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U.S. DEPARTMENT OF ENERGY

In Situ Analysis and Visualization with SENSEI

November 2017

Supercomputing 2017

Welcome! Why are we here?

Problem: FLOPS >> I/O, potential for lost science

Approach: do as much processing as possible while data still resident in memory?

Why This Tutorial? To inform you of issues involved, to show you what technologies are available and how to use them.

Outline

- Introduction to *In Situ* Analysis and Visualization
- SENSEI *In Situ* Data Interface
- Instrumenting data sources and endpoints (C++)
- SENSEI *In Situ* Demonstrations with Coupled Infrastructures
  - Autocorrelation with ADIOS
  - Data extracts with Libsim
  - Computational monitoring with ParaView Catalyst
  - Using SENSEI via Python
- *In Situ* Costs and Performance
- Closing thoughts

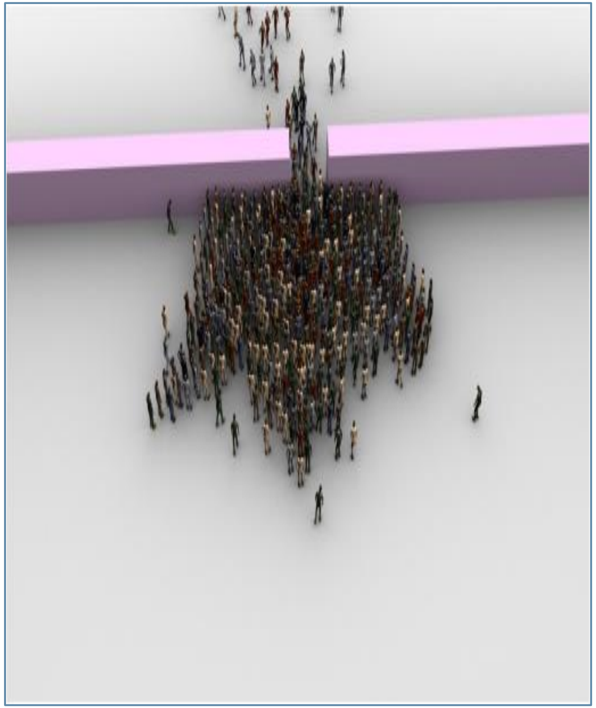
What are the problems?

Not enough I/O capacity on current HPC systems, and the trend is getting worse.

If there's not enough I/O, you can't write data to storage, so you can't analyze it: lost science.

Energy consumption: it costs a lot of power to write data to disk.

Opportunity for doing better science (analysis) when have access to full spatiotemporal resolution data.



Five orders of magnitude between compute and I/O capacity on Titan Cray system at ORNL

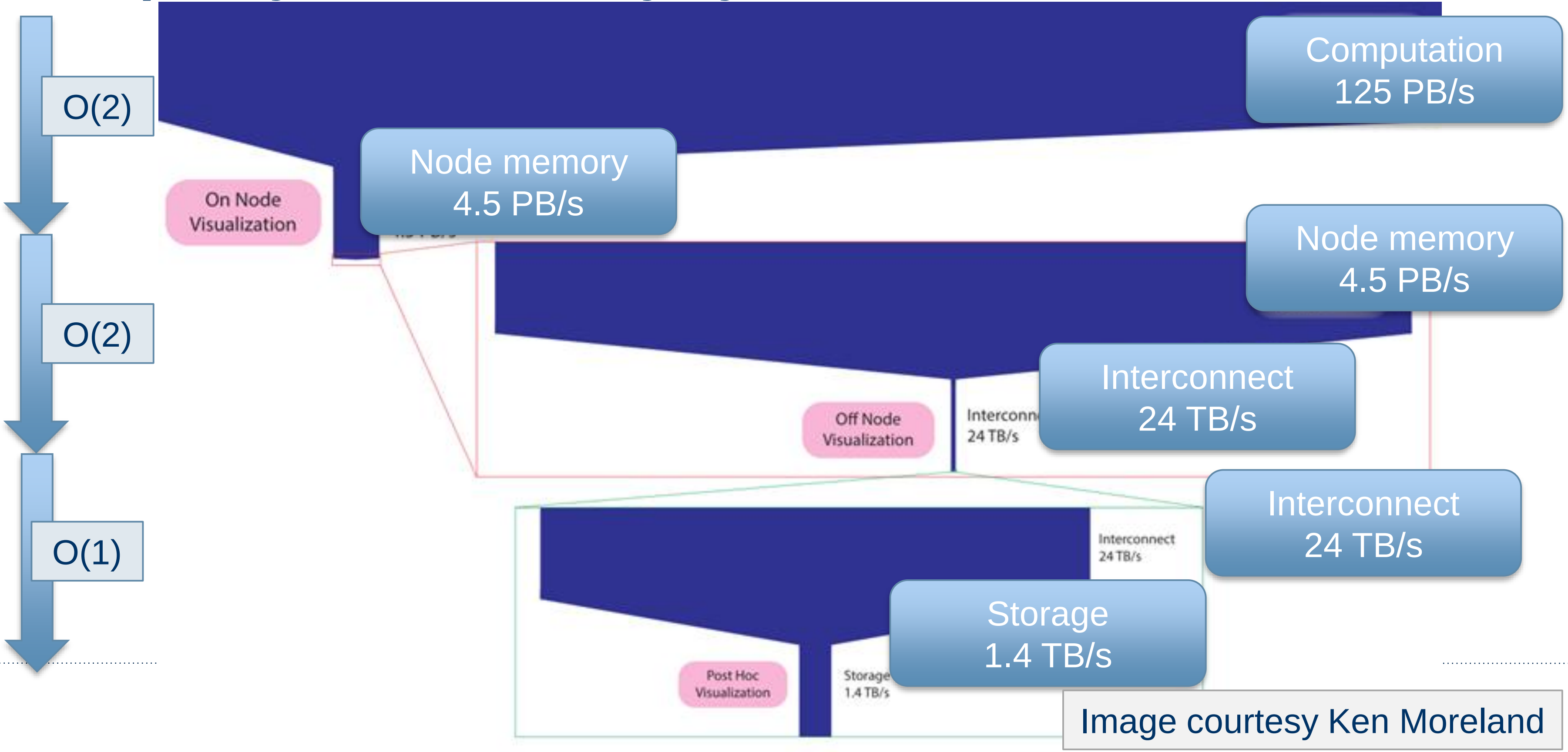


Image courtesy Ken Moreland

The problem is not going away

How does Summit compare to Titan

Feature	Summit	Titan
Application Performance	5-10x Titan	Baseline
Number of Nodes	~3,400	18,688
Node performance	> 40 TF	1.4 TF
Memory per Node	>512 GB (HBM + DDR4)	38GB (GDDR5+DDR3)
NVRAM per Node	800 GB	0
Node Interconnect	NVLink (5-12x PCIe 3)	PCIe 2
System Interconnect (node injection bandwidth)	Dual Rail EDR-IB (23 GB/s)	Gemini (6.4 GB/s)
Interconnect Topology	Non-blocking Fat Tree	3D Torus
Processors	IBM POWER9™ NVIDIA Volta™	AMD Opteron™ NVIDIA Kepler™
File System	120 PB, 1 TB/s, GPFS™	32 PB, 1 TB/s, Lustre®
Peak power consumption	10 MW	9 MW

Data courtesy A. Geist (ORNL)

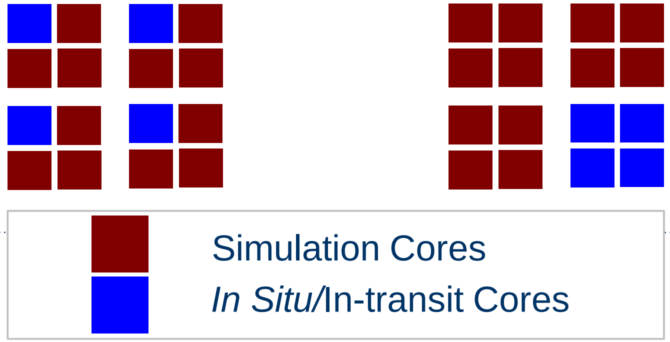
OAK RIDGE National Laboratory | OAK RIDGE LEADERSHIP COMPUTING FACILITY

What is *in situ* data analysis and visualization?

Two use models:

- <u>Post processing (*post hoc*)</u>: save to disk, then later, a separate analysis/vis program reads that data and operates on it.
- <u>*In situ* processing</u>: process data as it produced without writing to and reading from storage. Processed "<u>in place</u>".
  - Many flavors/terms: tightly coupled, loosely coupled, in transit, co-processing, etc.
  - Practical view: anything processed but not written to persistent storage is *in situ*

<u>*In situ*</u> *– no data movement*: Simulation and *in situ* methods share memory



<u>In transit</u> – data is moved: Simulation and *in situ* methods do not share memory

The story is much more interesting than “in situ” vs. “in transit”

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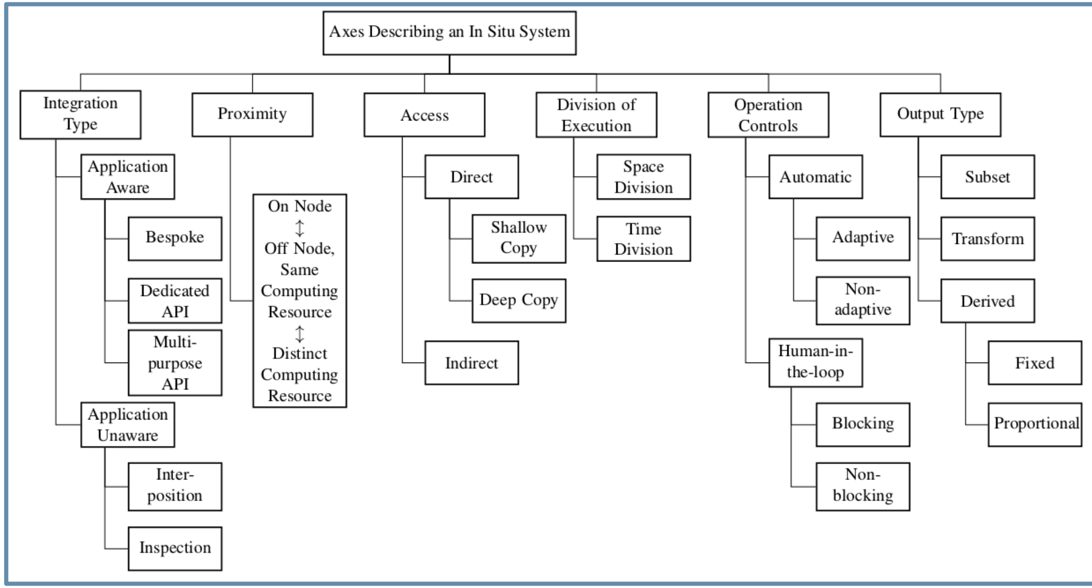
In situ vs. in transit is an oversimplification of a much richer problem space

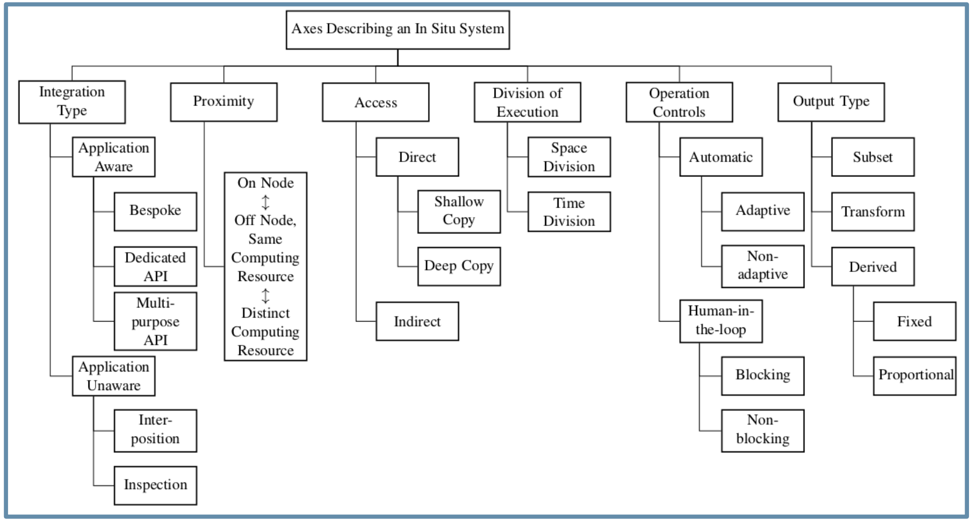
The “In Situ Terminology Project”

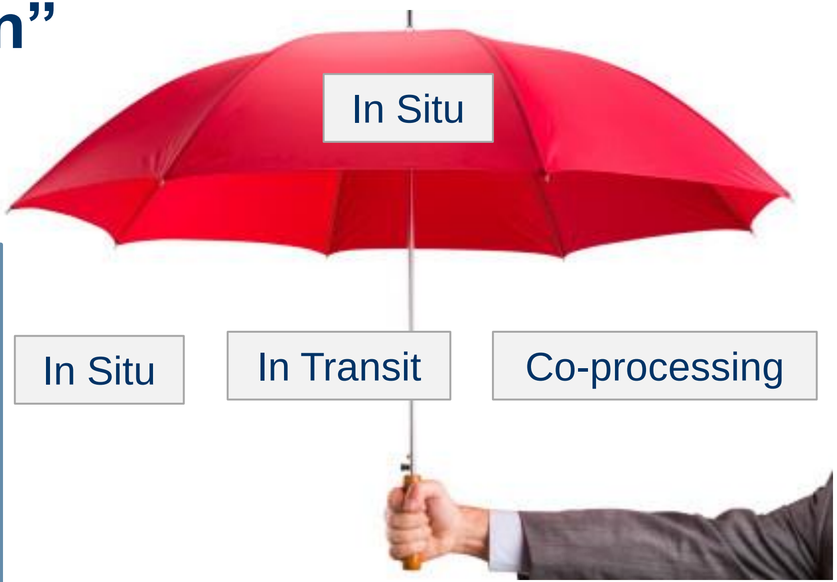
- A community effort (>50 participants)
- Identify “basis vectors” for describing aspects of in situ processing
  - Integration Type, Proximity, Access, Division of Execution, Operation Controls, Output Type



In situ: an ”umbrella definition”

In situ is term that covers a lot of territory:





In Situ Terminology project:
http://ix.cs.uoregon.edu/~hank/insituterminology/
Community effort to identify basis vectors and name them.

In situ has been around a long time: ancient history

E. Zajac, CACM 7(3), Mar 1964.

Direct-to-film process (simulation, calligraphic display exposes film) movie of a satellite orbiting a planet.

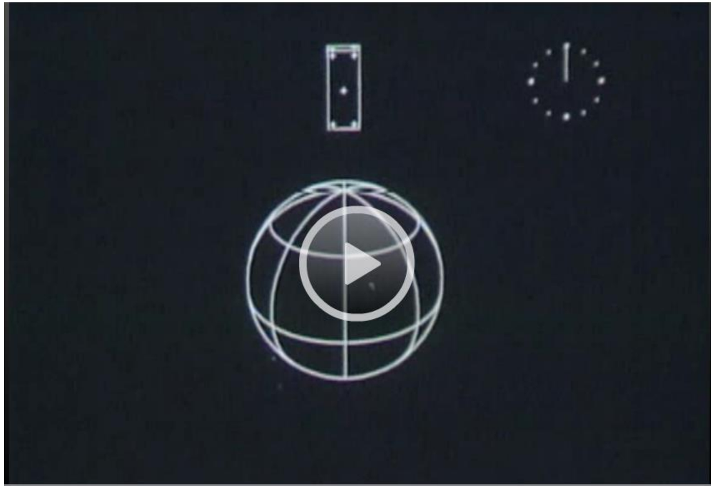
Is this *in situ?*

- Yes: no data ever landed on disk.

Why did he do it?

- "Standard practice" for that era, and many years that followed: direct-to-media more efficient.

Link to movie page

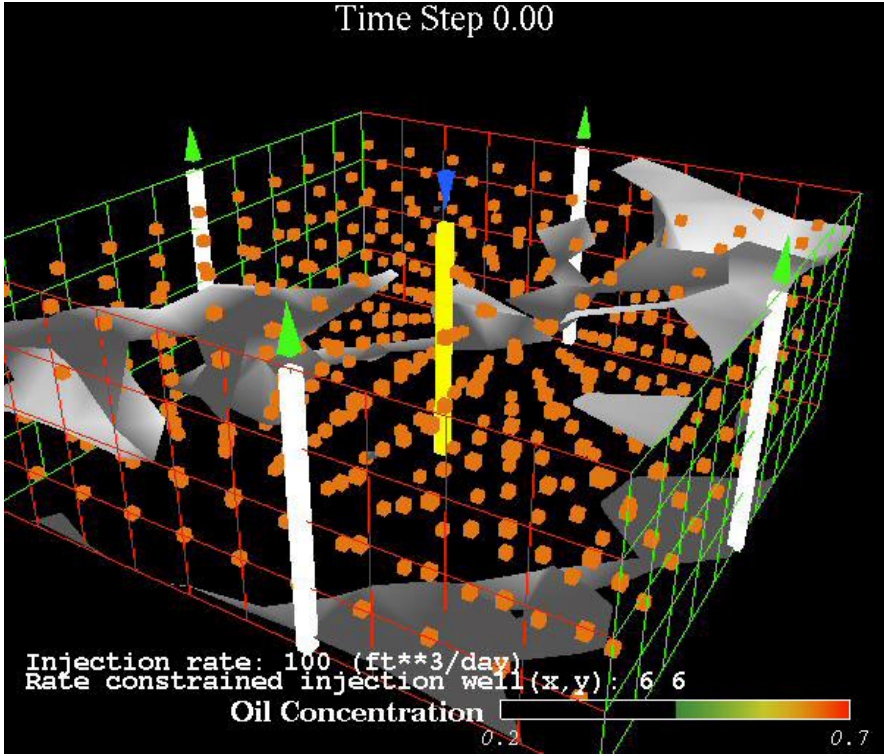


The 1990s: the golden era of coprocessing

Main idea: systems/methods that support interactive computation, computational monitoring and steering.

