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SENSEI: Cross-Platform View of In Situ Analytics

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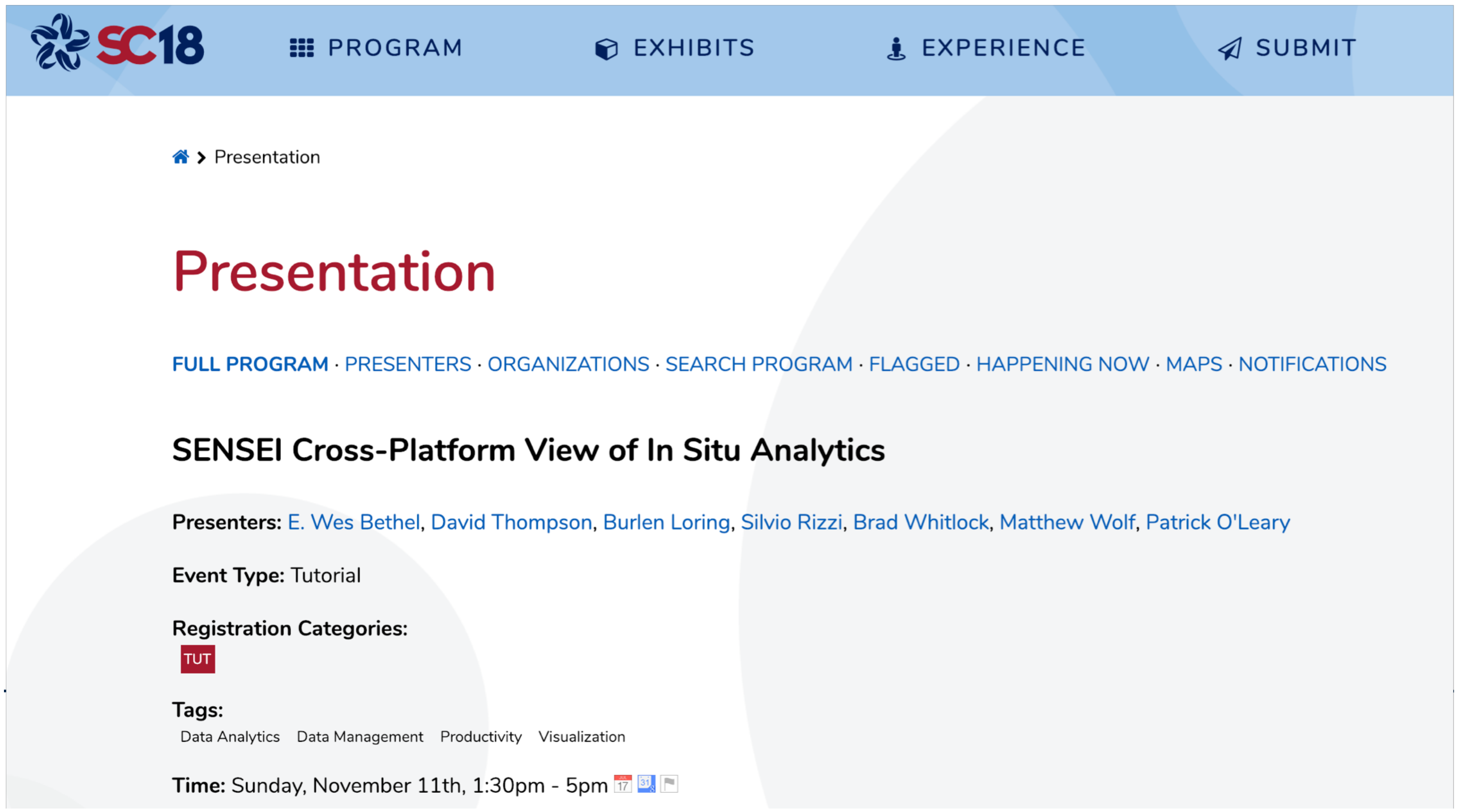
SENSEI: Scalable Analysis Methods and *In Situ* Infrastructure for Extreme Scale Knowledge Discovery

- Today we will cover a subset of a half day tutorial presented at SC18 by the SENSEI team
- Download SC18 slides and virtual machine image:

https://sensei-insitu.org/tutorials/sc18.html



Relevant links

- Main page – http://www.sensei-insitu.org/
- Software repository – https://gitlab.kitware.com/sensei/sensei
- 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/
- SENSEI in situ tutorial at CSCS

https://www.youtube.com/watch?v=nA22JqzhjqQ&list=PL1tk5lGm7zvRSS-M2bvW3JCt93gpgGHjM

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.

