In Situ Analysis and Visualization with SENSEI

Why in situ?

The difference between our ability to generate data and our ability to move it results in lost science.
SENSEI: Scalable Environments for Scientific Explorations In Situ

4 Project Pillars

• R&D for scalable infrastructure and methods to work around FLOPS-I/O bottleneck
• Generic infrastructure maximizes portability and preserves investment in DOE codes
• Science code team partnerships focus and prove R & D
• Outreach and community engagement make the technology accessible
Science Engagements

Phasta + Catalyst, 1M Cores, Mira

AVF Leslie + Libsim, 131K Cores Cori

LAMMPS + OSPray, interactive, Theta

Henson Gadget, 8192 Cores Edison

Warp + Libsim, 16k Cores Edison

Where do these codes come from?
DOE Office of Science: HEP, BES, BER
High Energy Physics (HEP)
Basic Energy Sciences (BES)
Biological and Environmental Research (BER)
Academic research community, then picked up and extended/used by DOE, DoD, others.
SENSEI In situ Infrastructure

*Write once run everywhere* - use any simulation with any visualization/analysis and easily swap back-ends at run time

SENSEI enables connection of simulation data sources to visualization and analysis back ends through a data model and API.

Simulations get run-time interchangeability of analysis/vis codes.

Analysis/vis codes can consume data from any simulation.
## Delivables

<table>
<thead>
<tr>
<th>Focus Area</th>
<th>Co-leads</th>
</tr>
</thead>
<tbody>
<tr>
<td>expanding the data model</td>
<td>Andrew Bauer (Kitware), Brad Whitlock (Intelligent Light)</td>
</tr>
<tr>
<td>bidirectional data movement</td>
<td>Patrick O’Leary (Kitware), Matthew Wolf (ORNL)</td>
</tr>
<tr>
<td>design/execution patterns</td>
<td>Dmitriy Morozov (LBNL), Dave Pugmire (ORNL)</td>
</tr>
<tr>
<td>scaling to next-generation systems</td>
<td>Nicola Ferrier (ANL), John Wu (LBNL)</td>
</tr>
<tr>
<td>outreach, code team partnerships, cookbook, workshops</td>
<td>Gunther Weber (LBNL), Matthew Wolf (ORNL)</td>
</tr>
<tr>
<td>software products, distribution, releases</td>
<td>Earl Duque (Intelligent Light), Patrick O’Leary (Kitware)</td>
</tr>
</tbody>
</table>
Expanding the data model
Bidirectional data movement supports more science use case scenarios; eg, computational steering
Design and execution patterns

Research focus areas:
• MxN data redistribution
• Depth of copies
• Bidirectional: interface, pipeline management
• Leveraging arch features like NVRAM for staging
• Leveraging 3rd party tools like TensorFlow for ML-based analytics
• Specific science app use case drivers

N producer ranks, N consumer ranks
Unidirectional data movement/control
(N:N:1)

M producer ranks, N consumer ranks
Unidirectional data movement/control
(M:N:1)

M producer ranks, N consumer ranks
Bidirectional data movement/control
(M:N:2)

M producer ranks, N1 and N2 consumer ranks,
Unidirectional data movement/control
(M:<N1, N2>:1)
data model
What simulation data types does SENSEI support?

- Many more purpose specific and esoteric data types are supported by VTK.
- No explicit dependence on other parts of VTK such as i/o, filters, rendering, etc etc.

vtkDataObject

- AMR
- Multi-"block"
- Uniform Cartesian
- Stretched Cartesian
- Curvilinear (logically Cartesian)
- Unstructured/FEM
- PIC/Point cloud
- Molecular
- Tabular
- Graphs
- Array Collection (no geometry)
Speed & Efficiency

zero copy layouts provide pointer equivalent performance

• Array of Structures (AOS)
  — single array with components interleaved
  \[ v = \begin{pmatrix} x_1 & y_1 & z_1 & x_2 & y_2 & z_2 & \ldots & x_n & y_n & z_n \end{pmatrix} \]

• Structure of Arrays (SOA)
  — each component in its own arrays
  \[ \begin{align*}
v_x & = \begin{pmatrix} x_1 \end{pmatrix}, \begin{pmatrix} x_2 \end{pmatrix}, \ldots, \begin{pmatrix} x_n \end{pmatrix} \\
v_y & = \begin{pmatrix} y_1 \end{pmatrix}, \begin{pmatrix} y_2 \end{pmatrix}, \ldots, \begin{pmatrix} y_n \end{pmatrix} \\
v_z & = \begin{pmatrix} z_1 \end{pmatrix}, \begin{pmatrix} z_2 \end{pmatrix}, \ldots, \begin{pmatrix} z_n \end{pmatrix} \end{align*} \]

// VTK's default is AOS, no need to use vtkAOSDataArrayTemplate
vtkDoubleArray *aos = vtkDoubleArray::New();
aos->SetNumberOfComponents(3);
aos->SetArray(v, 3*n, 0);