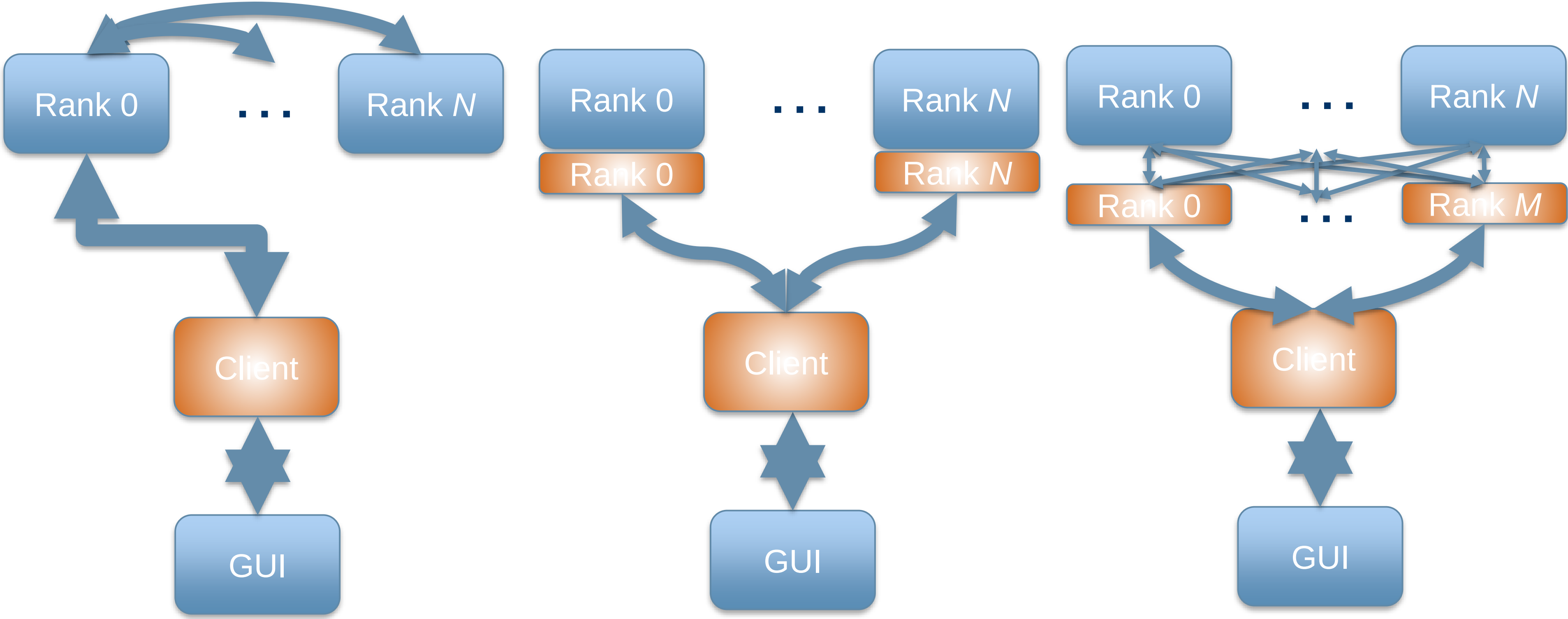
Packages from this era (partial list):

- pV3: custom distributed memory code (Haimes)
- AVS: co-routine processing (serial, mostly)
- CUMULVS: distributed memory M-to-N visualization, steering (based on PVM) (Kohl, et al.)



Bethel and Jacobsen (1994, 1995). Coupling a multi-phase reservoir simulator with AVS.

Common design patterns of 1990s



Many-to-one: AVS

“Tightly coupled”: pV3, custom projects

“Loosely coupled”, M-to-N: CUMULVS

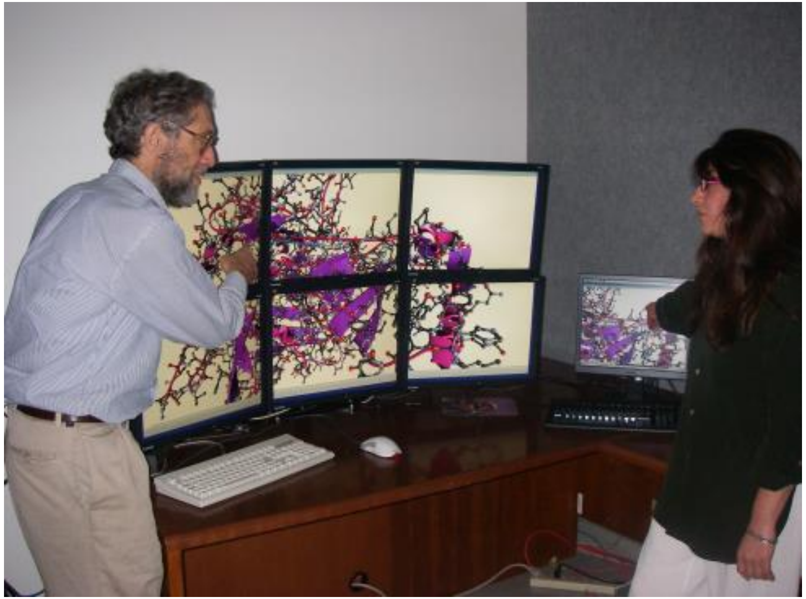
Computational steering – human in the loop

Main idea: rapid convergence

Example: protein structure prediction, find optimal-energy conformation from initial conditions (NP-hard problem)

Approach:

- parallel computations that minimize energy for individual conformations
- User can examine any of these, perform manual tweaks to get “unstuck” from local minimum, then resume calculations.



O. Kreylos, N. Max, B. Hamann, S. Crivelli, W. Bethel. *Interactive Protein Manipulation.* IEEE Vis 2003, Best Application Paper award.

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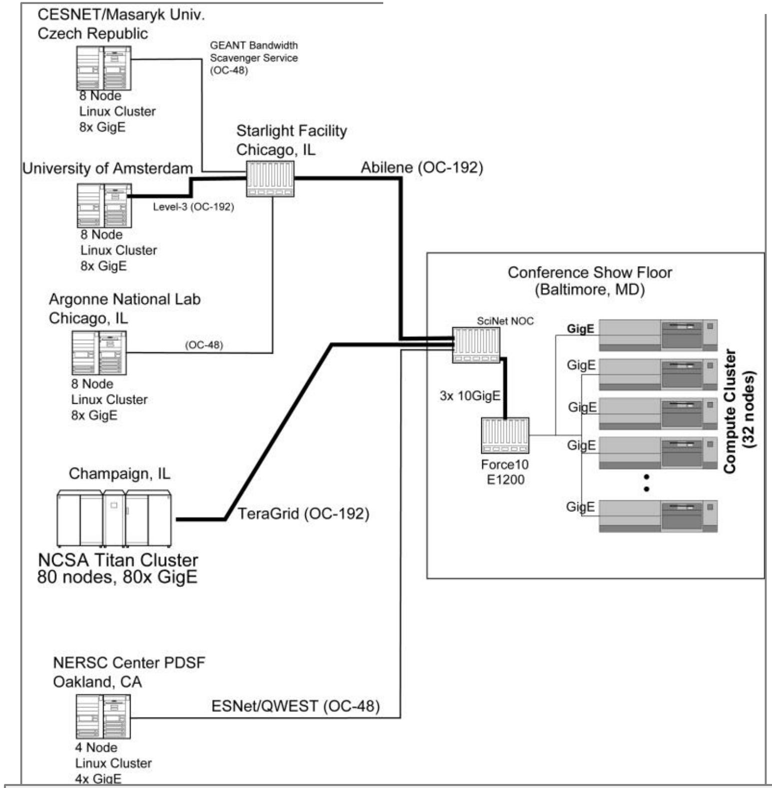
Integrated computational environments

- Simplify building, running codes
- Many add-on capabilities for vis, analysis, debugging, data I/O, etc.

Examples: SCIRun, Cactus

Application (sample): parallel binary black hole merger computation, in transit vis wins SC Bandwidth Challenge (2000, 2001, 2002)



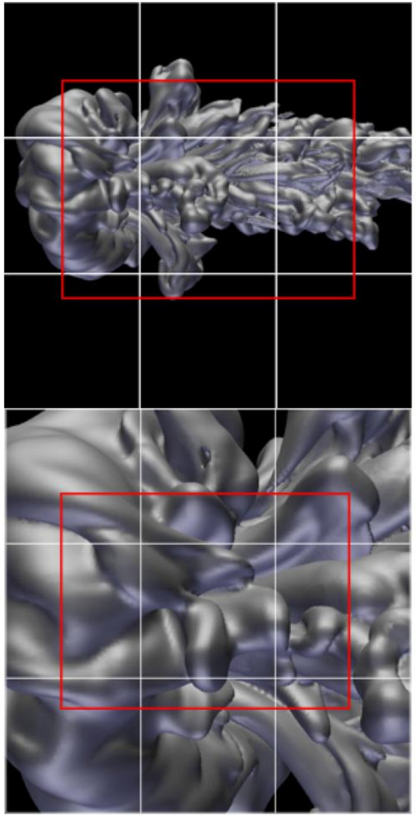
Resources used in SC 2002 Bandwidth Challenge, in transit workflow

Explorable extracts

Basic ideas:

- Overcome *in situ* primary weakness: know before you go.
- Use *in situ* computation to produce reduced-size datasets, e.g., images, data subsets, “extracts” like collections of features, etc.
- These “data extracts” are much smaller in size compared to doing full resolution data I/O.
- Use some post-processing tool to view/analyze/interact with these extracts.

Climate modeling example using Catalyst and Cinema in our STAR paper.



Chen et al., *Interactive, Internet Delivery of Visualization via Structured, Prerendered Multiresolution Imagery.* TVCG 14(2), 2008.

In situ projects over the years (approximate, partial)

- 1964: Zajac, direct-to-film animations
- 1990s: Code coupling, computational steering:
  - AVS
  - pV3
  - CUMULVS
- 2000s (early): Integrated Computational Environments:
  - SCIrun
  - CACUTS
- 2000s (late): Computing Extracts for Post Hoc Use
  - Multiresolution, precomputed images
  - Topology
  - Geometry
- Present day:
  - VisIt/Libsim, Paraview/Catalyst: scalable vis infrastructure accessible *in situ*
  - ADIOS: I/O library approach
  - SENSEI: generic *in situ* interface
  - Other nascent efforts

Generic processing sequence (sim code view)

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SENSEI *In Situ* Data Interface

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how to choose?

Can WE….

Enable use of any in situ framework?

Develop analysis routines that are portable between codes?

Make it easy to use?

The *current* problem set

ADIOS

LibSim

In situ infrastructures

Relatively new

- Until recently, **ad hoc**, **proof-of-concept prototypes**
- However, several **production quality** *in situ* **infrastructures** have emerged

ADIOS and **GLEAN** both provide tools for *in situ* **I/O** and some **analysis**

- ADIOS and GLEAN allow simulations to adopt *in situ* techniques by **leveraging** their **advanced I/O infrastructures** that enable co-analysis pipelines **rather than changing the simulator**.
- The non-intrusive integration **provides resilience** to third party library bugs and possible jitter in the simulation.

ParaView and **VisIt** both provide tools for *in situ* **analysis** and **visualization**

- ParaView **Catalyst** can be **tightly** or **loosely** linked to a simulation, allowing the simulation to **share data** with Catalyst for analysis and visualization.
- Similar capabilities are available within VisIt with the **Libsim** library.
- Catalyst (through **Live**), Libsim, and ADIOS enable the **opposite flow of information**, sending data from the client to the simulation, enabling the possibility of *in situ* and/or **monitoring/simulation steering**.

Our approach

Data model

- The lingua franca allowing an analyses to access simulation data consistently across a variety of simulations

Data adaptor

- Convert simulation data to/from the data model

API

- For instrumenting simulation and driving analyses

Library

- Providing off the shelf access to Libsim, Catalyst and ADIOS capabilities

Write once run everywhere

The **SENSEI API** enables connection of simulation data sources to visualization and analysis back ends

- From the perspective of the simulation, the back ends(analysis/vis codes) are interchangeable

The **SENSEI data model** enables viz & analysis codes to access data through a unified API.

- From the perspective of the analysis/visualization code, data sources(simulations) are interchangeable

Data model: VTK

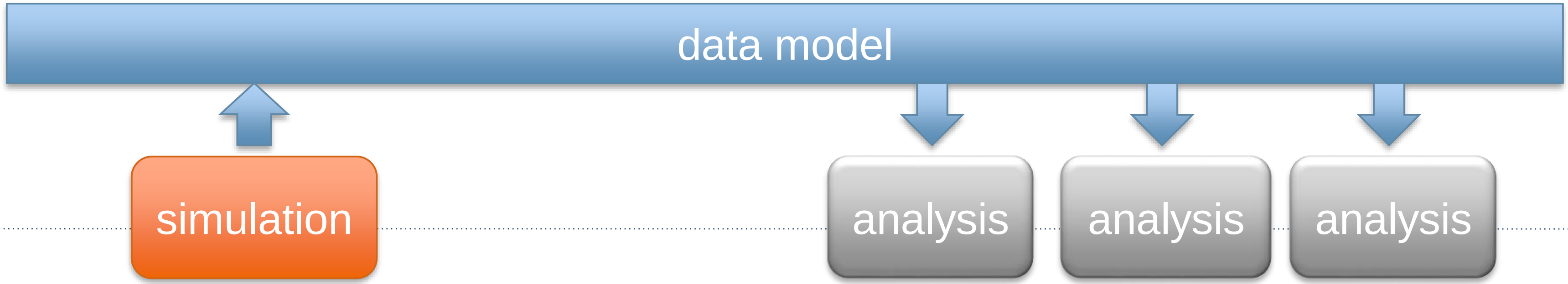
www.vtk.org/

Used by ParaView Catalyst and VisIt/Libsim

Supports common scientific dataset types

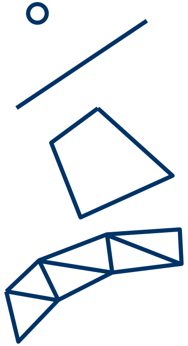
On going independent efforts to evolve for exascale

Supports using simulation memory directly (zero-copy) for multiple memory layouts

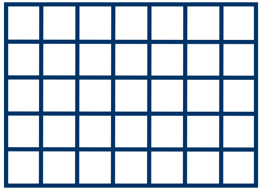


vtkDataSet subclasses

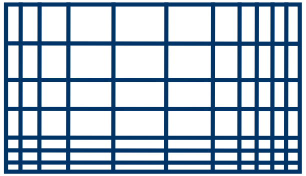
vtkPolyData



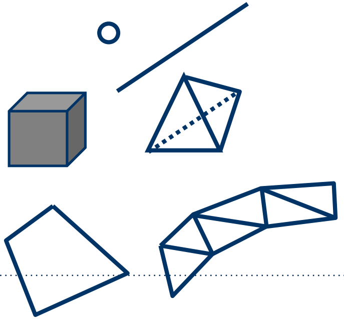
vtkImageData
vtkUniformGrid



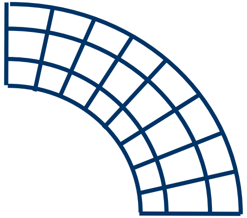
vtkRectilinearGrid



vtkUnstructuredGrid



vtkStructuredGrid



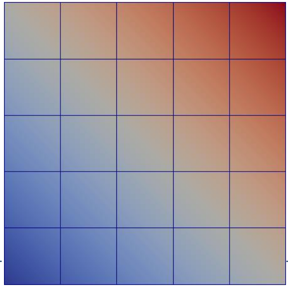
www.vtk.org/doc/nightly/html/classvtkDataSet.html

Field information

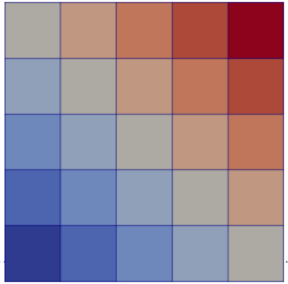
Store information defined over grids

Stored in concrete classes that derive from vtkDataArray

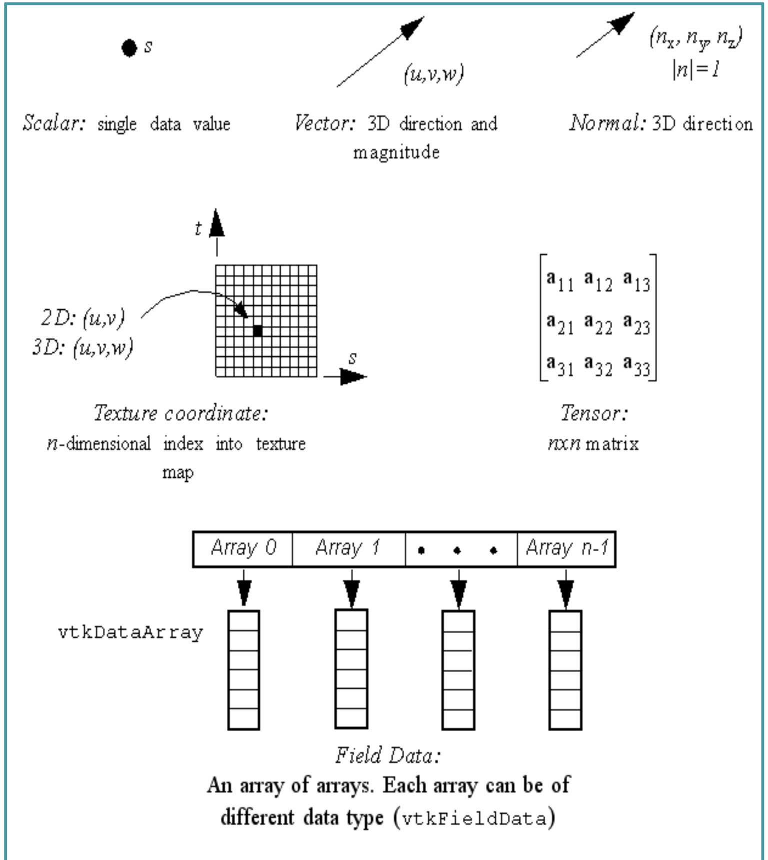
- vtkFloatArray
- vtkIntArray
- vtkDoubleArray
- vtkUnsignedCharArray
- …