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

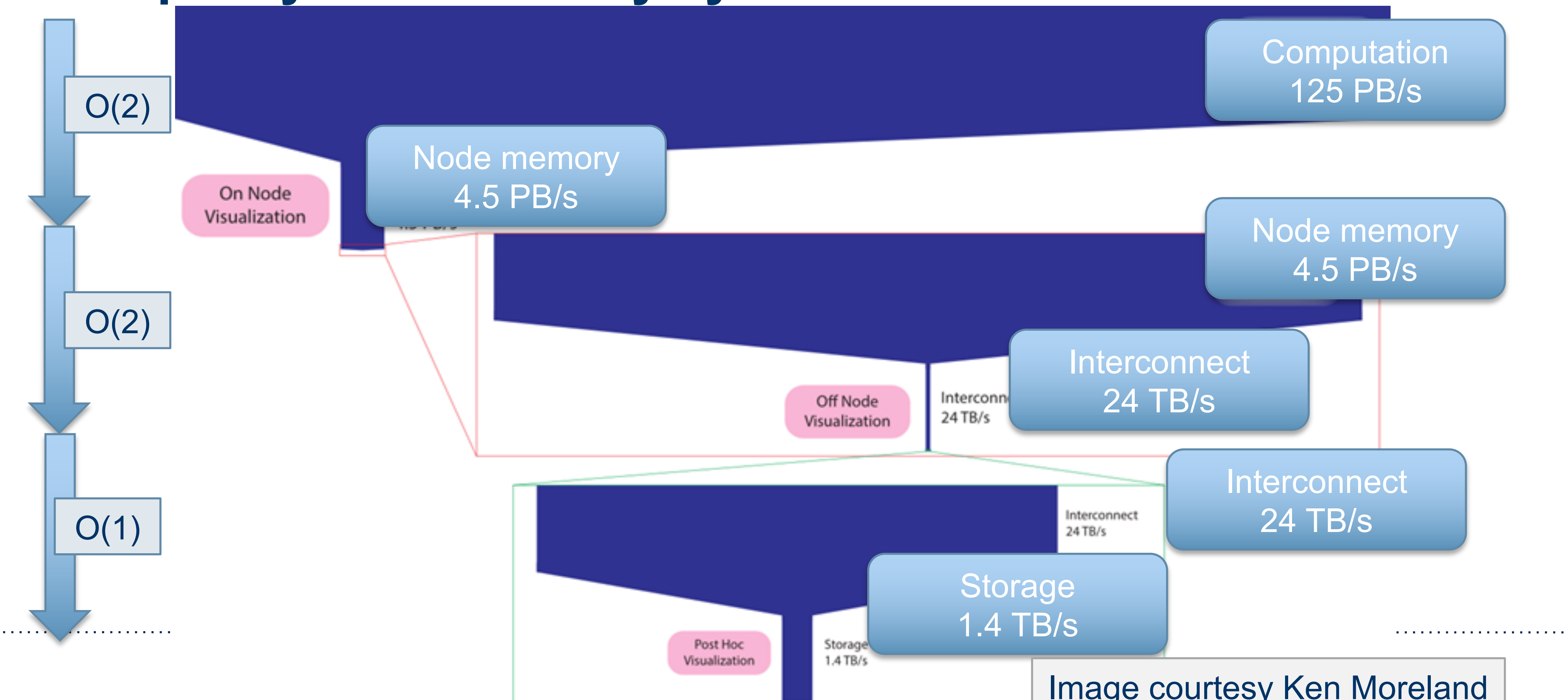


Image courtesy Ken Moreland

What is *in situ* data analysis and visualization?

- **Post processing**: save to disk, then later, a separate analysis/vis program reads that data and operates on it.
- ***In situ* processing**: process data as it produced without writing to and reading from storage. Processed "in place".
  - 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*

Generic processing sequence

```
1. initialize sim
2. do
3.   compute new state
4.   if do_io write plot file
5. while !done
6. finalize sim
```