// use the new SOA class
vtkSOADataArrayTemplate<double> *soa =
  vtkSOADataArrayTemplate<double>::New();
soa->SetNumberOfComponents(3);
soa->SetArray(0, vx, n, true);
soa->SetArray(1, vy, n);
soa->SetArray(2, vz, n);
SENSEI Overhead

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

- Original: subroutine called, Baseline: through SENSEI bridge

**Performance Analysis, Design Considerations, and Applications of Extreme-scale In Situ Infrastructures. SC16**
SENSEI architecture
In situ Architecture
The bridge

Manages data and analysis adaptors, periodically pushes data to the analysis

• Typically 3 functions: Initialize, Update and Finalize
The data adaptor

DataAdaptors – API giving analyses access to simulation data and metadata

• Convert simulation data to/from the data model
The analysis adaptor

AnalysisAdaptor – API for simulation to invoke vis & analysis

- Consume/process data
Analyses

**ConfigurableAnalysisAdaptor** – select an analysis at run time via an XML config file
In transit Architecture

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these

Simulation

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

Simulation

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

ADIOS data adaptor

FLEXPATH transport

XML selects one of these
ADIOS Adaptors

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Catalyst analysis adaptor
Libsim analysis adaptor
Histogram analysis adaptor

Simulation
VTK data adaptor
Configurable analysis adaptor
bridge code

ADIOS analysis adaptor
ADIOS data adaptor

Simulation runs in 1st job
End-point runs in 2nd job

FLEXPATH transport moves data across network
XML selects one of these

Catalyst analysis adaptor
Libsim analysis adaptor
Histogram analysis adaptor
End-Point

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job

FLEXPATH transport moves data across network

XML selects one of these

Bridge code

VTK data adaptor

Configurable analysis adaptor

ADIOS analysis adaptor

ADIOS end-point

ADIOS data adaptor

Configurable analysis adaptor

Catalyst analysis adaptor

Libsim analysis adaptor

Histogram analysis adaptor

Simulation runs in 1st job

End-point runs in 2nd job
In situ demo
Newton mini-app

N-body Gravitational Simulation. A single file, <400 lines.

Solves Newton's law of gravitation

Velocity Verlet method

\[ F_i = F_j = G m_i m_j / r_{ij}^2 \]

\[ x_i' = v_i \]

\[ v_i' = F_i / m_i \]
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

# 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()

# create an analysis adaptor(bridge code)
bridge = newton_bridge()
bridge.initialize(args.analysis, args.analysis_opts)

# run the sim and analysis
bridge.update(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)
    bridge.update(i,i*h,ids,x,y,z,m,vx,vy,vz,fx,fy,fz)
i += 1

# finish up
bridge.finalize()
class newton_bridge:
    def __init__(self):
        self.DataAdaptor = sensei.VTKDataAdaptor.New()

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

    def finalize(self):
        self.AnalysisAdaptor.Finalize()

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

Footer
Invoking in situ analysis

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

    # 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()
In situ demo

- Run the simulation 2 times
- Use XML to switch back end between Libsim and Catalyst

Catalyst
<sensei>
   <analysis type="catalyst" pipeline="pythonscript" filename="catalyst_config.py" enabled="1" />
</sensei>

Libsim
<sensei>
   <analysis type="libsim" plots="Pseudocolor" plotvars="ids" image-filename="image_%ts"
      image-width="800" image-height="800" slice-project="1" image-format="png" frequency="1" enabled="1"/>
</sensei>
In transit demo
In transit demo

Simulation: XML configures ADIOS analysis with FLEXPATH

ADIOS

<sensei>
   <analysis type="adios" filename="newton.bp" method="FLEXPATH" enabled="1" />
   <analysis type="adios" filename="newton.bp" method="DATASpaces" enabled="0" />
   <analysis type="adios" filename="newton.bp" method="MPI" enabled="0" />
</sensei>

End-point: XML configures either Catalyst or Libsim

Catalyst

<sensei>
   <analysis type="catalyst" pipeline="pythonscript" filename="catalyst_config.py" enabled="1" />
</sensei>

Libsim

<sensei>
   <analysis type="libsim" plots="Pseudocolor" plotvars="ids" image-filename="image_%ts"
            image-width="800" image-height="800" slice-project="1" image-format="png" frequency="1" enabled="1"/>
</sensei>
Links

- Main page – http://www.sensei-insitu.org/
- Software repo – https://gitlab.kitware.com/sensei/sensei
- VisIt/Libsim – https://www.visitusers.org/index.php?title=Category:Libsim
- ParaView Catalyst – http://www.paraview.org/in-situ/
Conduit data adaptor

CONDUIT DATA ADAPTOR

BRIDGE

SIMULATION

Consume conduit/blue-print data from simulations already instrumented for ascent

ANALYSIS

ANALYSIS ADAPTOR

SENSEI INSITU
VTK-m as an analysis back-end