Point data

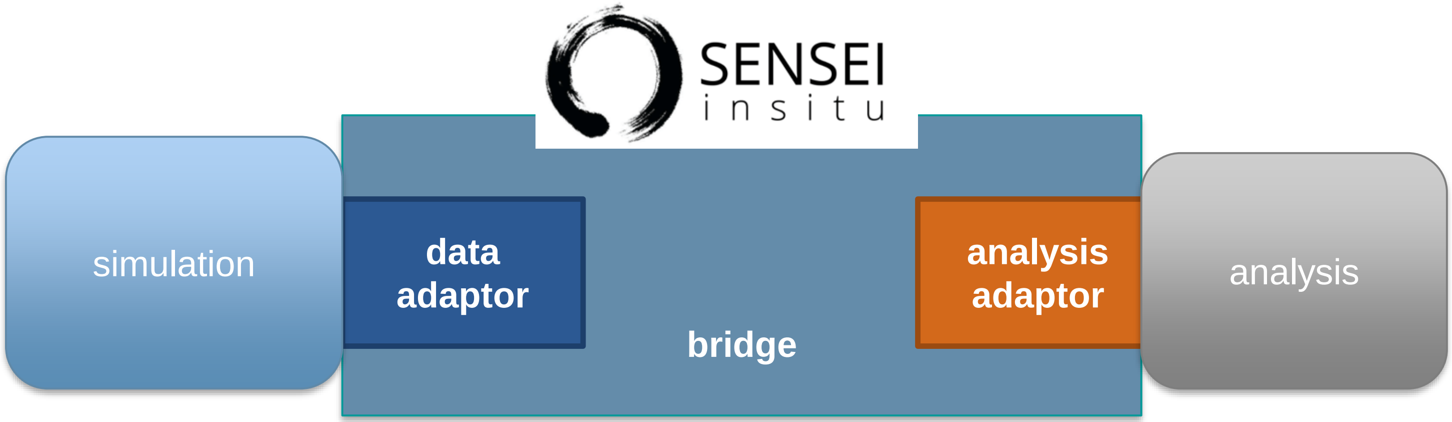


Cell data



Data attributes associated with the points and cells of a dataset.

Architecture



The data adaptor

- Provides the API through which data is accessed
- Converts simulation data structures into VTK data structures on demand
  - Try make use of VTK’s array zero copy facility
- Is used by the analysis adaptor to access simulation data on demand

sensei::DataAdaptor pure virtual class

```cpp
/// DataAdaptor is an abstract base class that defines the SENSEI data interface.
class DataAdaptor : public vtkObjectBase
{
public:
    /// Return the data object with appropriate structure.
    virtual vtkDataObject* GetMesh(bool structure_only = false) = 0;

    /// Adds the specified field array to the mesh.
    virtual bool AddArray(vtkDataObject* mesh, int association, const std::string& arrayname) = 0;

    /// Return the number of field arrays available.
    virtual unsigned int GetNumberOfArrays(int association) = 0;

    /// Return the name for a field array.
    virtual std::string GetArrayName(int association, unsigned int index) = 0;

    /// Release data allocated for the current time step.
    virtual void ReleaseData() = 0;

    /// Convenience method to get the time
    double GetDataTime();
    void SetDataTime(double time);

    /// Convenience method to get the time step
    int GetDataTimeStep();
    void SetDataTimeStep(int index);
};
```

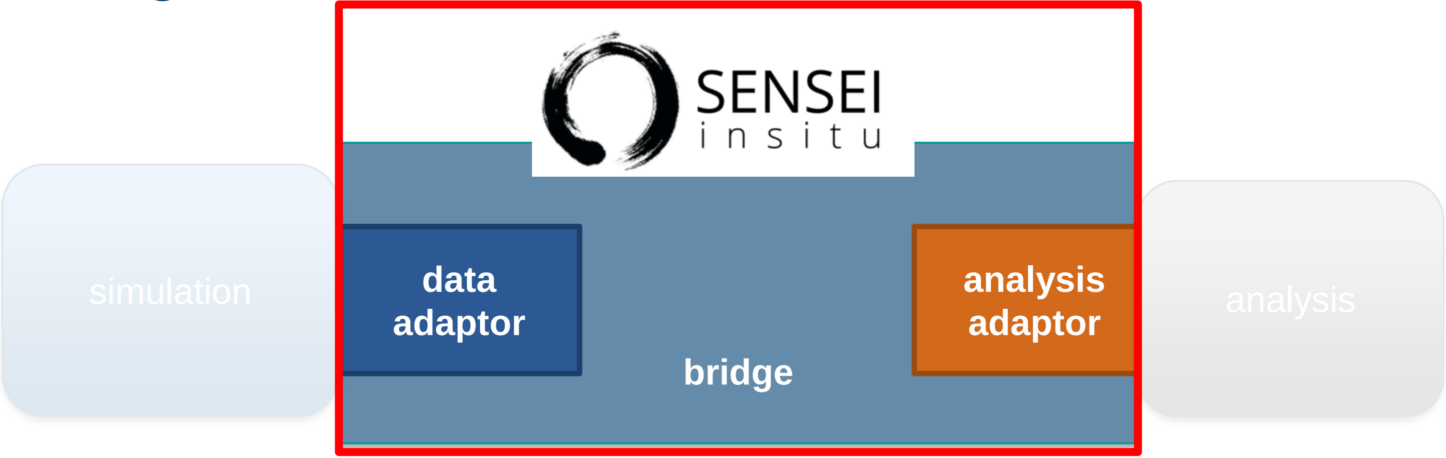
The analysis adaptor

- Provides the API for driving the analysis
- Invoked by the simulation when it is time for analysis
- You pass in a data adaptor instance, which the analysis code uses to access simulation data structures

sensei::AnalysisAdaptor pure virtual class

```
/// @brief AnalysisAdaptor is an abstract base class that defines
/// the analysis interface.
class AnalysisAdaptor : public vtkObjectBase
{
public:
   /// @brief Execute the analysis routine.
   virtual bool Execute(DataAdaptor* data) = 0;
};
```

The bridge



- Is where you create, initialize, and manage your data and analysis adaptors
- Is where you execute the analyses adaptors as needed
- Typically consists of 3 functions: Initialize, Compute and Finalize

Off the shelf solutions

Hidden

- **VTKDataAdaptor:** Implements SENSEI logic for you. your bridges code passes it a VTK dataset
- **ConfigurableAnalysisAdaptor:** read in XML file specifying what available analyses to compute during a simulation run

```
<sensei>
 <analysis type="catalyst" pipeline="pythonscript" filename="slice_contourcut.py"/>
 <analysis type="autocorrelation" array="data" association="cell" window="10" k-max="3"/>
 <analysis type="adios" filename="oscillators.bp" method="MPI"/>
 <analysis type="libsim" options="-no-icet" plots="Pseudocolor" plotvars="cell_data"
           visitdir="/global/homes/w/whitlocb/Development/SC16/install_static"
           slice-origin="32.5,32.5,32.5" slice-normal="0,0,1" image-filename="slice%ts"
           image-width="1600" image-height="1600" image-format="png"/>
</sensei>
```

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Instrumenting Data Sources and Endpoints with SENSEI

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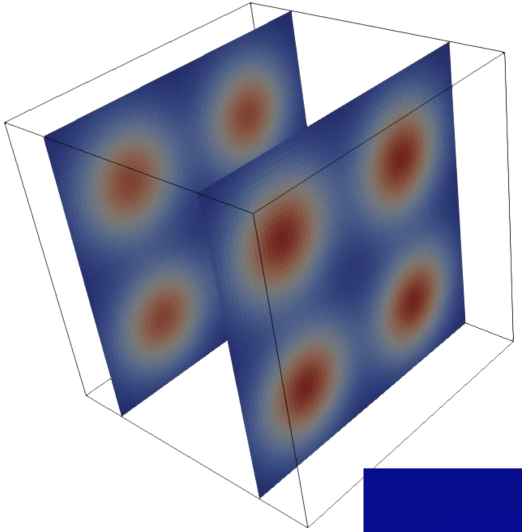
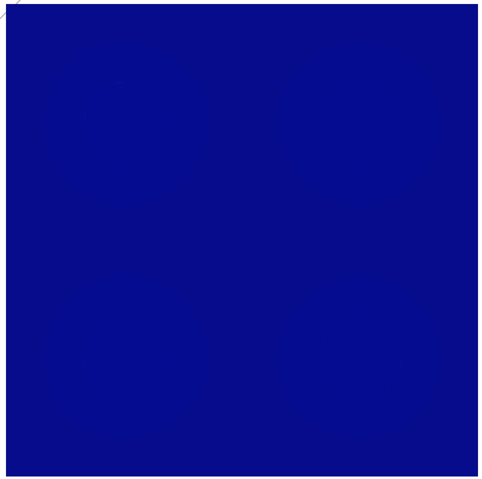
Instrumentation tasks

1. Data
   - Decide if you can use `sensei::VTKDataAdaptor`
   - Or write an adaptor derived from `sensei::DataAdaptor`
2. Analysis
   - Decide if you can use existing analyses: Libsim, Catalyst, Adios, etc
   - And/Or implement new analyses derived from `sensei::AnalysisAdaptor`
3. Bridge
   - Implement Initialize, Compute, and Finalize methods/functions
   - Instrument the simulation to call the bridge code at the right times

Oscillator miniapp overview



- MPI based C++ code that simulates a collection of periodic, damped, or decaying oscillators over a Cartesian grid
- Each oscillator is convolved with a Gaussian of a prescribed width
- Executable inputs are oscillator parameters, time resolution, length of the simulation, grid dimensions and grid partitioning



Instrumenting the oscillator mini-app to use SENSEI

Most of the work is in creating VTK objects to represent simulation grid and field data

- Create a class that derives from `sensei::DataAdaptor` and implements:
  - `virtual vtkDataObject* GetMesh(bool structure_only=false) = 0;`
  - `virtual bool AddArray(vtkDataObject* mesh, int association, const std::string& arrayname) = 0;`
  - `virtual unsigned int GetNumberOfArrays(int association) = 0;`
  - `virtual std::string GetArrayName(int association, unsigned int index) = 0;`
  - `virtual void ReleaseData() = 0;`

Creating the VTK grid – GetMesh() method

```
vtkDataObject* DataAdaptor::GetMesh(bool vtkNotUsed(structure_only))
{
  if (!this->internals->Mesh)
    {
    this->internals->Mesh = vtkSmartPointer<vtkMultiBlockDataSet>::New();
    this->internals->Mesh->SetNumberOfBlocks(static_cast<unsigned int>(internals.CellExtents.size()));
    for (size_t cc=0; cc < internals.CellExtents.size(); ++cc)
      {
      internals.Mesh->SetBlock(static_cast<unsigned int>(cc), this->GetBlockMesh(cc));
      }
    }
  this->AddArray(this->internals->Mesh, vtkDataObject::FIELD_ASSOCIATION_CELLS, "data");
  return this->internals->Mesh;
}

vtkDataObject* DataAdaptor::GetBlockMesh(int gid)
{
  vtkSmartPointer<vtkImageData>& blockMesh = this->internals->BlockMesh[gid];
  const diy::DiscreteBounds& cellExts = this->internals->CellExtents[gid];
  if (!blockMesh && areBoundsValid(cellExts))
    {
    blockMesh = vtkSmartPointer<vtkImageData>::New();
    blockMesh->SetExtent(
      cellExts.min[0], cellExts.max[0]+1,
      cellExts.min[1], cellExts.max[1]+1,
      cellExts.min[2], cellExts.max[2]+1);
    }
  return blockMesh;
}
```

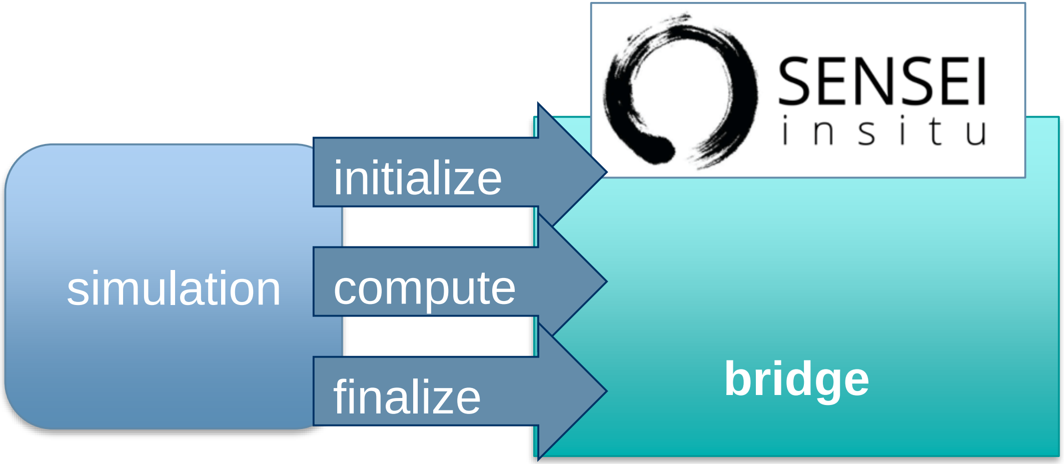
Creating the VTK cell data – AddArray() method

```
bool DataAdaptor::AddArray(vtkDataObject* mesh, int association, const std::string& arrayname)
{
  (void)association;
  bool retVal = false;
  DInternals& internals = (*this->Internals);
  vtkMultiBlockDataSet* md = vtkMultiBlockDataSet::SafeDownCast(mesh);
  for (unsigned int cc=0, max=md->GetNumberOfBlocks(); cc < max; ++cc)
    {
    if (!internals.Data[cc])
      {
      continue;
      }
    vtkSmartPointer<vtkImageData>& blockMesh = internals.BlockMesh[cc];
    if (vtkCellData* cd = (blockMesh? blockMesh->GetCellData(): NULL))
      {
      if (cd->GetArray(arrayname.c_str()) == NULL)
        {
        vtkFloatArray* fa = vtkFloatArray::New();
        fa->SetName(arrayname.c_str());
        fa->SetArray(internals.Data[cc], blockMesh->GetNumberOfCells(), 1);
        cd->SetScalars(fa);
        cd->SetActiveScalars("data");
        fa->FastDelete();
        }
      retVal = true;
      }
    }
  return retVal;
}
```

Implementing the bridge to SENSEI

Typically 3 calls:

- Initialize()
  - For the Oscillator we store the static Cartesian grid parameters
  - Specify what analysis will be done. For the Oscillator we use the ConfigurableAnalysis class.
- Compute()
  - For the Oscillator we do this with two calls: set_data() and analyze(), so that SENSEI may be disabled in benchmarks
- Finalize()



Initializing the bridge

```
void initialize(MPI_Comm world, size_t window, size_t nblocks, size_t n_local_blocks,
   int domain_shape_x, int domain_shape_y, int domain_shape_z, int* gid, int* from_x,
   int* from_y, int* from_z, int* to_x,   int* to_y,   int* to_z,
   const std::string& config_file)
{
  (void)window;
  GlobalDataAdaptor = vtkSmartPointer<oscillators::DataAdaptor>::New();
  GlobalDataAdaptor->Initialize(nblocks);
  GlobalDataAdaptor->SetDataTimeStep(-1);

  for (size_t cc=0; cc < n_local_blocks; ++cc)
    {
    GlobalDataAdaptor->SetBlockExtent(gid[cc],
      from_x[cc], to_x[cc], from_y[cc], to_y[cc],
      from_z[cc], to_z[cc]);
    }

  int dext[6] = {0, domain_shape_x, 0, domain_shape_y, 0, domain_shape_z};
  GlobalDataAdaptor->SetDataExtent(dext);

  GlobalAnalysisAdaptor = vtkSmartPointer<sensei::ConfigurableAnalysis>::New();
  GlobalAnalysisAdaptor->Initialize(world, config_file);
}
```

Executing the in situ

```
void set_data(int gid, float* data)
{
  GlobalDataAdaptor->SetBlockData(gid, data);
}

void compute(float time)
{
  GlobalDataAdaptor->SetDataTime(time);
  GlobalDataAdaptor->SetDataTimeStep(GlobalDataAdaptor->GetDataTimeStep() + 1);
  GlobalAnalysisAdaptor->Execute(GlobalDataAdaptor.GetPointer());
  GlobalDataAdaptor->ReleaseData();
}
```

Finalizing the bridge

```
void finalize(size_t k_max, size_t nblocks)
{
  (void)k_max;
  (void)nblocks;
  GlobalAnalysisAdaptor = NULL;
  GlobalDataAdaptor = NULL;
}
```

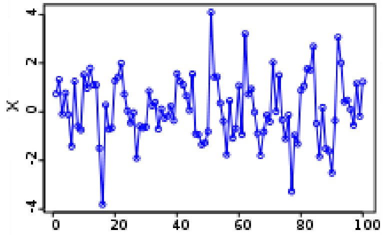
Overview of autocorrelation

Autocorrelation is a statistical test of a function with itself

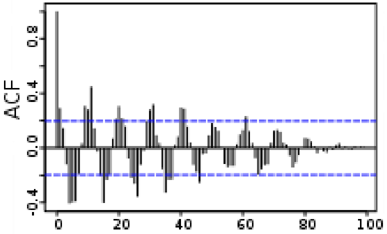
- Generally done in time, although can also be done over a spatial integral, or in some cases both.