Generic processing sequence w/ in situ

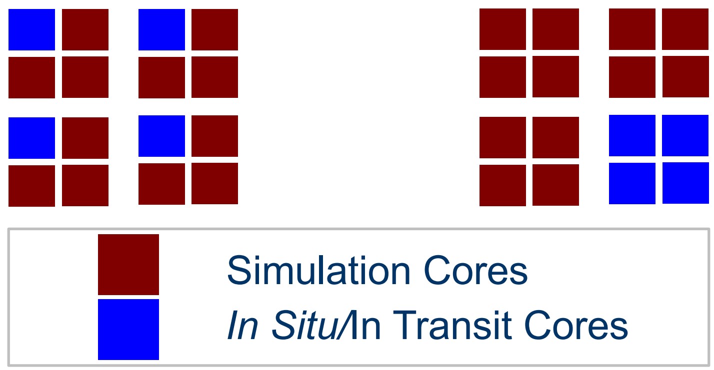
```
initialize sim
if do_insitu initialize in situ
do
  compute new state
  if do_io write plot file
  if do_insitu execute in situ
while !done
if do_insitu finalize insitu
finalize sim
```

execute is where things get interesting

- shared address space zero copy data transfers to shared or unique compute resources
- staging transfer sends data to a de-coupled parallel job, potentially asynchronous, potentially different jobs size

In situ vs In transit

In situ – no data movement: Simulation and *in situ* methods share memory



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

What is the cost of *in situ* processing?

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:

Ayachit, Bauer, Duque, Eisenhauer, Ferrier, Gu, Jansen, Loring, Lukic, Menon, Morozov, O'Leary, Ranjan, Rasquin, Stone, Vishwanath, Weber, Whitlock, Wolf, Wu, and Bethel, *"Performance Analysis, Design Considerations, and Applications of Extreme-scale In Situ Infrastructures"*. In Proceedings of SC16, November 2016.

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SENSEI System Overview

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Kitware

In situ infrastructures

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

ADIOS provides tools for *in situ* **I/O** , **data movement** and **analysis**

- ADIOS allows 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**

- Can be **tightly** or **loosely** linked to a simulation, allowing the simulation to **share data** with Catalyst for analysis and visualization.
- Catalyst, 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**.

Ascent an emerging in situ framework with an elegant data model, taking advantage of emerging **VTK-m** many core analysis and rendering capabilities

Can WE….

Enable use of any in situ framework?

Enable use of any analysis library/tool, even those not designed for in situ?

Develop analysis routines that are portable between codes?

Make it easy to use?

The *current* problem set

SENSEI seamlessly & efficiently enables in situ data processing with a diverse set of tools & libraries

Our approach

Data model

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

Data adaptor

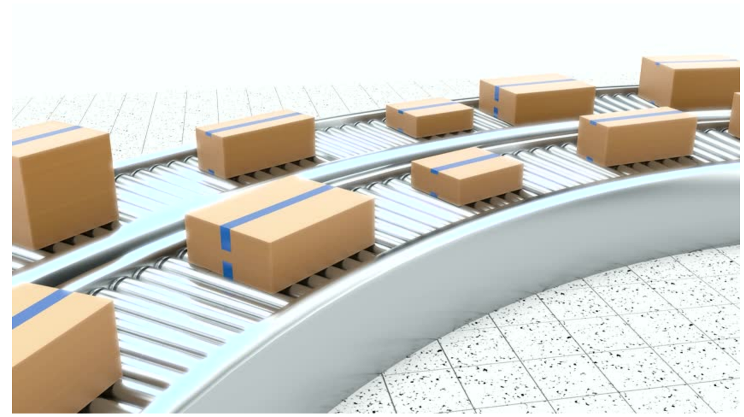
- Convert simulation data to/from the data model
- API for accessing the simulation data from the backend

Analysis adaptor

- Present the back-end data consumer to the simulation
- API for pushing data through the system from the sim

Library

- Providing off the shelf access to a diverse set of back-ends. eg Libsim, Catalyst, and ADIOS capabilities



