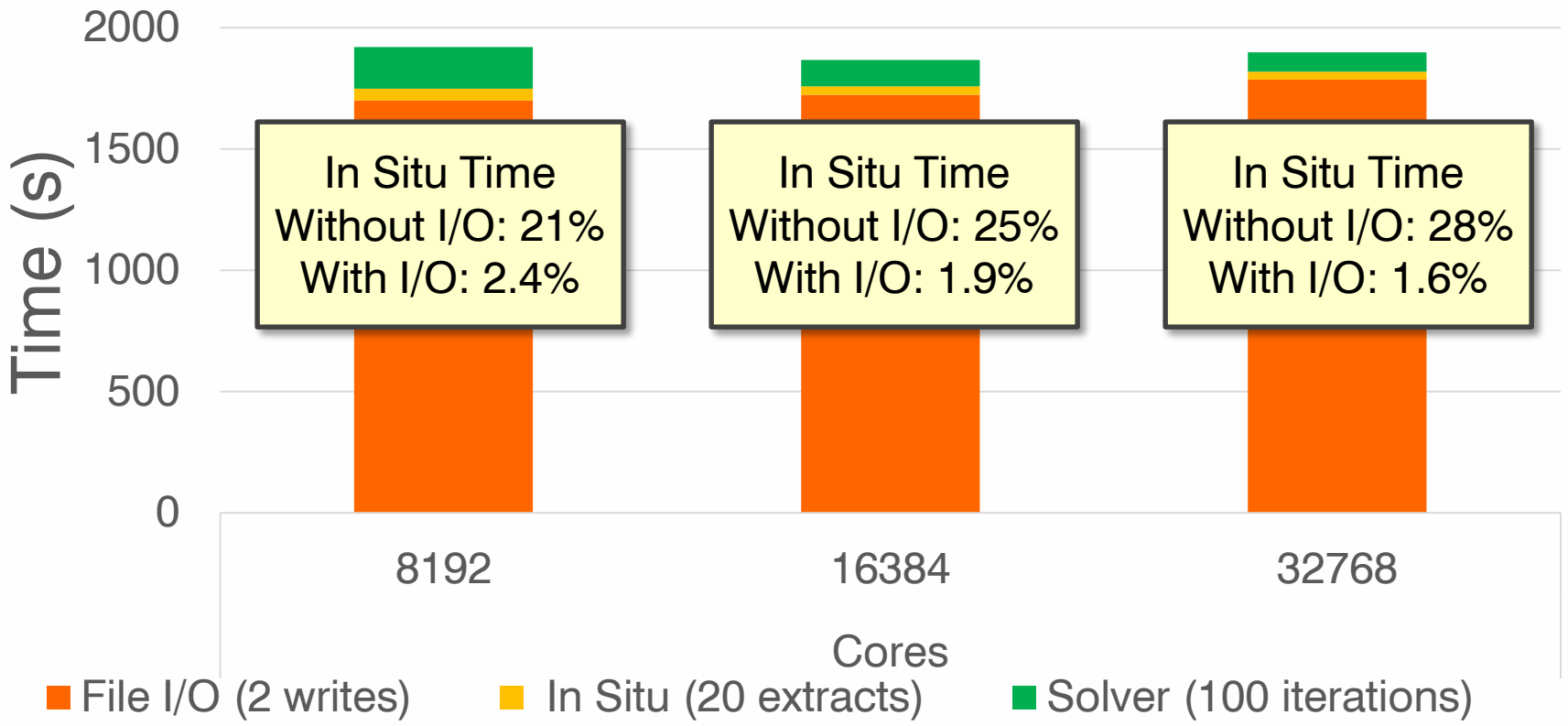
In Situ Extract Generation Overhead

- Save vorticity isosurface every 5th iteration to FieldView XDB format
- Use write groups size 96 to partially aggregate extract I/O



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File Size Comparison

- Each 100 iterations of the solver produced 1 volume results file
- Each 100 iterations of the solver produced 20 XDB files

Cores	1 Volume File Size (bytes)	1 Extract File Size (avg bytes)	1 Extract / 1 Volume	20 Extracts / 1 Volume
8192	51842236960	260100740	0.005017159	0.105360337
16384	51842236960	262613625	0.005065631	0.106378244
32768	51842236960	266710142	0.00514465	0.108037641

~200x reduction ~10x reduction

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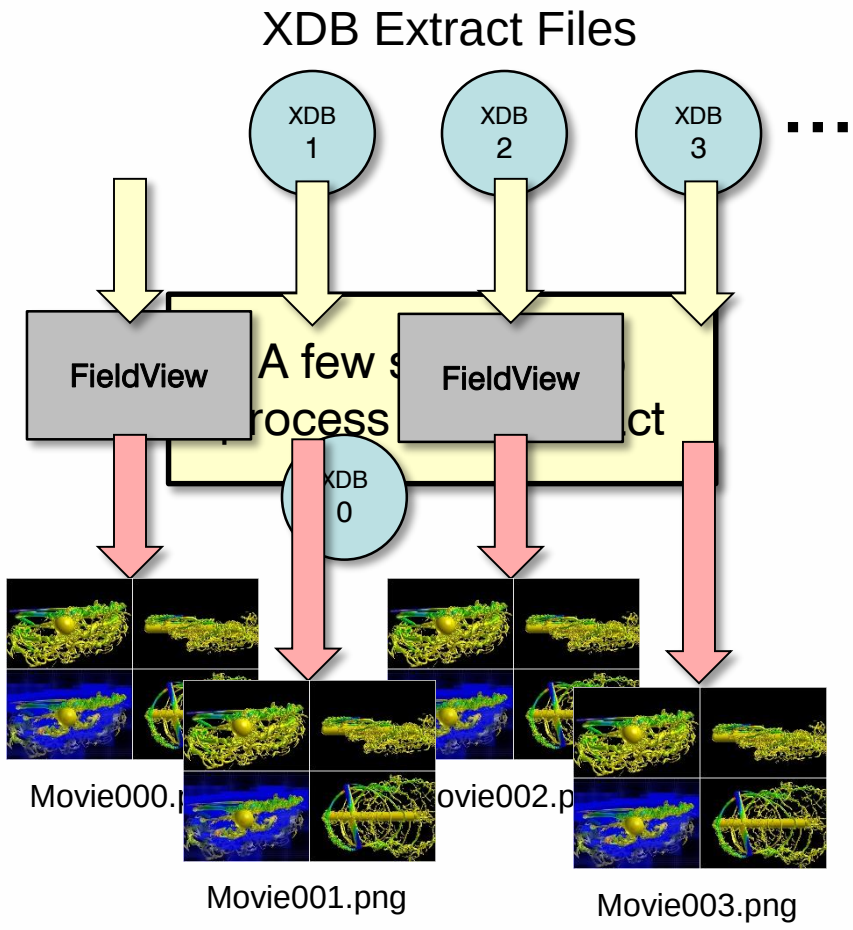
Extract Post Processing

- Multiple FieldView instances used
- XDB extracts used to make movie
  - Further analysis is possible since extracts contain geometry with data
- Time saved by reducing data in situ
  - Surfaces of interest already computed
  - No need to compute vorticity



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Acknowledgements

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