Simple definition:

- $C(\tau) = \frac{\sum_{i=1}^{N} F(i)F(i-\tau)}{N * C(\emptyset)}$



A plot of a series of 100 random numbers concealing a sine function



The sine function revealed in a correlogram produced by autocorrelation

Image and captions from https://en.wikipedia.org/wiki/Autocorrelation

Initializing the autocorrelation analysis adaptor

In order to compute autocorrelation need to provide:

- MPI communicator
- Autocorrelation window size
- Field type and name

```
void Autocorrelation::Initialize(MPI_Comm world,
  size_t window, int association, std::string& arrayname,
  size_t kmax)
{
  AInternals& internals = (*this->Internals);
  internals.Master = make_unique<diy::Master>(world,
    -1, -1, &AutocorrelationImpl::create,
    &AutocorrelationImpl::destroy);

  internals.Association = association;
  internals.ArrayName = arrayname;
  internals.Window = window;
  internals.KMax = kmax;
}
```

Executing the autocorrelation analysis adaptor

Implement the Execute() method

- Use the passed in DataAdaptor object to get the desired data (grid and field data to compute the autocorrelation)
- Operate on grid and field information to compute desired result

```
bool Autocorrelation::Execute(DataAdaptor* data)
{
  AInternals& internals = (*this->Internals);
  const int association = internals.Association;

  vtkDataObject* mesh = data->GetMesh(/*structure-only*/ true);
  if (!data->AddArray(mesh, association, internals.ArrayName))
    {
    return false;
    }

  internals.InitializeBlocks(mesh);

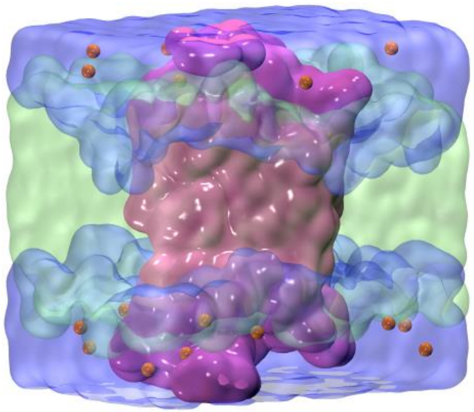

  if (vtkCompositeDataSet* cd = vtkCompositeDataSet::SafeDownCast(mesh))
    {
    vtkSmartPointer<vtkCompositeDataIterator> iter;
    iter.TakeReference(cd->NewIterator());
    iter->SkipEmptyNodesOff();

    int bid = 0;
    for (iter->InitTraversal(); !iter->IsDoneWithTraversal(); iter->GoToNextItem(), ++bid)
      {
      if (vtkDataSet* dataObj = vtkDataSet::SafeDownCast(iter->GetCurrentDataObject()))
        {
        int lid = internals.Master->lid(static_cast<int>(bid));
        AutocorrelationImpl* corr = internals.Master->block<AutocorrelationImpl>(lid);
        vtkFloatArray* fa = vtkFloatArray::SafeDownCast(
          dataObj->GetAttributesAsFieldData(association)->GetArray(internals.ArrayName.c_str()));
        if (fa)
          {
          corr->process(fa->GetPointer(0));
          }
        else
          {
          cerr <<"Current implementation only supports float arrays" << endl;
          abort();
          }
        }
      }
    }
  else if (vtkDataSet* ds = vtkDataSet::SafeDownCast(mesh))
    {
    int bid = internals.Master->communicator().rank();
    int lid = internals.Master->lid(static_cast<int>(bid));
    AutocorrelationImpl* corr = internals.Master->block<AutocorrelationImpl>(lid);
    vtkFloatArray* fa = vtkFloatArray::SafeDownCast(
      ds->GetAttributesAsFieldData(association)->GetArray(internals.ArrayName.c_str()));
    if (fa)
      {
      corr->process(fa->GetPointer(0));
      }
    else
      {
      cerr <<"Current implementation only supports float arrays" << endl;
      abort();
      }
    }
  return true;
}
```

Another example: instrumenting LAMMPS with SENSEI

- Large-scale Atomic/Molecular Massively Parallel Simulator
- Classical molecular dynamics code
- Runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain
- Accelerated performance on CPUs, GPUs, and Intel Xeon Phis
- Distributed by Sandia National Laboratories

http://lammps.sandia.gov/



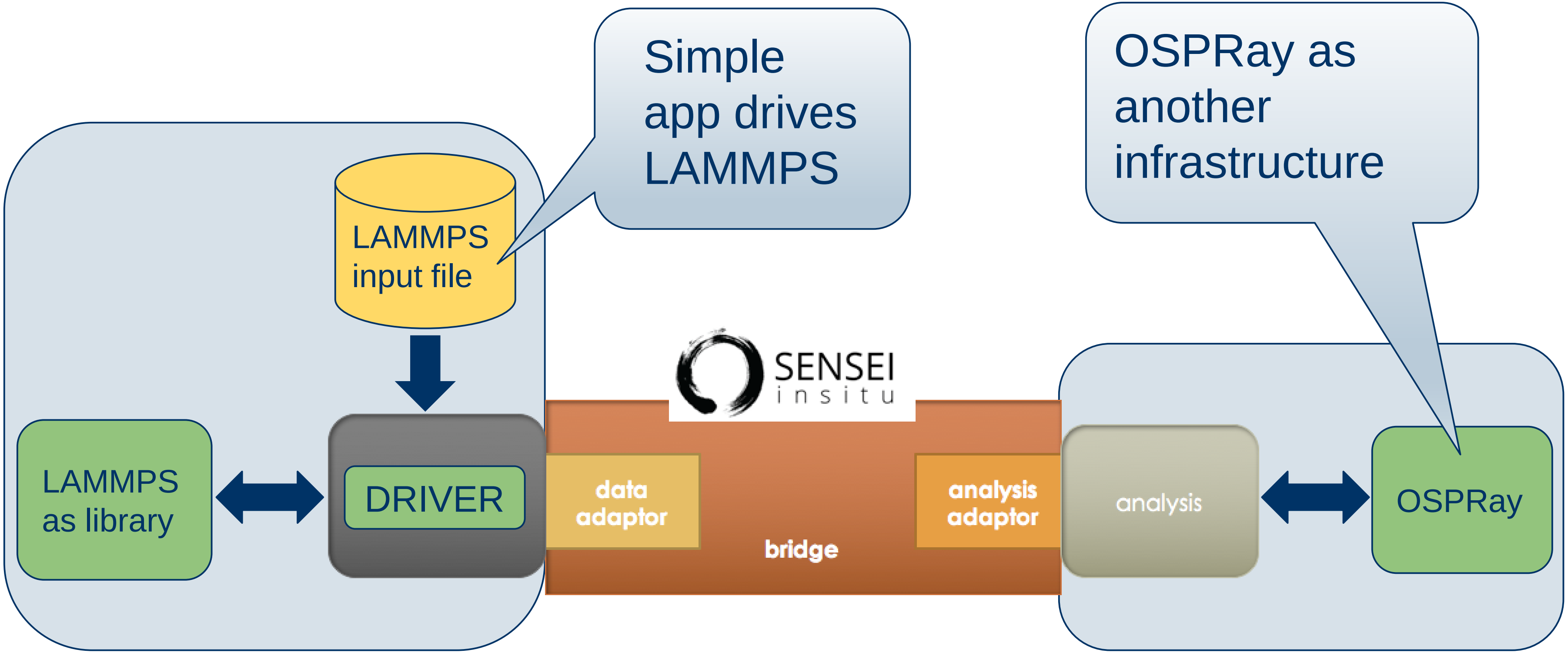
LAMMPS rhodopsin benchmark (32,000 atoms).
Courtesy Malakar et al. "Optimal scheduling of in situ analysis for large-scale scientific simulations." SC 2015.

Enabling in situ interactive visualization for large-scale molecular simulations

- LAMMPS is a good representative application of large scale molecular dynamics simulations
- Use LAMMPS as a library
  - Big advantage: No need to recompile or instrument LAMMPS original code
- Drive LAMMPS from a simple application instrumented with SENSEI
- Integrate OSPRay (Intel Software-Defined visualization) as an additional SENSEI infrastructure for interactive visualization

SENSEI architecture

Architecture of LAMMPS instrumentation with SENSEI



Data format

- LAMMPS particle format is basically x,y,z coordinates with additional fields like atom type or radius)
- Add LAMMPS *fix/external* command in input file for LAMMPS to share pointers to its internal data after computing every timestep of the simulation

- Additional information here: ***Coupling LAMMPS to other codes***

http://lammps.sandia.gov/doc/Section_howto.html#howto-10

Callback function from LAMMPS (every timestep)

```
void LAMMPSCallback(void *ptr, bigint ntimestep,
                    int nlocal, int *id, double **x, double **f)
{
    Info *info = (Info *) ptr;

    // extents
    double boxxlo = *((double *) lammps_extract_global(info->lmp,"boxxlo"));
    double boxxhi = *((double *) lammps_extract_global(info->lmp,"boxxhi"));
    double boxylo = *((double *) lammps_extract_global(info->lmp,"boxylo"));
    double boxyhi = *((double *) lammps_extract_global(info->lmp,"boxyhi"));
    double boxzlo = *((double *) lammps_extract_global(info->lmp,"boxzlo"));
    double boxzhi = *((double *) lammps_extract_global(info->lmp,"boxzhi"));

    // get pointer to atom types
    int    *type = (int *) lammps_extract_atom(info->lmp,"type");

    // update SENSEI bridge
    bridge::Set_data(nlocal, id, type, x, boxxlo, boxylo, boxzlo, boxxhi, boxyhi, boxzhi);

    // visualize
    bridge::Execute();
}
```

XYZ atom coords from LAMMPS

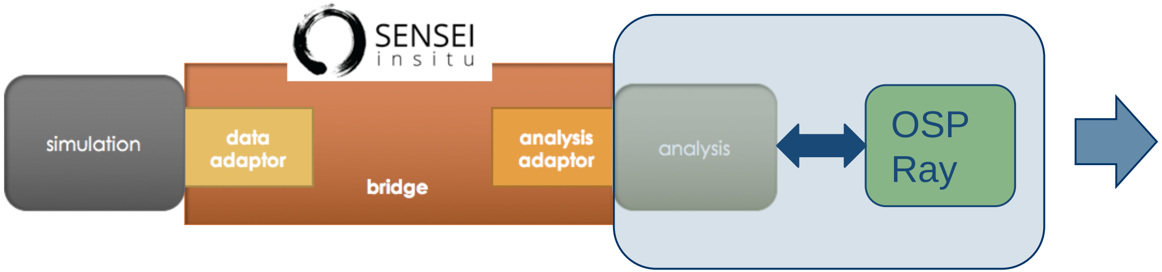
get atom types from LAMMPS

Update SENSEI bridge

Visualize

OSPRay as an additional infrastructure

- Connect to SENSEI endpoint to query data
- Pull data back to distributed OSPRay client app running using OSPRay's distributed device to provide an interactive viewer of the latest timestep



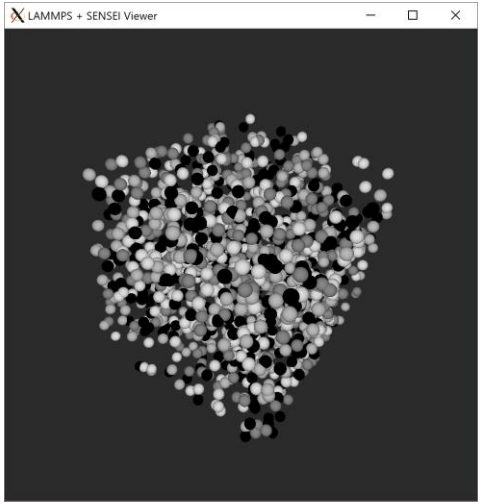


Image courtesy Will Usher, SCI, Univ. of Utah

Live demo

- Live demo on virtual machine

BERKELEY LAB
Bringing Science Solutions to the World

U.S. DEPARTMENT OF ENERGY

SENSEI In Situ Demonstrations with Coupled Infrastructures

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ADIOS

Autocorrelation with ADIOS

BERKELEY LAB
Argonne NATIONAL LABORATORY
OAK RIDGE National Laboratory
Intelligent Light
Kitware

What is ADIOS

An extendable framework that allows developers to *plug-in*

- **I/O methods**: N-to-M, N-to-N, N-to-1, In Situ (aka Staging)
- **Transformations**: Compression, Decompression, Indexing
- **Self describing** data format: ADIOS-BP
- **Indexing/Querying**: MinMax, FastBit, Alacrity

Incorporates the “best” practices in the I/O middleware layer

Released twice a year, now 1.12, under the completely free BSD license

- https://www.olcf.ornl.gov/center-projects/adios
- https://github.com/ornladios/ADIOS

Available at ALCF, OLCF, NERSC, CSCS, Tianhe-1,2, Pawsey SC, Ostrava

Applications are supported through OLCF INCITE program

Outreach via on-line manuals, and live tutorials

How to use ADIOS

ADIOS is provided as a library to users; use it like other I/O libraries, except

ADIOS has a simple approach for I/O

- User defines in application source code: “what” and “when”
  - **Every process defines what data and when to output**
- ADIOS takes care of the “how”

Biggest hurdle for users:

- Forget all of your manual **tricks** to gain I/O performance on your particular target system and target scale and just say what you want to write/read
- Trust ADIOS to deliver the performance

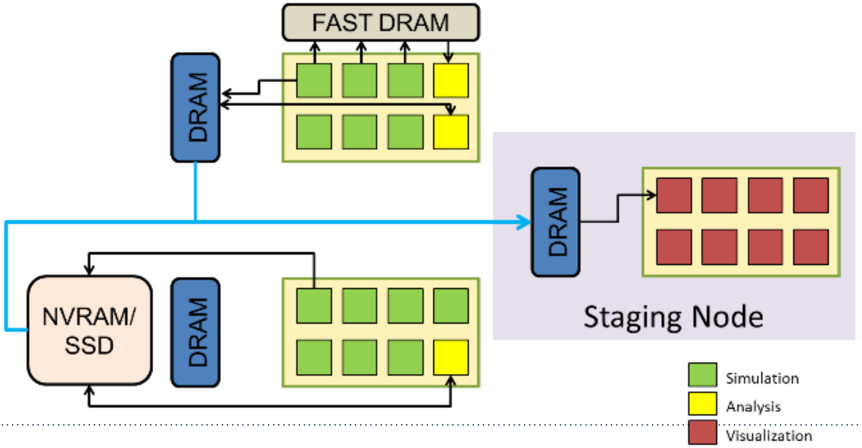
Performance Portability:

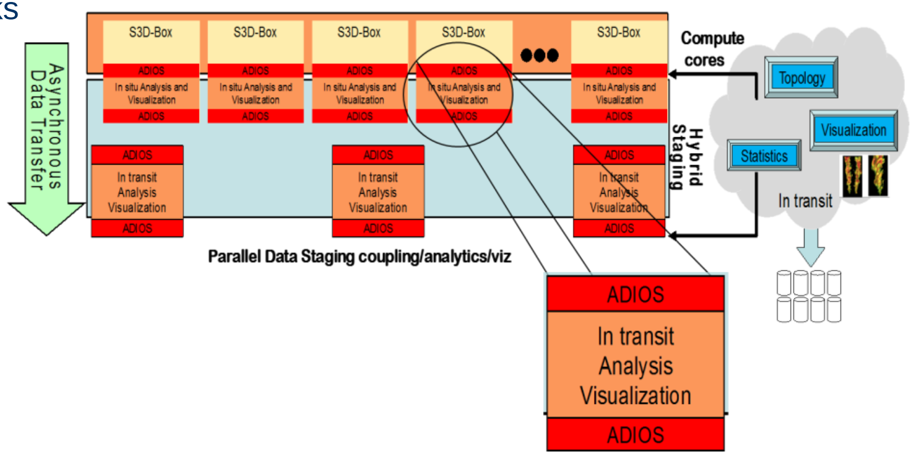
- Write once, perform well anywhere
  - It comes naturally with ADIOS
  - ADIOS has many different I/O methods (strategies)

Data management tradeoffs at exascale → to hybrid staging

Explore node layout choices for data management

- Balance of memory size and speed
- Feedback for node designs with NVRAM, larger memory, on-chip NIC
- Network throughput and latency impact on SDMA tasks
- Placement of operations in concert with solver and network topology





Goals of the ADIOS Read API design

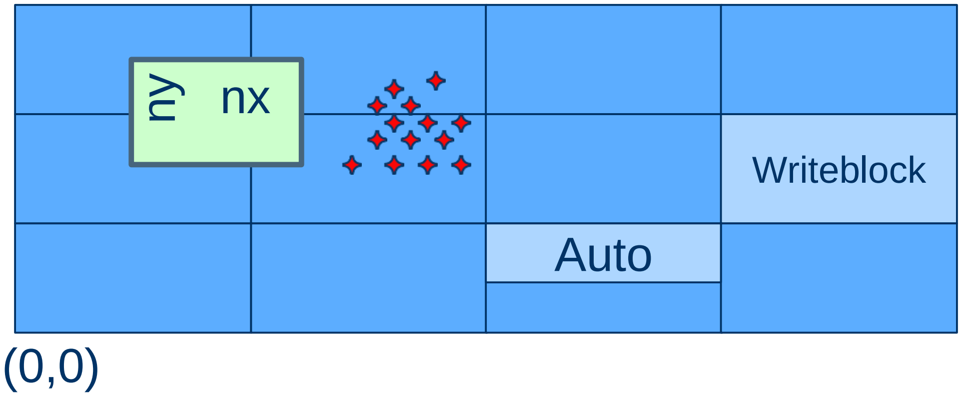
Staging I/O

- Insulate the scalable application from the variability inherent in the file system
- Enable the utilization of in situ and in-transit analytics and visualization