Write once run everywhere

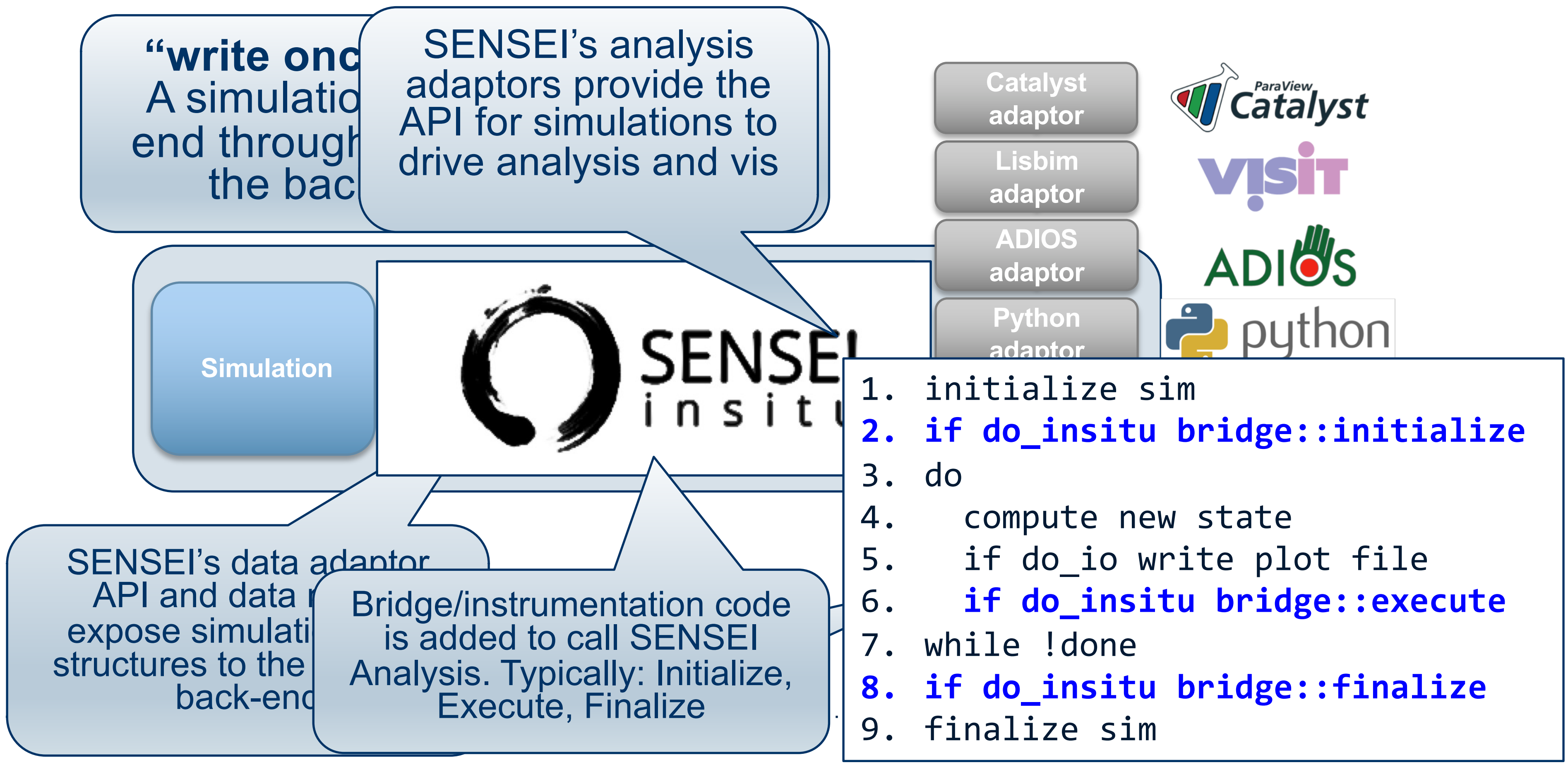
The **SENSEI API** enables connection of simulation data sources to visualization and analysis back ends

- 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

SENSEI Architecture



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SENSEI API’s

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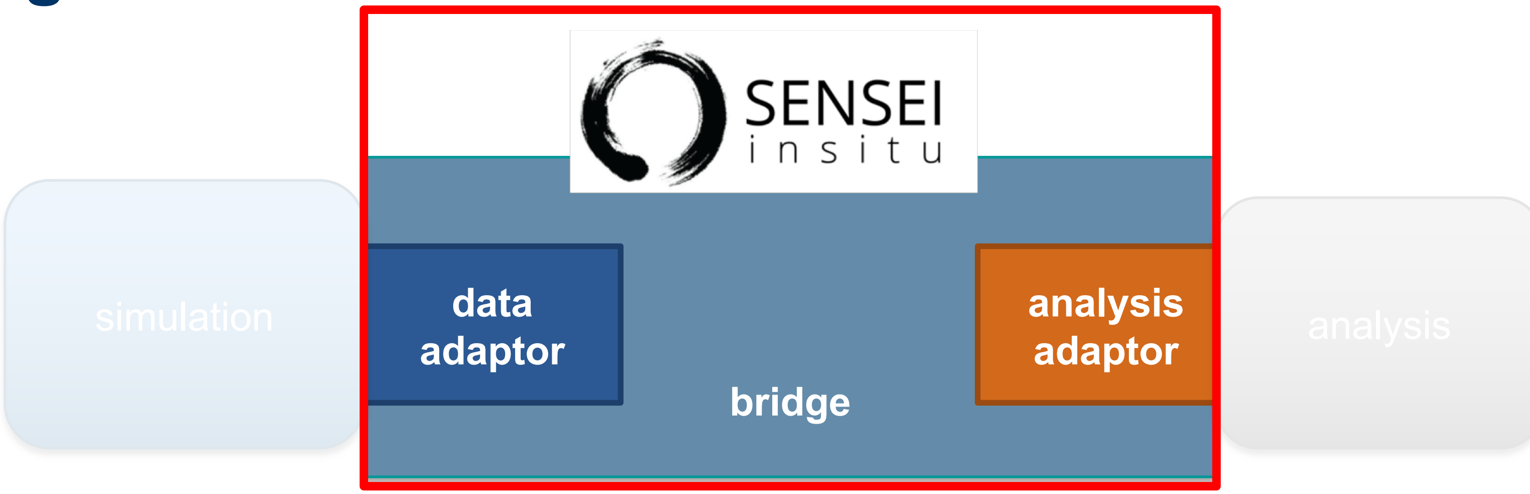
Bridge API