Same API for reading data from files and from staging

Allow for read optimizations:

- Multiple read operations can be scheduled before performing them
- Allow for blocking and non-blocking reads
- Use generic selections in the read statements instead of describing a bounding box
- Option to let ADIOS deliver data in chunks, with memory allocated inside ADIOS not in user-space



Selections

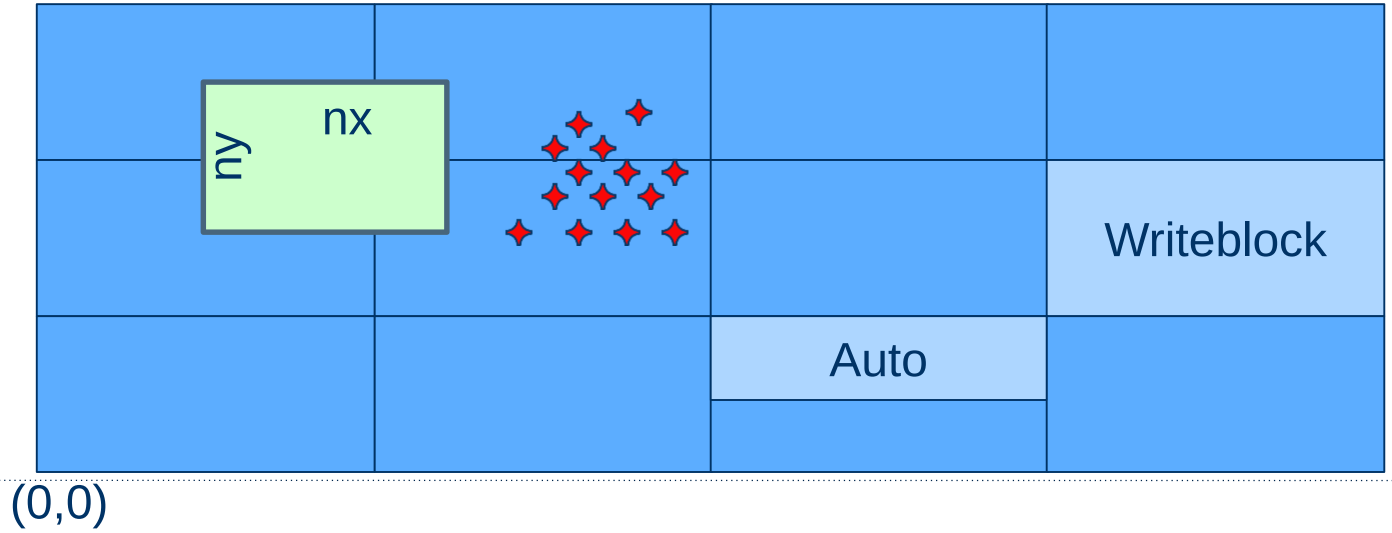
ADIOS_SELECTION *

adios_selection_boundingbox (int ndim, uint64_t * offsets, uint64_t * readsize)

adios_selection_points (uint64_t ndim, uint64_t npoints, uint64_t *points)

adios_selection_writeblock (int index)

adios_selection_auto (char * hints)



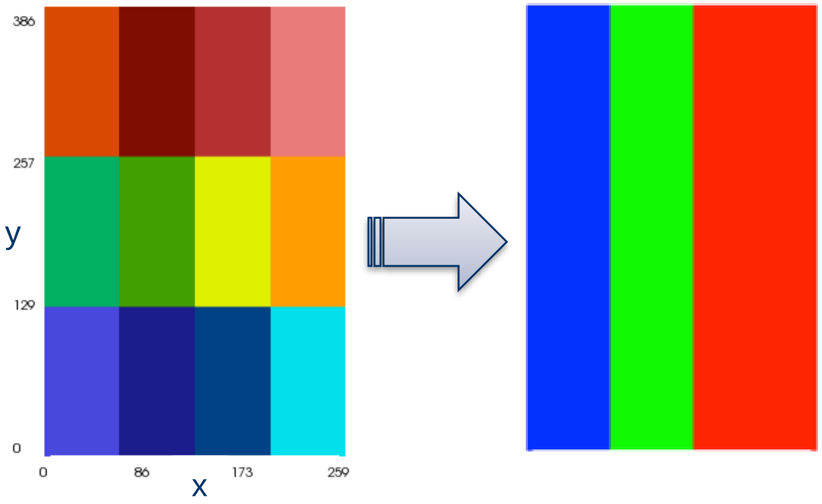
Example of Read API: read a variable step-by-step

```
int count[] = {10,10,10};
int offs[] = {5,5,5};
P = (double*) malloc (sizeof(double) * count[0] * count[1] * count[2]);
Q = (double*) malloc (sizeof(double) * count[0] * count[1] * count[2]);
ADIOS_SELECTION *sel = adios_select_boundingbox (3, offs, count);
while (fp != NULL) {
    adios_schedule_read (fp, sel, "P", 0, 1, P);
    adios_schedule_read (fp, sel, "Q", 0, 1, Q);
    adios_perform_reads (fp, 1, NULL);   // 1: blocking read
    // P and Q contains the data at this point
    adios_release_step (fp); // staging method can release this step
    // ... process P and Q, then advance the step
    adios_advance_step (fp, 0, 60.0);
    // 60 sec blocking wait for the next available step
}
// free ADIOS resources
adios_free_selection (sel);
```

N to M reorganization with stage_write

heat transfer + stage_write running together

- Write out 6 time-steps.
- Write from 12 cores, arranged in a 4 x 3 arrangement.
- Read from 3 cores, arranged as 1x3



N to M reorganization with stage_write

```
$ cd ~/Tutorial/heat_transfer
edit heat_transfer.xml  (vi, gedit)
set method to MPI
<method group="heat" method="MPI"/>

$ mpirun -np 12 ./heat_transfer_adios1   heat  4 3    40 50   6 500
$ bpls -D  heat.bp   T
 double    T              6*{150, 160}
        step 0:
          block  0: [  0: 49,    0: 39]
          block  1: [  0: 49,   40: 79]
          ...
          block 11: [100:149, 120:159]


$ mpirun -np 3    stage_write/stage_write    heat.bp    h_3.bp    BP  ""    FLEXPATH ""   3
$ bpls -D   h_3.bp   T
 double    T              6*{150, 160}
        step 0:
          block 0: [  0:149,    0: 52]
          block 1: [  0:149,   53:105]
          block 2: [  0:149,  106:159]
```

Live demo

- Live demo on virtual machine

VisIt

Data Extracts with VisIt/Libsim

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

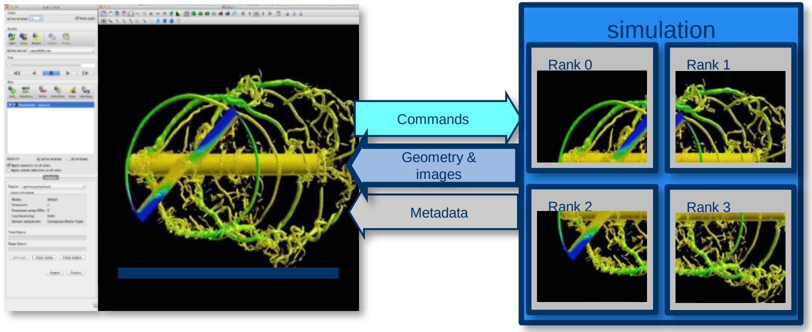
- Versatile open source software for visualizing and analyzing petascale simulation datasets

Libsim

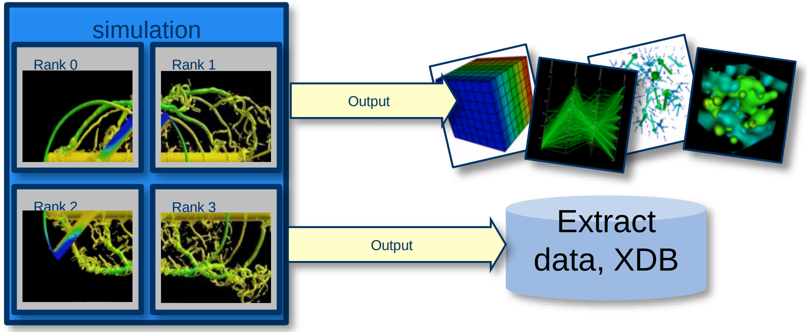
- Enables simulations to perform data analysis and visualization in situ by applying VisIt algorithms to data.

Libsim enables flexible workflows

- Use the VisIt GUI to connect to your simulation and explore!
- Simulations are like any other data source



- Create automated routines to generate data in batch
- Program directly using Libsim
- Use VisIt session files



XDB workflow

- Use Libsim to instrument simulation so it produces **FieldView XDB** files for later visualization in Fieldview
- XDB is a CFD format made of surfaces and streamlines, which provides geometry and field data that e
- Extra
- XDB'
- Field
  - All ope
  - Nume

XDB's 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

FieldView

XDB produced in situ XDB XDB visualized

Flexible XDB export

- Hard-coding plots and extracts limits flexibility
- New functions manage extract creation and export via an extract input file
  - Provides hints to Libsim
  - Specifies extracts, variables, files to write

```
 $LIBSIM_CONTROL
    ENABLE = TRUE
    VISITDIR = /usr/gapps/visit
    MODE = BATCH  # Or INTERACTIVE
    SIMV2 = avf-leslie.sim2
    DESCRIPTION = We are connecting VisIt and AVF-
LESLIE
    OPTIONS = -debug 5 -clobber_vlogs
    PREFIX = './',
    FREQUENCY = 100,
    $END

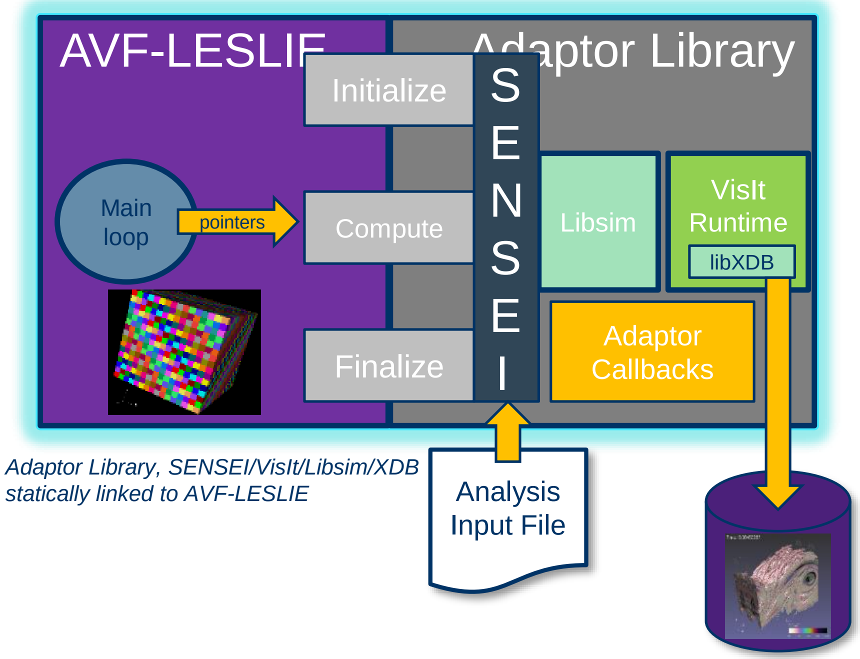
 $LIBSIM_COORDSURF
    FILE = slice
    NORMAL = 4,5,6
    POINT  = 1,2,3
    VARS = Density, Pressure
    $END

 $LIBSIM_COORDSURF_AXIS
    FILE = slicex
    AXIS = X
    INTERCEPT = 4.5
    VARS = Pressure, Density
    $END

 $LIBSIM_ISOSURF
    FILE = iso
    VALUES = 0.2, .4, .6, .8, 1, 1.2, 1.4, 1.6, 1.8, 2
    VARS = Density, Pressure, Enthalpy
    $END
```

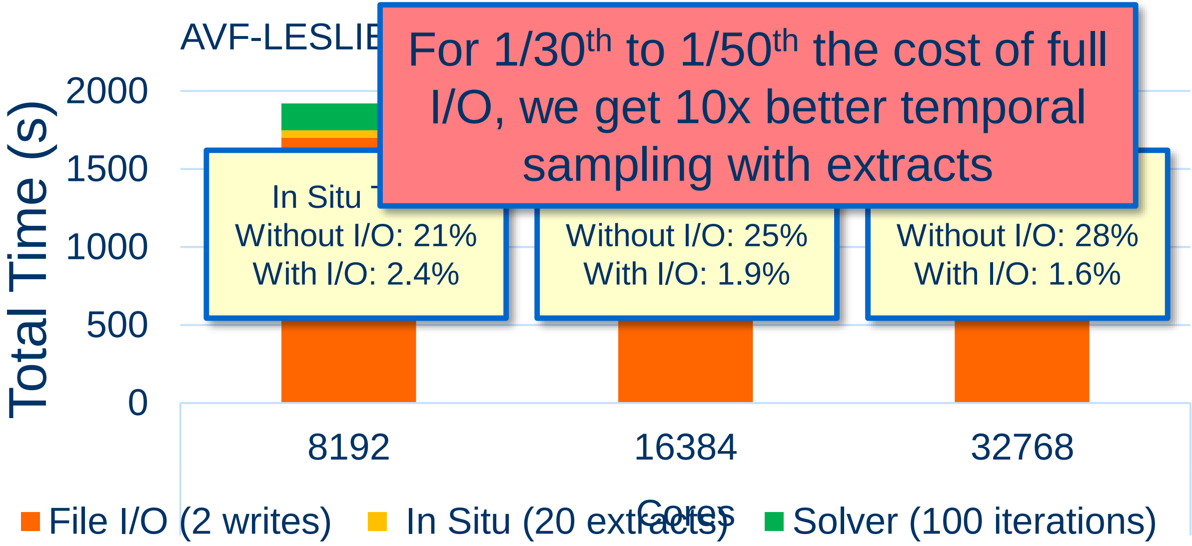
Instrumenting AVF-LESLIE simulation

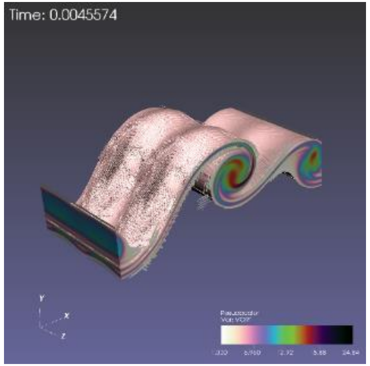
- Created adaptor library for AVF-LESLIE
- Calls Compute function when we want to generate extracts via SENSEI+Libsim
- Libsim adaptor in SENSEI directs Libsim to render or produce extracts and which are saved to XDB format

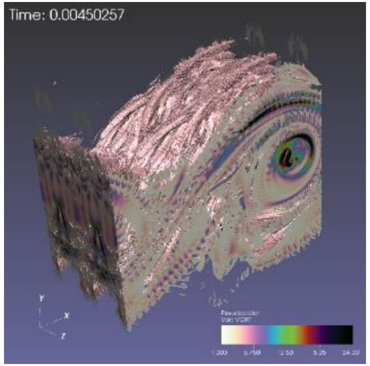


AVF-LESLIE in situ extract generation

- Combustion code / Turbulent mixing use case
- Save vorticity isosurface every 5th iteration to FieldView XDB format
- Write groups to partially aggregate extract I/O







Libsim information

- Information about instrumenting a simulation can be found at the following sources:
- Getting Data Into VisIt (https://wci.llnl.gov/codes/visit/2.0.0/GettingDataIntoVisIt2.0.0.pdf)
- VisIt Example Simulations (http://visit.ilight.com/trunk/src/tools/DataManualExamples/Simulations)
- VisIt Wiki (http://www.visitusers.org)
- VisIt Email List (visit-users@email.ornl.gov)

Computational Monitoring with ParaView Catalyst

ParaView Catalyst information

Functionality:

- Batch and interactive *in situ* analysis and visualization
- In transit workflows done with standalone ParaView, ADIOS and GLEAN
- Generate Catalyst Python scripts to drive *in situ* analysis and visualization output
- Image, data extract and Cinema database outputs
- Instrumented with Fortran, C, C++ and Python based simulation codes

Notable achievements:

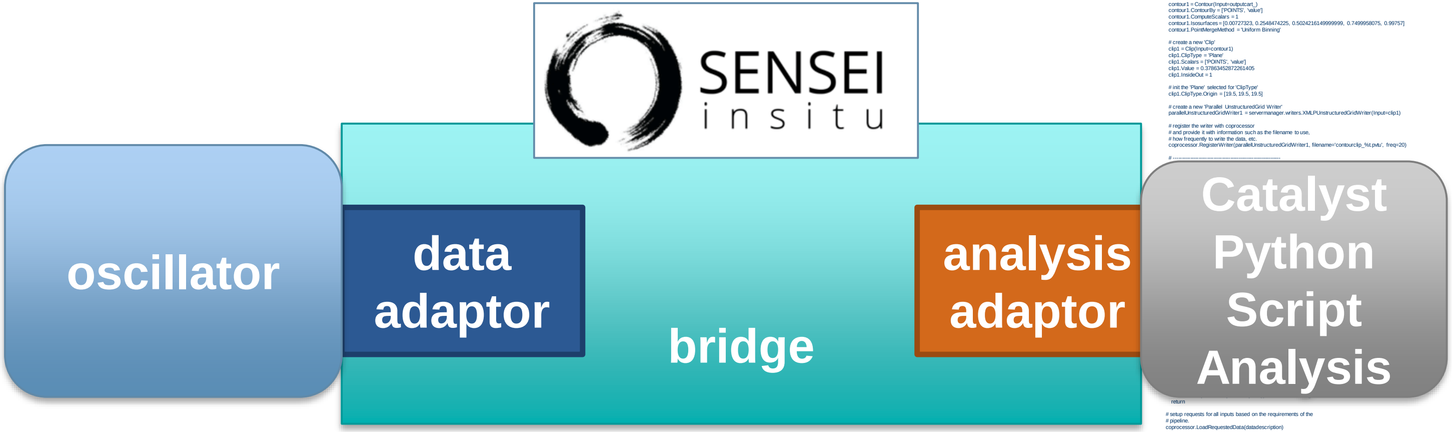
- Scaled to 1Mi MPI ranks on ALCF's Mira BG/Q
- SC16 visualization showcase winner generated animation using Catalyst
- HPCWire Best HPC Visualization Product or Technology
  - 2011 (VTK), 2012, 2014 (runner-up), 2016 Editor's Choice (ParaView)
  - 2015 Reader's Choice – tie (Paraview)
- Used on Cray, BlueGene, SGI, etc. HPC architectures

ParaView Catalyst computational steering

Capabilities:

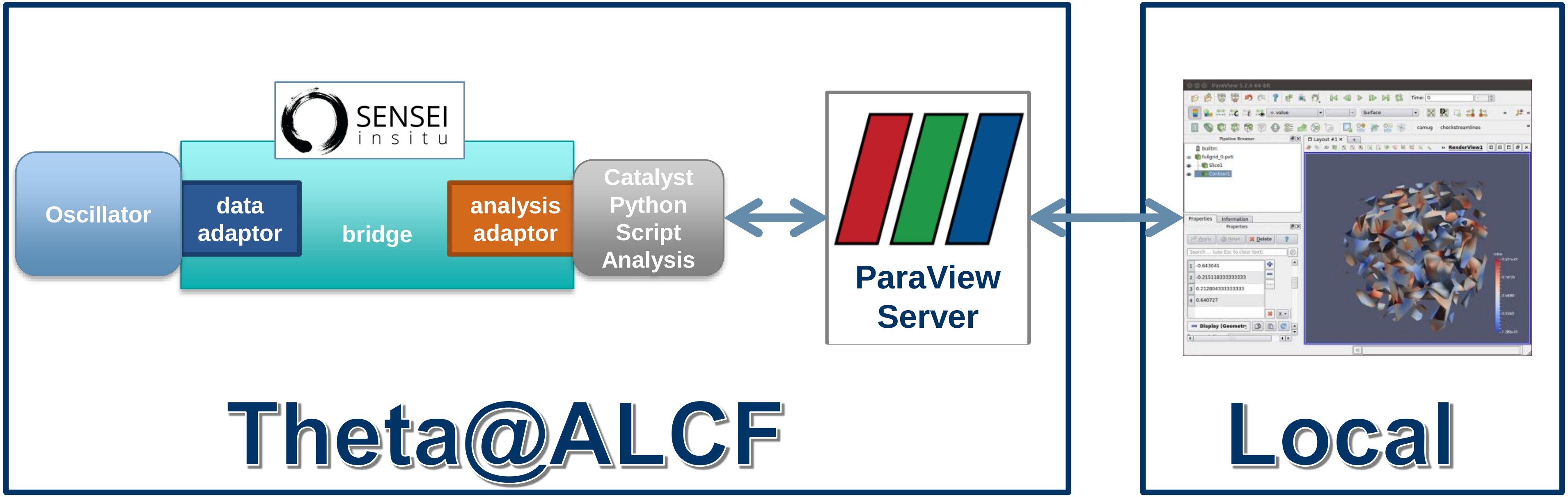
- Connect ParaView server to a running simulation
- ParaView server can be run separately (e.g. on HPC platform) or use the GUI’s built-in server
- Data can be extracted from Catalyst instrumented simulation to ParaView server
- Examine and change in situ analysis and visualization parameters
- Ability to disconnect and reconnect multiple times to a running simulation
- Can pause the simulation to examine results at specific points in the simulation

SENSEI example with Catalyst Python script



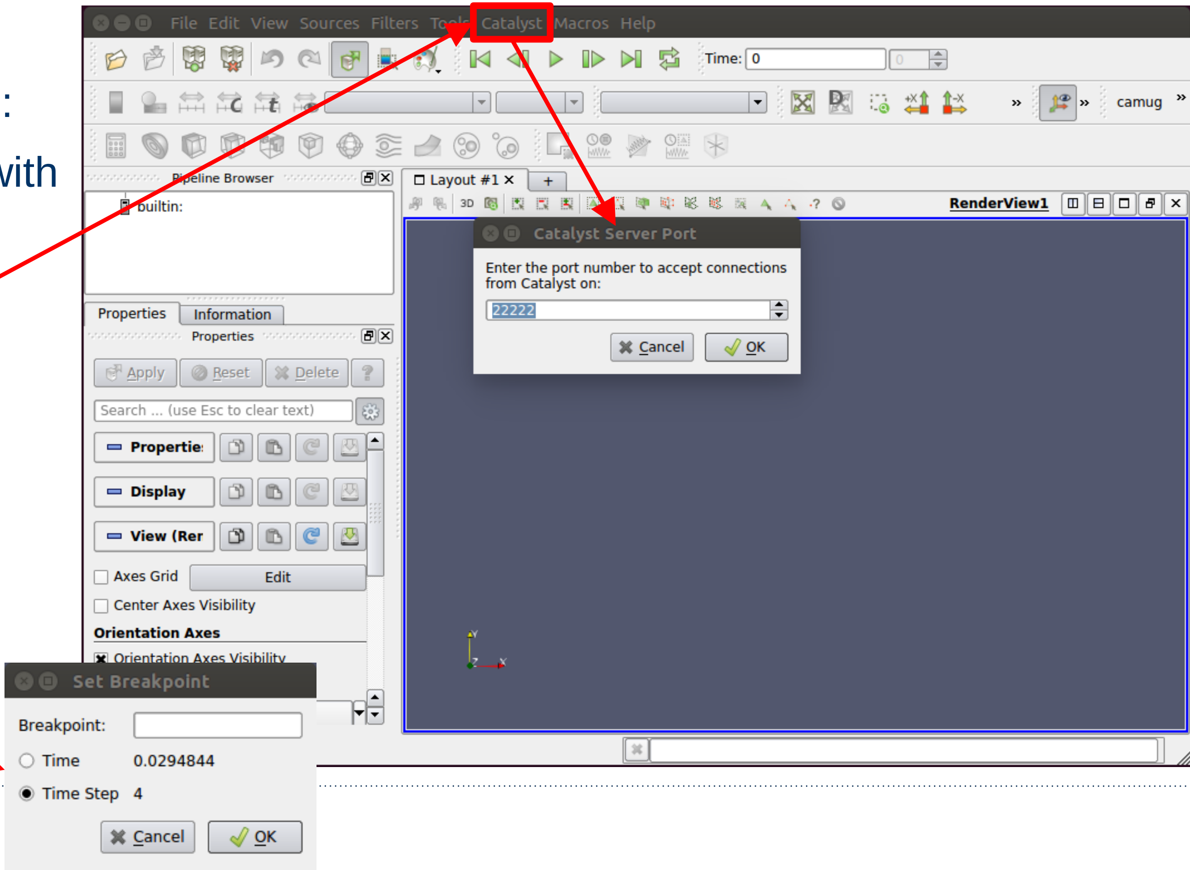

```
<sensei>
 <analysis type="catalyst" pipeline="pythonscript" filename="slice_contourcut.py"/>
</sensei>
```

Catalyst Live through Python script



Computational monitoring VM example

- In ~/SENSEIBuild directory, run:
- Simulation with Catalyst script with “mpirun –np 4 ./bin/oscillator -f steeringExample.xml OSCILLATORS.txt”
- ParaView with “paraview”
  - Catalyst Menu
    - Connect…
    - Pause Simulation
    - Continue
    - Set Breakpoint
    - Remove Breakpoint



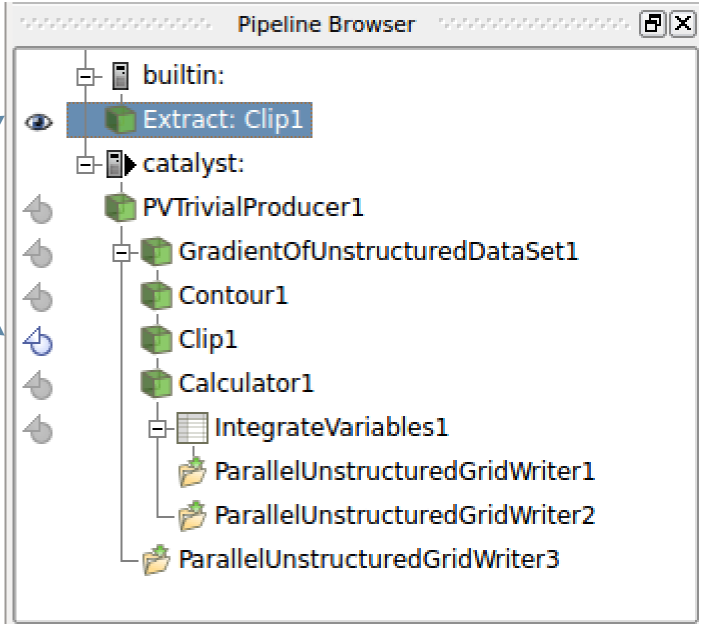
Live *in situ* example

Only transfer requested data from server (simulation run) to client

- Clip1 is already getting extracted

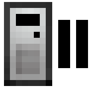
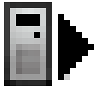
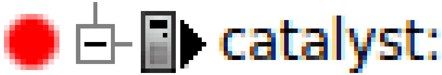
Click on to transfer to client from Catalyst

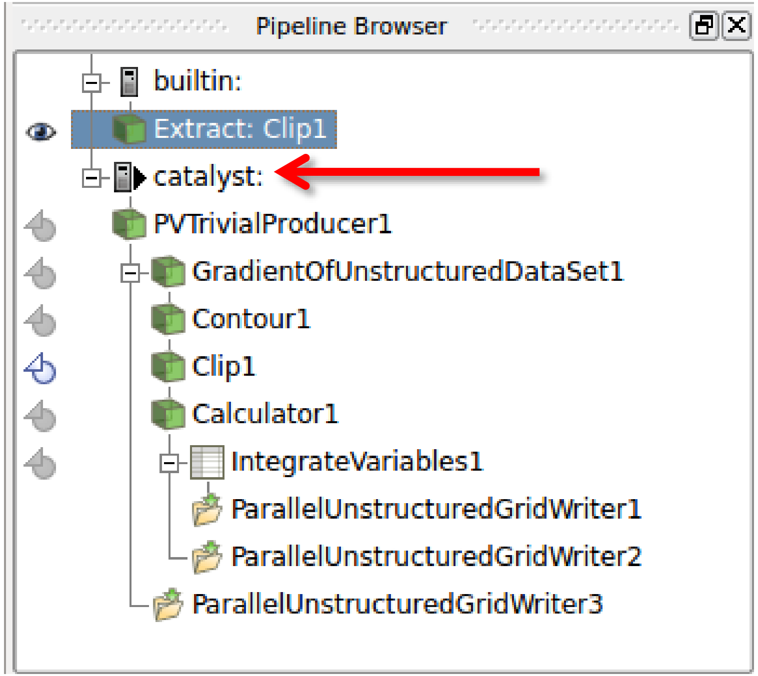
Use Delete on client to stop transferring to client

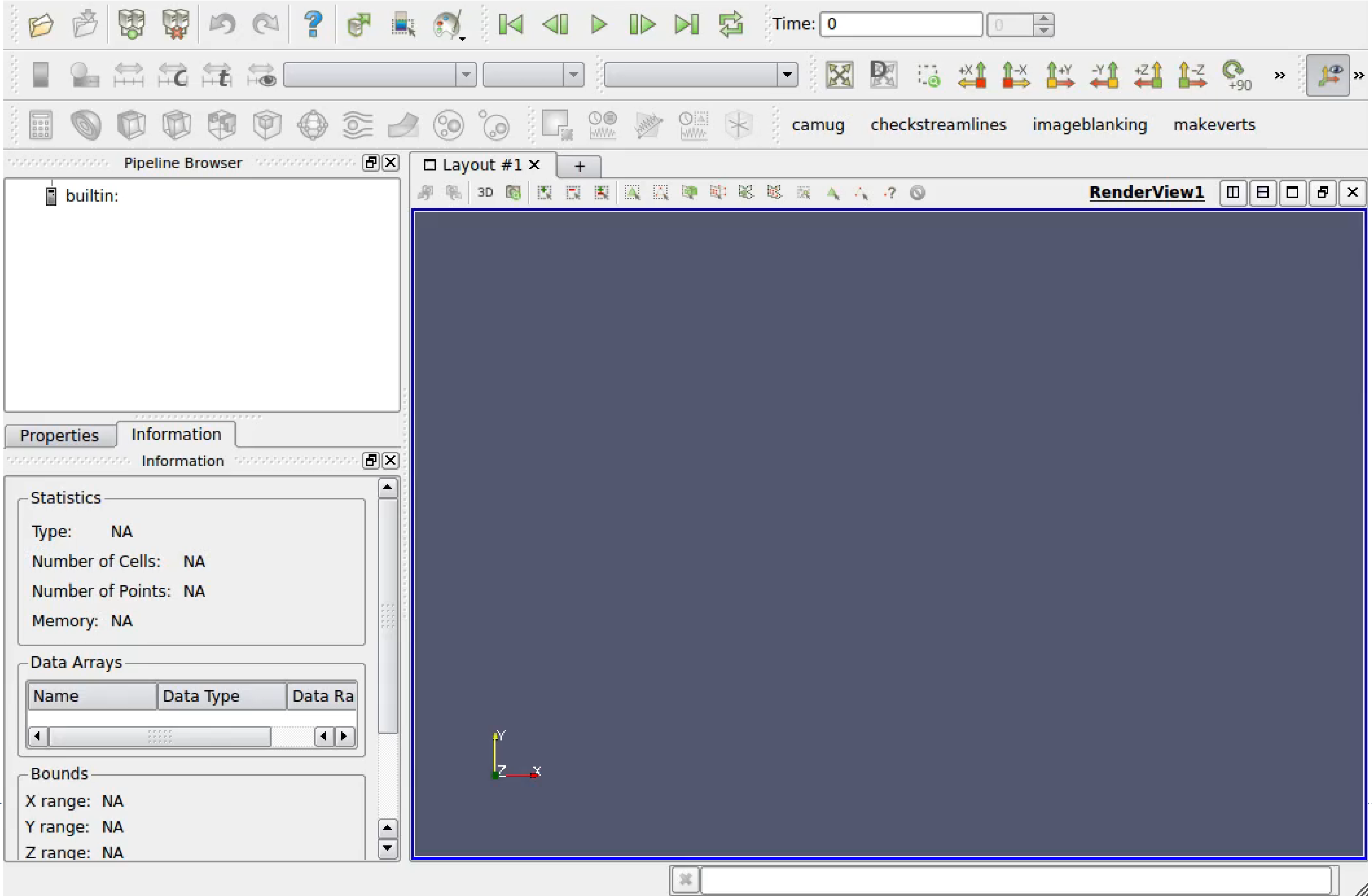


Catalyst Live GUI feedback

Three pieces of feedback

- Simulation paused 
- Simulation running 
- Simulation running with a breakpoint set 




Time: 0
camug
checkstreamlines
imageblanking
makeverts
Pipeline Browser
builtin:
Layout #1
RenderView1
3D
Properties
Information
Information
Statistics
Type: NA
Number of Cells: NA
Number of Points: NA
Memory: NA
Data Arrays
Name
Data Type
Data Ra
Bounds
X range: NA
Y range: NA
Z range: NA
Y
Z
X

ParaView Catalyst online help

ParaView User's Guide:

– http://www.paraview.org/paraview-guide

ParaView Catalyst User's Guide:

– http://www.paraview.org/files/catalyst/docs/ParaViewCatalystUsersGuide_v2.pdf

Email list:

– paraview@paraview.org

Websites:

– http://www.paraview.org
– http://www.paraview.org/in-situ/
– http://www.cinemascience.org/

Doxygen:

– http://www.vtk.org/doc/nightly/html/classes.html
– http://www.paraview.org/ParaView3/Doc/Nightly/html/classes.html

Sphinx:

– http://www.paraview.org/ParaView3/Doc/Nightly/www/py-doc/index.html

Articles & blog posts:

– http://www.kitware.com/source/home/post/170
– http://www.kitware.com/blog/home/post/606
– http://kitware.com/blog/home/post/722
– http://www.kitware.com/blog/home/post/737
– http://www.kitware.com/blog/home/post/752
– http://www.kitware.com/blog/home/post/733
– http://www.kitware.com/blog/home/post/709

SENSEI + Python

SENSEI is a powerful tool to connect simulations to visualization tools for in situ use. Here we show how to leverage this from a Python based simulation.

Python

Hidden

- it’s easy to use
- provides reasonable performance for the time you spend coding
- has numerous scientific computing packages saving even more time
- can be extended and/or optimized by C/C++ if needed

SENSEI's Python bindings

VTK's Python wrapper generator

- well suited for VTK’s needs, and not much else
- doesn’t wrap many methods due to types it doesn’t understand

SWIG - Simple Wrapper Interface Generator

- it’s automated and handles all types we have in our API
- can be taught to place nice with VTK’s wrapper generator

SENSEI uses SWIG to generate wrappers, and has code to make the two wrapping systems play nice with each other.