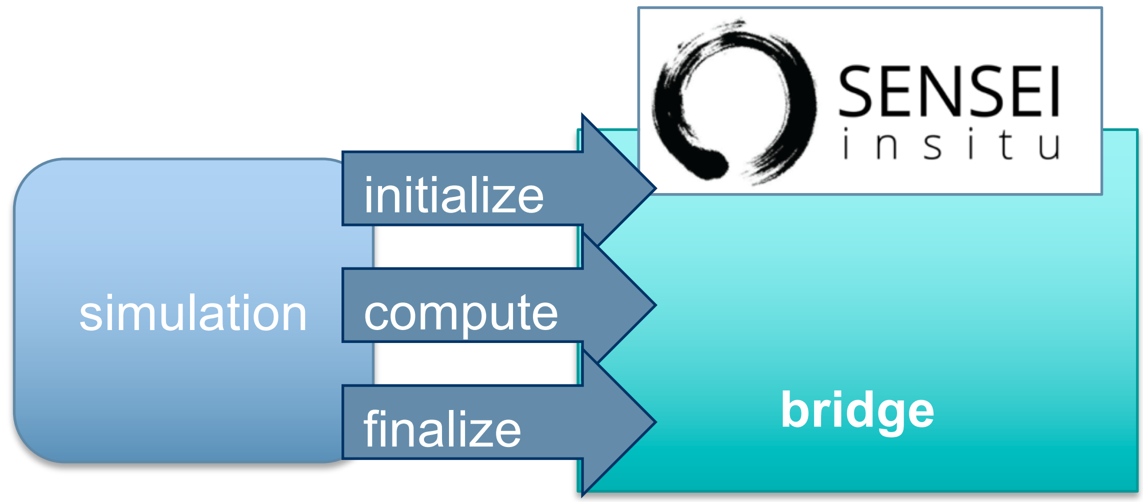


- Is part of the simulation code
- Is where you create, initialize, and manage your data and analysis adaptors
- Is where you execute the analyses adaptors as needed
- Typically consists of 3 functions: Initialize, Compute and Finalize

Implementing the bridge to SENSEI

Typically 3 calls:

- Initialize()
  - Set the DataAdaptor
  - Initialize DataTimeStep
  - 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() / set_particles() and analyze(), so that SENSEI may be disabled in benchmarks
- Finalize()



Simulation loop with bridge code

```
initialize sim
if do_insitu bridge::initialize
do
  compute new state
  if do_io write plot file
  if do_insitu bridge::execute
while !done
if do_insitu bridge::finalize
finalize sim
```

Run time configuration

Adaptors

- SENSEI Configurable analysis. Parses XML and creates and configures one of the other analysis adaptors interfacing to the back-ends (Libsim, Catalyst, ADIOS, custom, etc).
- Direct integration

Back-ends

- May expose control API via their SENSEI adaptor. In the Configurable analysis adaptor these are exposed via XML attributes.
- May be scriptable via their own Python bindings adding another layer of control.
- May be configured via "state" or "session" files.
- Special purpose

ConfigurableAnalysisAdaptor

- A meta analysis. A manager. It configures and invokes one or more of the other analysis adaptors
- XML specifies analyses and their run time options
- Supports ADIOS, Catalyst, Libsim, VTK I/O, and other data consumers
- In in transit use cases one XML configures the transport a second configures the analysis/backend

ConfigurableAnalysis XML

```xml
<sensei>
  <!-- Custom Analyses -->
  <analysis type="histogram" mesh="bodies" array="v" association="point"
    bins="10" enabled="0" />

  <!-- VTK XMLP I/O -->
  <analysis type="PosthocIO" mode="paraview" output_dir="./" enabled="0">
    <mesh name="bodies">
        <point_arrays> ids, m, v, f </point_arrays>
    </mesh>
  </analysis>

  <!-- CATALYST -->
  <analysis type="catalyst" pipeline="pythonscript"
    filename="../sensei/miniapps/newton/newton_catalyst.py" enabled="1" />

  <!-- LIBSIM -->
  <analysis type="libsim" plots="Pseudocolor" plotvars="ids"
    image-filename="newton_%ts" image-width="800" image-height="800"
    slice-project="1" image-format="png" enabled="0"/>
</sensei>
```

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Generating an in situ pipeline in ParaView

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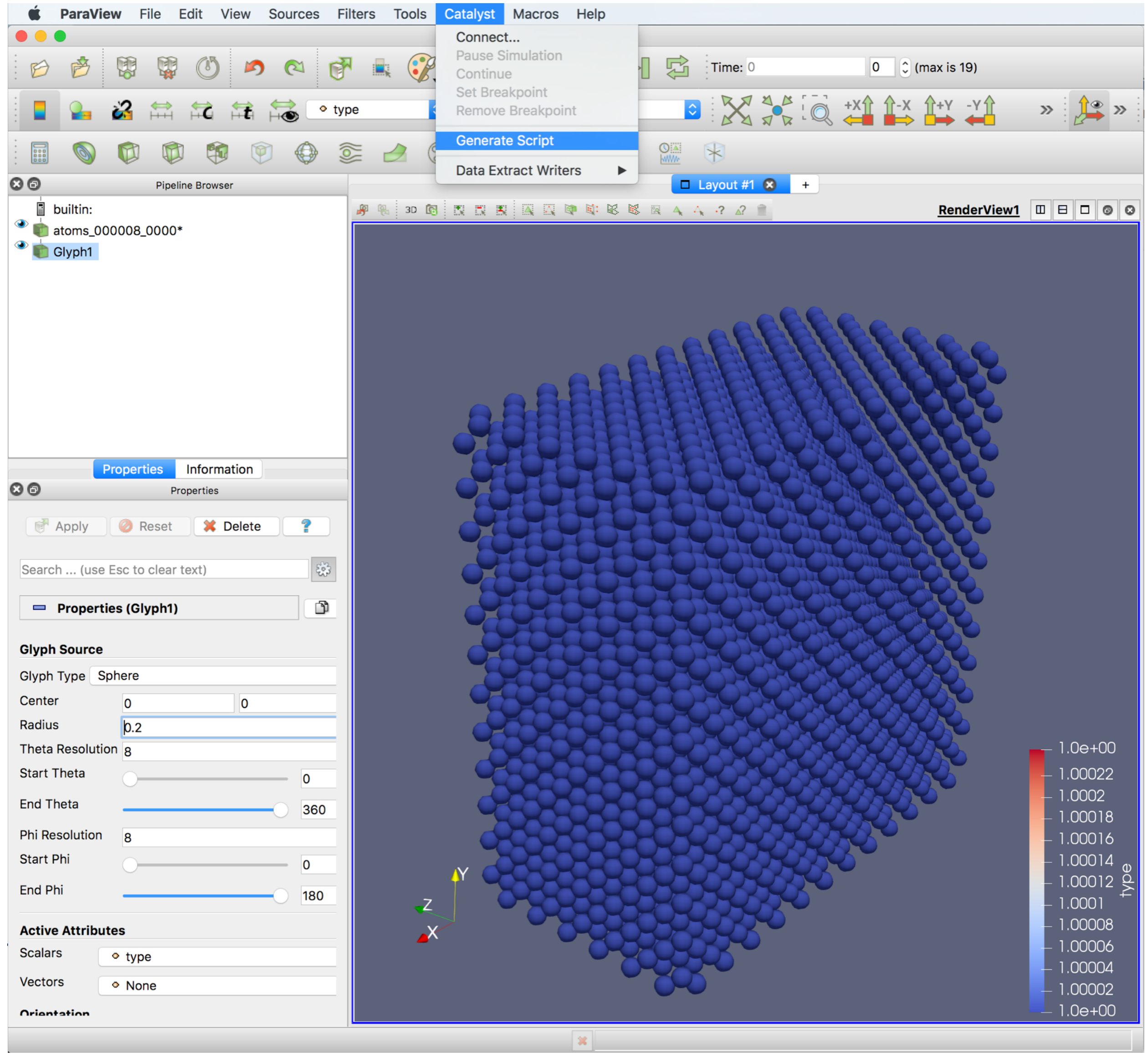
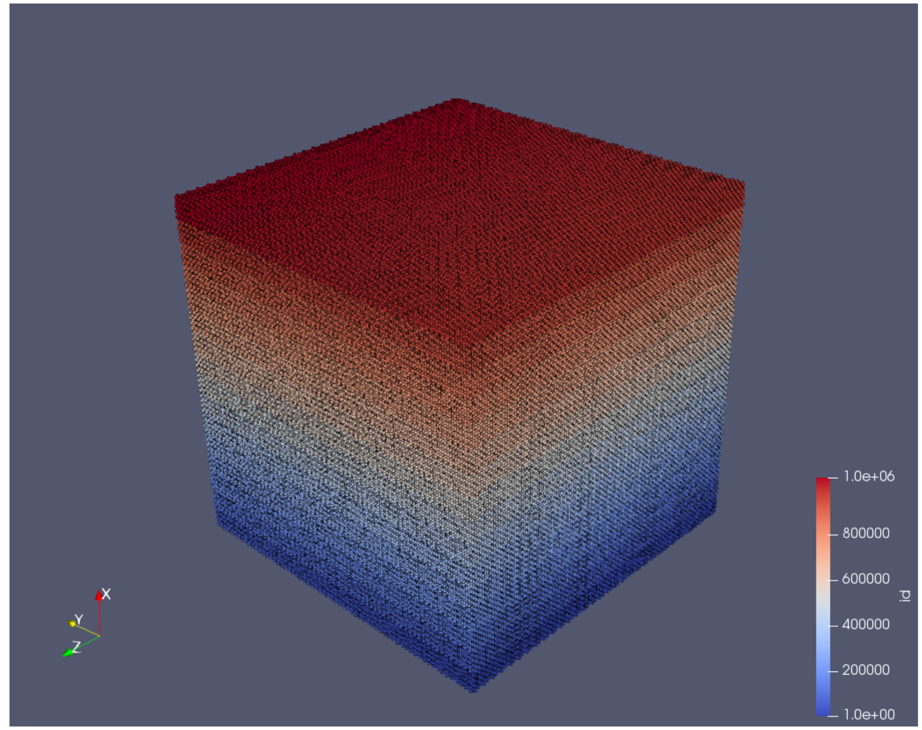
Instructions for ParaView v5.5.2