Adding a new analysis or data adaptor

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vtk.i A SWIG interface file defining 2 macros:

1. `VTK_SWIG_INTEROP(vtk_t)`

- defines typemaps for using VTK wrapped VTK classes in SWIG generated API (tells SWIG how to play nice with VTK)

2. `VTK_DERIVED(derived_t)`

- enable SWIG memory management for wrapped classes derived from VTK classes (VTK has unique reference counting implementation)

✅ Pass a VTK class to SENSEI

❌ Pass a SENSEI class to VTK

The path to SENSEI+Python

1. Optionally compile your back end (Catalyst, Libsim, ADIOS) with Python enabled.
   – or use existing analyses and API's exposed via C++
2. Compile SENSEI with Python features enabled
3. Use existing SENSEI analysis and data adaptors
   – or write your own
4. Instrument your simulation
5. Create back end specific analyses
   – See Catalyst, Libsim, ADIOS documentation for more info

Newton mini-app

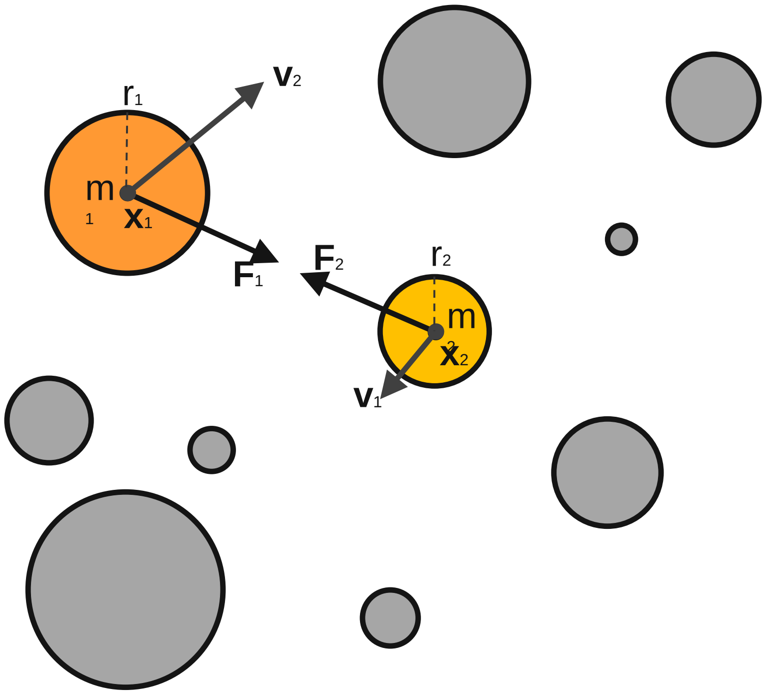
N-body Gravitational Simulation

```
x' = v

v' = F/m
```

Newton's law

```
F1 = F2 = G*m1*m2/r**2
```



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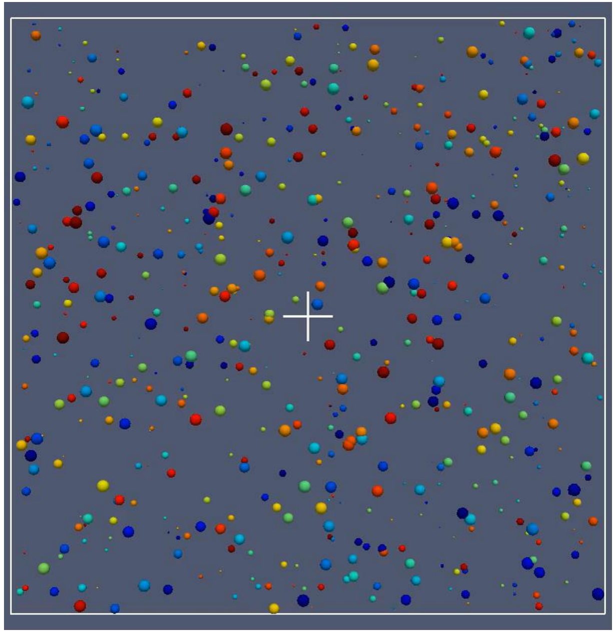
Newton mini-app

- direct solver, O(N**2)
  - Velocity Verlet
    - » second order, symplectic, conserves momentum exactly, time reversible
- the simplest possible code
  - a single file, <400 lines, to better focus on use of SENSEI interface
  - a production quality code could easily be thousands of lines (see NBODY6 ~6K lines)



Instrumenting the simulation

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```
if __name__ == '__main__':
    # parse the command line
    …

    # set up the initial condition
    n_bodies = args.n_bodies*n_ranks
    ic = uniform_random_ic(n_bodies, -5906.4e9, \
        5906.4e9, -5906.4e9, 5906.4e9, 10.0e24, \
        100.0e24, 1.0e3, 10.0e3)

    ids,x,y,z,m,vx,vy,vz,fx,fy,fz = ic.allocate()
    h = args.dt if args.dt else ic.get_time_step()

    # run the sim and analysis
    i = 1
    while i <= args.n_its:
        velocity_verlet(x,y,z,m,vx,vy,vz,fx,fy,fz,h)
        i += 1
```

Instrumenting the simulation

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# set up the initial condition
n_bodies = args.n_bodies*n_ranks
ic = uniform_random_ic(n_bodies, -5906.4e9, \
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ids,x,y,z,m,vx,vy,vz,fx,fy,fz = ic.allocate()
h = args.dt if args.dt else ic.get_time_step()

# create an analysis adaptor
adaptor = analysis_adaptor()
adaptor.initialize(args.analysis, args.analysis_opts)

# run the sim and analysis
adaptor.compute(0,0,ids,x,y,z,m,vx,vy,vz,fx,fy,fz)
i = 1
while i <= args.n_its:
    velocity_verlet(x,y,z,m,vx,vy,vz,fx,fy,fz,h)
    adaptor.compute(i,i*h,ids,x,y,z,m,vx,vy,vz,fx,fy,fz)
    i += 1

# finish up
adaptor.finalize()
```

Interface to SENSEI (aka the bridge)

```
class analysis_adaptor:
    def __init__(self):
        self.DataAdaptor = sensei.VTKDataAdaptor.New()
        self.AnalysisAdaptor = None

    def initialize(self, analysis, args=''):
        # select and configure SENSEI analysis adaptor
        …

    def finalize(self):
        if self.Analysis == 'posthoc':
            self.AnalysisAdaptor.Finalize()

    def compute(self,
   i,t,ids,x,y,z,m,vx,vy,vz,fx,fy,fz):
        # convert simulation data to VTK
        # invoke the analysis
        …
```

- Our analysis adaptor selects and configures and drives one of a number of SENSEI analysis adaptors
- Manages an instance of SENSEI VTK data adaptor to which we will create and pass VTK objects to
  - alternative is a custom data adaptor written in C++ that does this in a more transparent manner

Initializing the back end

```
def initialize(self, analysis, args=''):
    self.Analysis = analysis
    args = csv_str_to_dict(args)
    # Libsim
    if analysis == 'libsim':
        self.AnalysisAdaptor = sensei.LibsimAnalysisAdaptor.New()
        self.AnalysisAdaptor.AddPlots('Pseudocolor','ids', False,False, \
            (0.,0.,0.),(1.,1.,1.),sensei.LibsimImageProperties())
    # Catalyst
    elif analysis == 'catalyst':
        if check_arg(args,'script'):
            self.AnalysisAdaptor = sensei.CatalystAnalysisAdaptor.New()
            self.AnalysisAdaptor.AddPythonScriptPipeline(args['script'])
    # VTK I/O
    elif analysis == 'posthoc':
        if check_arg(args,'file','newton') and check_arg(args,'dir','./') \
            and check_arg(args,'mode','0') and check_arg(args,'freq','1'):
            self.AnalysisAdaptor = sensei.VTKPosthocIO.New()
            self.AnalysisAdaptor.Initialize(comm, args['dir'],args['file'], \
                [],['ids','fx','fy','fz','f','vx','vy','vz','v','m'], \
                int(args['mode']),int(args['freq']))
    # ADIOS, etc
    elif analysis == 'configurable':
        if check_arg(args,'config'):
            self.AnalysisAdaptor = sensei.ConfigurableAnalysis.New()
            self.AnalysisAdaptor.Initialize(comm, args['config'])

    if self.AnalysisAdaptor is None:
        status('ERROR: Failed to initialize "%s"\n'%(analysis))
        sys.exit(-1)
```

Select and configure one of the existing SENSEI analysis adaptors from command line arguments

Invoking in situ back end

```python
def compute(self, i,t,ids,x,y,z,m,vx,vy,vz,fx,fy,fz):

    status('% 5d\n'%(i)) if i > 0 and i % 70 == 0 else
   None
    status('.')

    # construct VTK a dataset
    node =
   points_to_polydata(ids,x,y,z,m,vx,vy,vz,fx,fy,fz)
    mb = vtk.vtkMultiBlockDataSet()
    mb.SetNumberOfBlocks(n_ranks)
    mb.SetBlock(rank, node)

    # pass it to the data adaptor
    self.DataAdaptor.SetDataTime(t)
    self.DataAdaptor.SetDataTimeStep(i)
    self.DataAdaptor.SetDataObject(mb)

    # execute the in situ analysis
    self.AnalysisAdaptor.Execute(self.DataAdaptor)

    # free up memory
    self.DataAdaptor.ReleaseData()
```

1. create and pass Multi-block (tree based) dataset to SENSEI data adaptor
   - each rank is responsible for a leaf in the tree
2. pass time and step number to data adaptor
3. invoke the SENSEI analysis adaptor
4. release memory held in the adaptor

VTK multi-block leaf data set

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```
def points_to_polydata(ids,x,y,z,m,vx,vy,vz,fx,fy,fz):
    nx = len(x)
    # convert simulation to VTK data structures
    v_pts = to_vtk_points(nx,x,y,z)
    v_cells = to_vtk_cells(nx)
    v_ids = to_vtk_scalars(nx,'ids',ids)
    v_m = to_vtk_scalars(nx,'m',m)
    v_v,v_mv = to_vtk_vector(nx,'v',vx,vy,vz)
    v_f,v_mf = to_vtk_vector(nx,'f',fx,fy,fz)
    # package it all up in a poly data set
    pd = vtk.vtkPolyData()
    pd.SetPoints(pts)
    pd.GetPointData().AddArray(v_ids)
    pd.GetPointData().AddArray(v_m)
    pd.GetPointData().AddArray(v_v)
    pd.GetPointData().AddArray(v_mv)
    pd.GetPointData().AddArray(v_f)
    pd.GetPointData().AddArray(v_mf)
    pd.SetVerts(cells)
    return pd
```

Strategy

1. create VTK arrays
2. pass them to a VTK dataset

Who owns what?

- VTK uses reference counting. Python does too. Unfortunately they don't talk to each other without some extra code.
- Tell VTK to make a deep copy if the array goes out of scope

Dataset geometry

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```
def to_vtk_points(nx,x,y,z):
    xyz = np.empty(3*nx, dtype=np.float32)
    xyz[::3] = x[:]
    xyz[1::3] = y[:]
    xyz[2::3] = z[:]
    vxyz = vtknp.numpy_to_vtk(xyz, deep=1)
    vxyz.SetNumberOfComponents(3)
    vxyz.SetNumberOfTuples(nx)
    pts = vtk.vtkPoints()
    pts.SetData(vxyz)
    return pts

def to_vtk_cells(nx):
    cids = np.empty(2*nx, dtype=np.int32)
    cids[::2] = 1
    cids[1::2] = np.arange(0,nx,dtype=np.int32)
    cells = vtk.vtkCellArray()
    cells.SetCells(nx, vtknp.numpy_to_vtk(cids, \
        deep=1, array_type=vtk.VTK_ID_TYPE))
    return cells
```

Strategy

1. create an empty array
2. interleave x,y,z components or cell length and point ids
3. pass new array to VTK data structure

TODO – test new zero copy stuff from DG

Array based data

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```
def to_vtk_scalars(nx,name,s):
    scalar = vtknp.numpy_to_vtk(s, deep=1)
    scalar.SetName(name)
    return scalar

def to_vtk_vector(nx,name,vx,vy,vz):
    # vector in interleaved layout
    vxyz = np.zeros(3*nx, dtype=np.float32)
    vxyz[::3] = vx
    vxyz[1::3] = vy
    vxyz[2::3] = vz
    vector = vtknp.numpy_to_vtk(vxyz, deep=1)
    vector.SetName('v')
    # magnitude
    mv = np.sqrt(vx**2 + vy**2 + vz**2)
    mag = vtknp.numpy_to_vtk(mv, deep=1)
    mag.SetName('mag%s'%(name))
    return vector,mag
```

Scalars

1. pass new array to VTK data structure

Vectors/Tensors

1. create an empty array
2. interleave components
3. pass new array to VTK data structure

TODO – test new zero copy stuff from DG

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Leveraging ADIOS for in transit rendering

Demo

Demo parameters

- Run Newton simulation on 2 cores on node 1
- ADIOS moves data to node 2
- Libsim or Catalyst render on 2 cores on node 2

Simulation→ADIOS Analysis Adaptor

End-point → ADIOS Data Adaptor → Catalyst/Libsim

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Measuring the cost of *in situ*

Two questions:

How much overhead associated with use of *in situ* methods, infrastructure (runtime, memory)?

Does this change with varying concurrency?

Additionally:

In situ and in transit configurations

In situ and *post hoc:* end-to-end comparison

U. Ayachit, A. Bauer, E. P. N. Duque, G. Eisenhauer, N. Ferrier, J. Gu, K. E. Jansen, B. Loring, Z. Lukic, S. Menon, D. Morozov, P. O'Leary, R. Ranjan, M. Rasquin, C. P. Stone, V. Vishwanath, G. H. Weber, B. Whitlock, M. Wolf, K. Wu, and E. W. Bethel. Performance Analysis, Design Considerations, and Applications of Extreme-scale In Situ Infrastructures. In Proceedings of SC16, November 2016.

Methodology for measuring cost of *in situ*

Miniapplication: data source (next slide)

In situ methods

- Histogram computation
- Autocorrelation computation (temporal analysis)
- Extract and render a 2D slice from a 3D volume

In situ infrastructures

- VisIt/Libsim
- ParaView/Catalyst
- ADIOS

Measure:

- Runtime and memory footprint
- At varying levels of concurrency
- One-time and recurring

Test Platform

Cori Phase I at NERSC
Cray XC system
1630 compute nodes
Dual 2.3Ghz 16-core Intel Haswell processors
128GB RAM/node

Concurrency levels of tests:
812 (~1K)
6496 (~6K)
45440 (~45K)

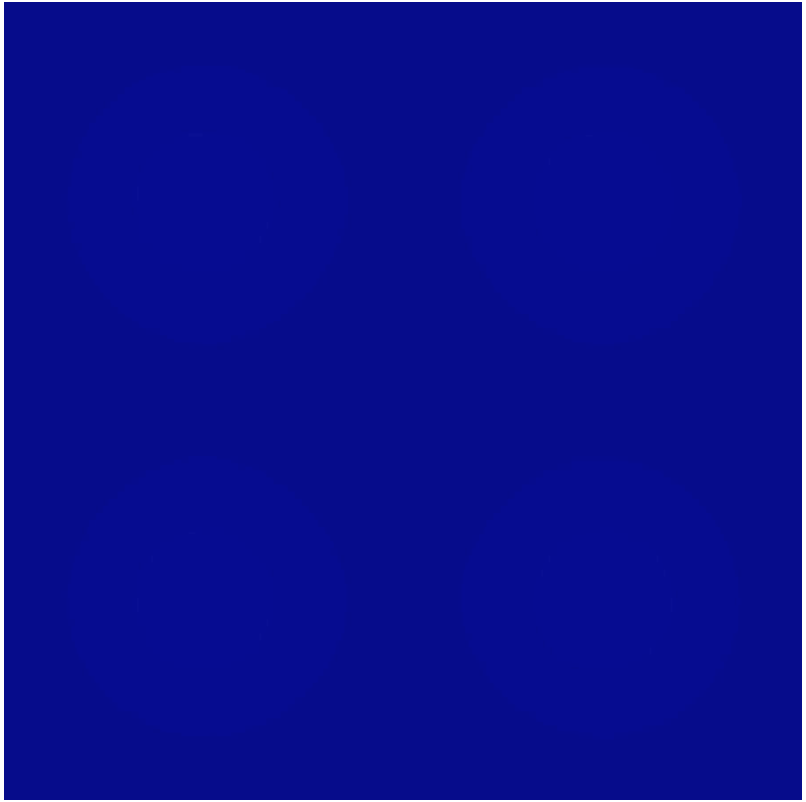
Miniapplication - oscillators

Bulk-synchronous parallel computation of periodic, damped oscillators (MPI-based app)

No interprocess communication - entirely analytic, embarassingly parallel

For *m* oscillators and per-rank grid size of N^3:

- Per-rank memory footprint: $2N^3$
- Per-rank complexity: mN^3



Miniapp configurations – *in situ* methods

Configuration	Intention
Original	Miniapp with no SENSEI interface, no I/O. Direct-coupling (subroutine call) to analysis methods Measure runtime/memory with no *in situ*
Baseline	Miniapp with the SENSEI interface enabled No analysis or I/O Measure overhead of *in situ* interface in isolation
Histogram	Miniapp+SENSEI interface+histogram computation No *in situ* infrastructures Compare performance to *Original, Baseline*
Autocorrelation	Miniapp+SENSEI interface+autocorrelation computation No *in situ* infrastructures Compare performance to *Original, Baseline*

Miniapp configurations – with *in situ* infrastructures

Configuration	Intention
Catalyst-slice	Miniapp + SENSEI interface + Catalyst Catalyst performs a 2D slice extraction of 3D volume Followed by parallel rendering, produces an image Compare to *Original, Baseline*
Libsim-slice	Miniapp + SENSEI interface + Libsim Libsim performs a 2D slice extraction of 3D volume Followed by parallel rendering, produces an image Compare to *Original, Baseline*
ADIOS-FlexPath	Miniapp + SENSEI interface + ADIOS/FlexPath In transit implementation of histogram, autocorrelation, Catalyst-slice Compare to *Original, Baseline*

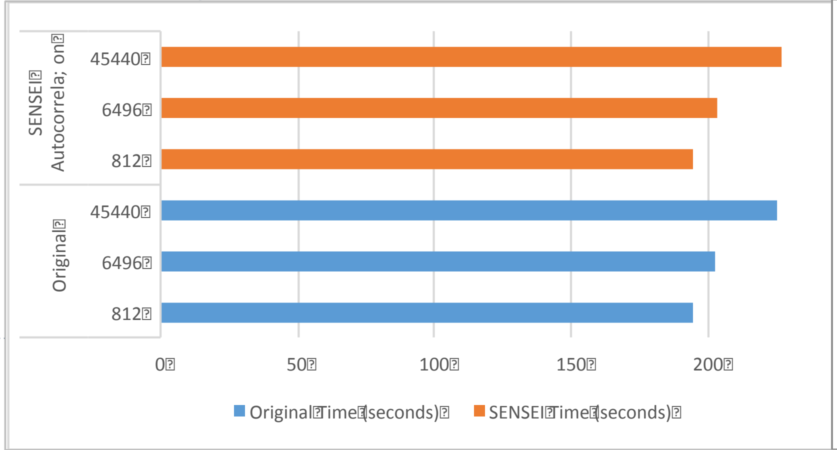
Measuring impact of SENSEI interface

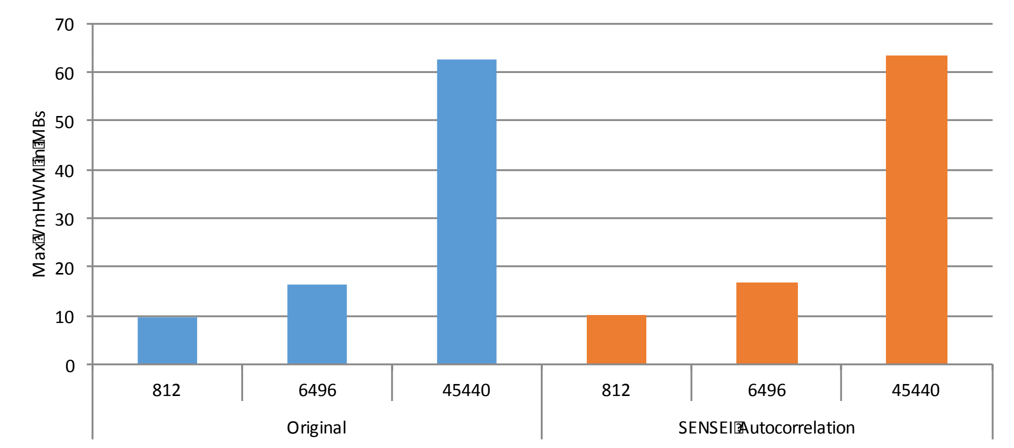
Run *Original* and *Baseline* configs, 3 levels of concurrency: 1K, 6K, 45K

- Original: miniapp + subroutine called autocorrelation
- Baseline: miniapp + SENSEI bridge to autocorrelation

Compare runtime (left), memory footprint (right)

No significant difference reflects zero-copy nature of the interface





Comparing *in situ* to *post hoc*

Post hoc configuration

- Simulation computes something
- Then writes results to disk
- Post hoc method reads from disk and performs analysis

In Situ configuration

- Simulation computes something
- Then *in situ* method computes something
- (No disk I/O involved)

Post hoc study concurrency

Simulation	Postprocess
812	82
6496	650
45440	4545

Weak-scaling Study

- Measure post hoc end-to-end cost
  - Sim writes, post hoc reads, processing
- Compare to *in situ* configurations
- Also measure time-to-solution for 100 timesteps

Post hoc: cost of writes

Baseline miniapp with the addition of parallel I/O

- VTK I/O, non-collective
- MPI-IO collective is slower (see the paper)
- This is not an I/O study. ☺ We used the fastest I/O approach we could get our hands on.

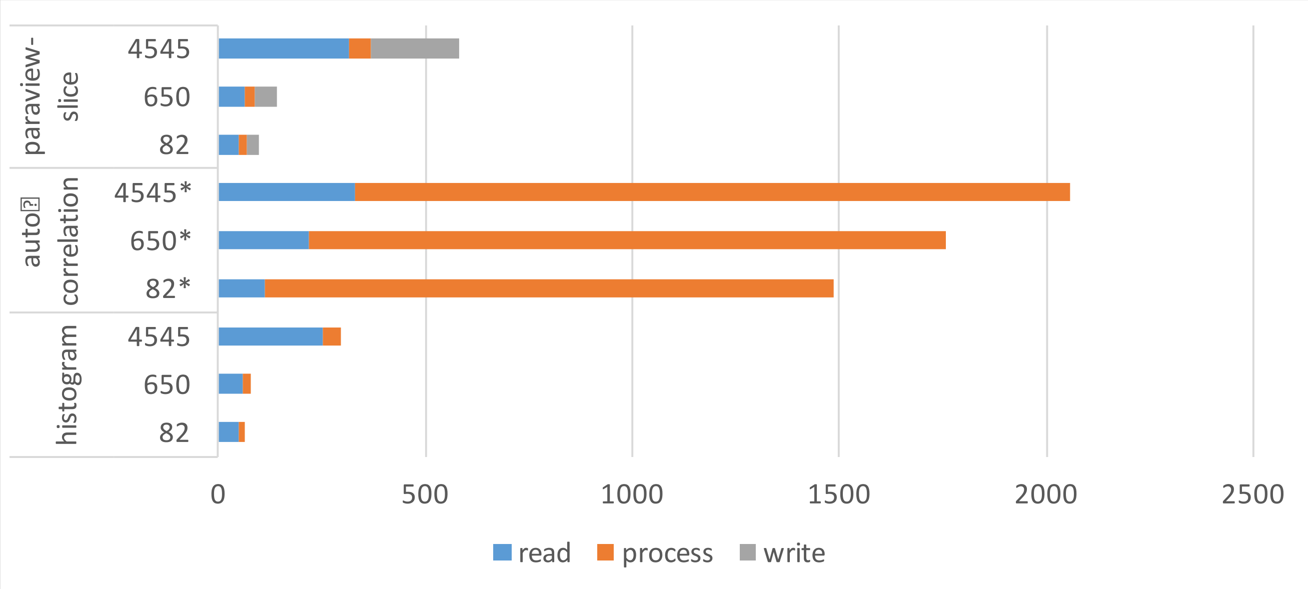
Weak-scaling: linear increase with problem size

I/O cost is significant at high concurrency

Cost of Writes

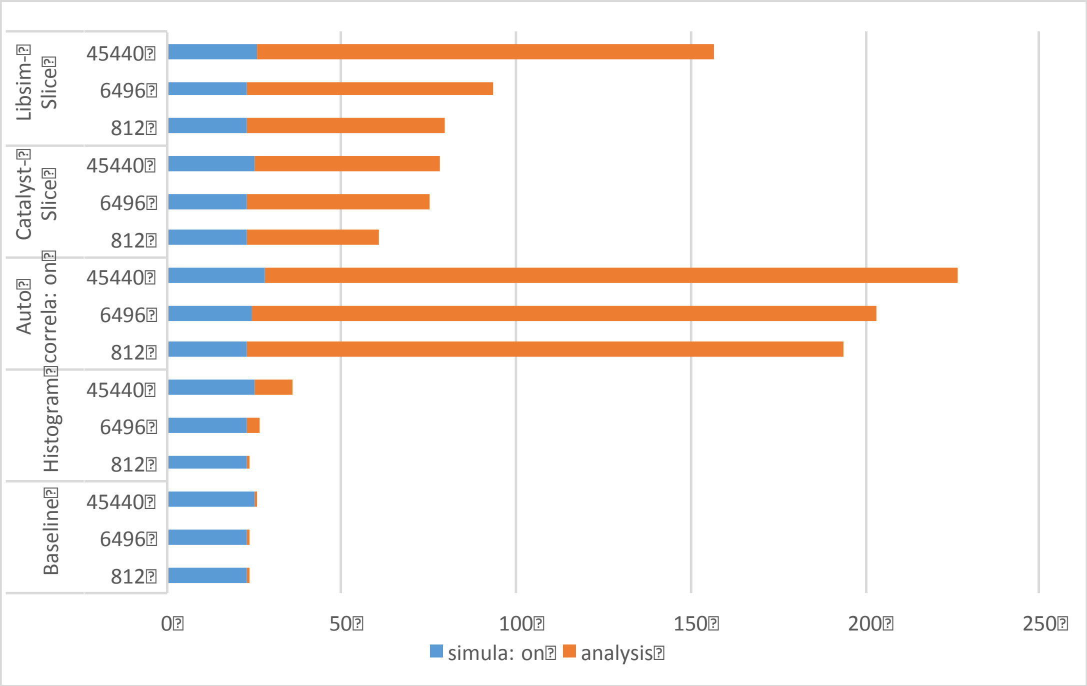
Concurrency	1 step	Aggregate
812	2 GB, 0.12s	0.2 TB, 12s
6496	16 GB, 0.67s	1.6 TB, 67s
45440	123 GB. 9.05s	12.3 TB, 905s

Post hoc: cost of reads + processing



Time required for reads, processing, and writing (results) for post hoc methods at varying level of concurrency.

In situ: time-to-solution



Post hoc vs. *in situ* time to solution

Configuration (45K)	*In Situ*	Post hoc: sim + write + read + process
Histogram	~40s	~1200s = ~25s + ~905s + ~300s + (a few secs)
Autocorrelation	~225s	~2930s = ~25s + ~905s + ~300s + ~1700s
Catalyst-slice	~80s	~1505s = ~25s + ~905s + ~300s + ~275s

Post hoc fixed costs (at 45K): about 1200s and 12.3 TB disk space

Fewer ranks for analysis processing results in longer analysis runtime (in this 1:10 configuration, which is typical for post hoc use cases)

Three key performance analysis focus areas

One-time costs: initialization

- Some *in situ* setups may entail non-zero initialization costs, e.g.:
  - Per-rank config file processing
- Hero-sized runs reveal such things, remedy with straightforward engineering work

Recurring costs

- Execution time:
  - Different methods require differing amounts of computation
  - Algorithmic complexity at scale
  - *In situ* methods that use reductions
- Memory consumption
  - Temporal analysis methods must buffer more data

One-time costs: finalization

- Some *in situ* setups may entail non-trivial initialization costs, e.g.:
  - Global reductions
- Gives insights into ways to optimize

What is the cost of *in situ* processing?

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Concern: simulations want to use all available resources, so having an understanding of *in situ* resource utilization is useful.

In other words: In situ infrastructure must play nicely with simulation

Full details in SC16 paper: Utkarsh Ayachit, Andrew Bauer, Earl P. N. Duque, Greg Eisenhauer, Nicola Ferrier, Junmin Gu, Kenneth E. Jansen, Burlen Loring, Zarija Lukic, Suresh Menon, Dmitriy Morozov, Patrick O'Leary, Rateesh Ranjan, Michel Rasquin, Christopher P. Stone, Venkat Vishwanath, Gunther H. Weber, Brad Whitlock, Matthew Wolf, K. John Wu, and E. Wes Bethel, Performance Analysis, Design Considerations, and Applications of Extreme-scale In Situ Infrastructures. In Proceedings of SC16, November 2016.

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Shared resources

- Initialization costs need to be monitored
  - Static build options important as HPC simulation size increases
  - Initialization costs do get amortized
- Finalization costs can be a factor for certain in situ algorithms
- Memory costs can be a factor
  - Shared memory usage for simulation and in situ arrays ("zero copy")
  - Request only needed arrays through the DataAdaptor's AddArray() method
  - Some analysis algorithms can require a lot of memory
  - Autocorrelation could potentially need to store full data at each time step. Use autocorrelation window size to reduce the amount of time steps stored

In situ compute

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- In situ computation may not need to be done every time step
  - Lower fidelity time stepping output
  - Only when something “interesting” is happening

- Can still reduce output size
  - Image output is fixed size and independent of simulation size
  - Coarsen data extracts
  - Compute summary statistics (e.g. autocorrelation, histogram)

Measuring impact of SENSEI interface

Hidden

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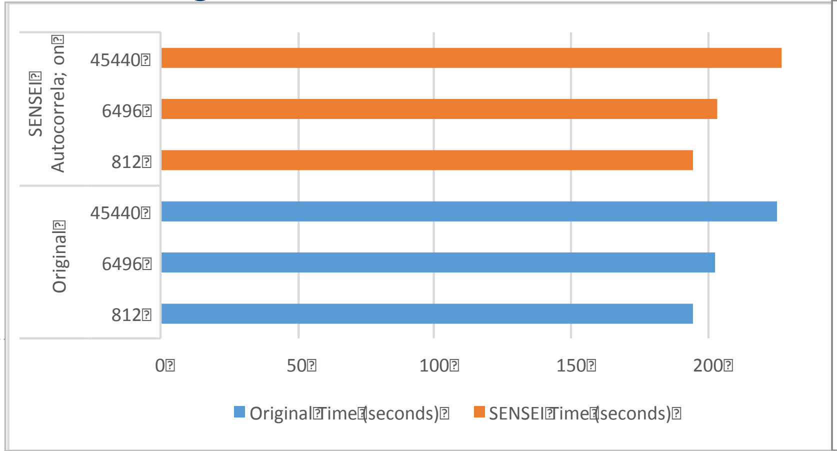

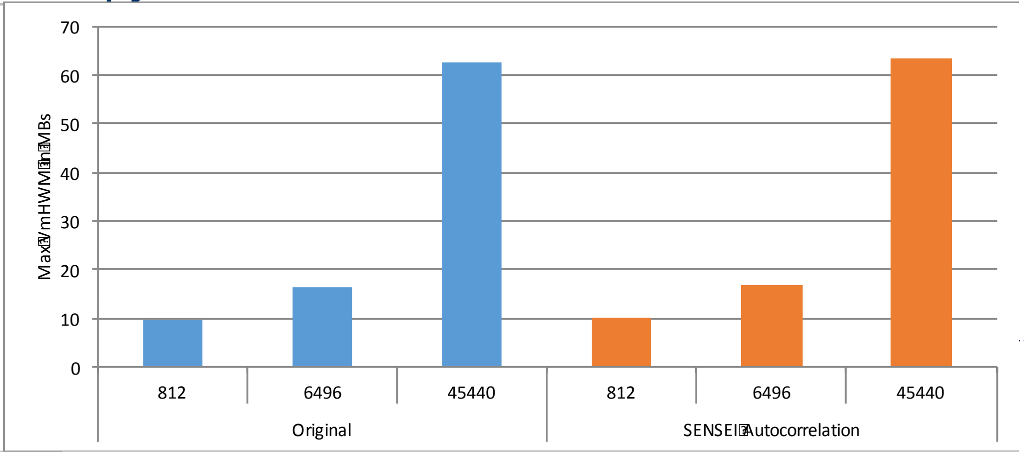

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SC17 In Situ Tutorial Summary

- Why should you care about *in situ?*
  - Flops >> I/O; *in situ* is a viable approach for coping with this problem
- What *in situ* infrastructures are available?
- What about interfacing my sim code to them?
- What are the performance issues to be thinking about?

Tutorial evaluation

- Was this tutorial useful to you?
- Were there any subjects you'd like to see covered?
  - More of some?
  - Less of others?
- Please provide SC17 with tutorial feedback
- Also, can provide feedback to us at:
  - Andy Bauer: andy.bauer@kitware.com
  - Wes Bethel: ewbethel@lbl.gov

Conclusions and future work

Write once, use everywhere

Easy to add new analysis/frameworks

Understanding data transformation costs

Data Model: supporting arbitrary layouts for connectivity

Bigger runs – current best is 1Mi MPI processes on Mira@ALCF

More examples, tutorials, improved docs, etc.

SENSEI: Scalable Analysis Methods and *In Situ* Infrastructure for Extreme Scale Knowledge Discovery

This work is supported by the Director, Office of Science, Office of Advanced Scientific Computing Research, of the U.S. Department of Energy, Office of Advanced Scientific Computing Research, under Contract No. DE-AC02-05CH11231, through the grant "**Scalable Analysis Methods and *In Situ* Infrastructure for Extreme Scale Knowledge Discovery**," program managers Dr. Lucy Nowell and Dr. Laura Biven.

Links

- Main page – http://www.sensei-insitu.org/
- Software repo – https://gitlab.kitware.com/sensei/sensei
- GLEAN – https://www.alcf.anl.gov/glean
- ADIOS – https://www.olcf.ornl.gov/center-projects/adios/
- VisIt/Libsim – https://www.visitusers.org/index.php?title=Category:Libsim
- ParaView Catalyst – http://www.paraview.org/in-situ/

Acknowledgment

This work is supported by the Director, Office of Science, Office of Advanced Scientific Computing Research, of the U.S. Department of Energy, Office of Advanced Scientific Computing Research, under Contract No. DE-AC02-05CH11231, through the grant "**Scalable Analysis Methods and *In Situ* Infrastructure for Extreme Scale Knowledge Discovery**," program managers Dr. Lucy Nowell and Dr. Laura Biven.

SENSEI: Scalable Analysis Methods and *In Situ* Infrastructure for Extreme Scale Knowledge Discovery

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THE
END