- Load a representative dataset in ParaView
- Define your visualization pipeline
- Export Catalyst Python script



Catalyst example

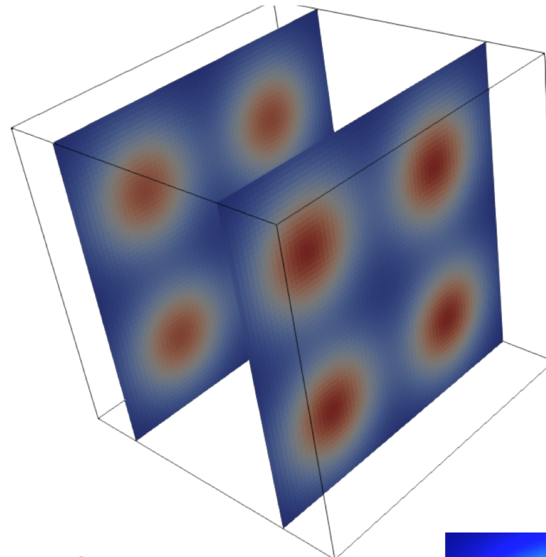
- Configure XML file
- Run instrumented simulation
- Result: one .png image per simulation timestep



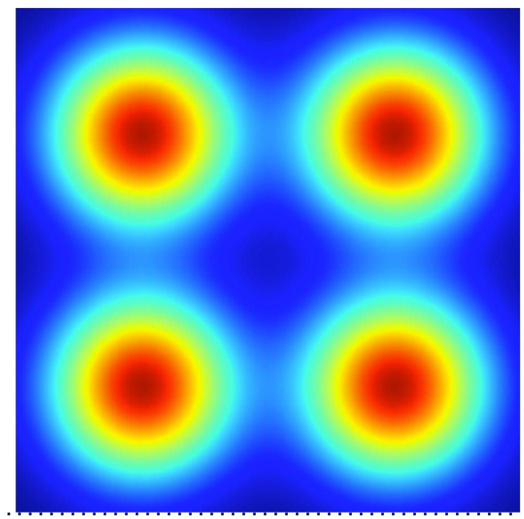

```xml
<sensei>
  <!-- Available with ENABLE_CATALYST -->
  <analysis type="catalyst" pipeline="pythonscript"
    filename="gaussianptsbyid.py" enabled="1" />
</sensei>
```

Demos

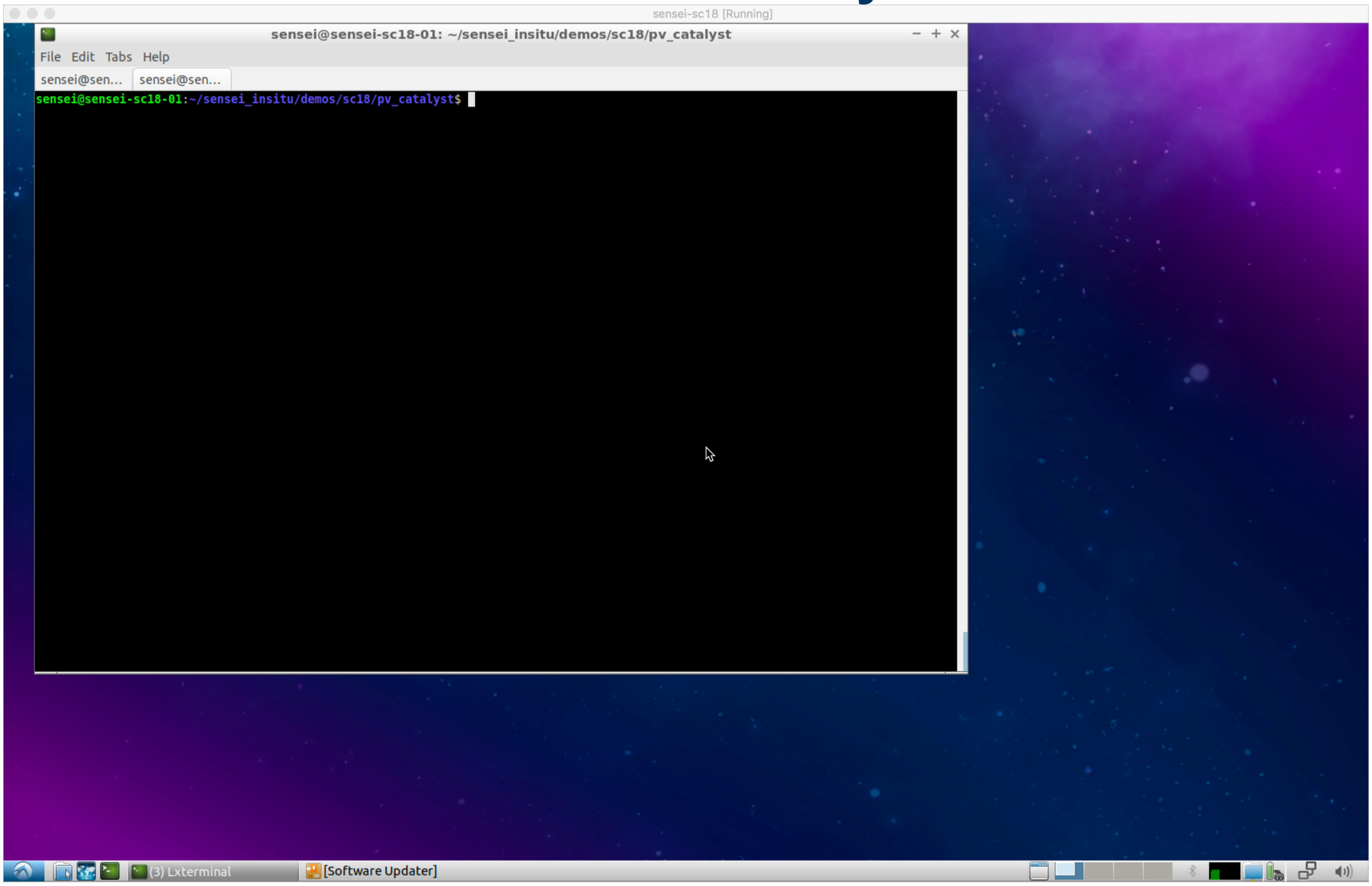
Oscillator miniapp overview



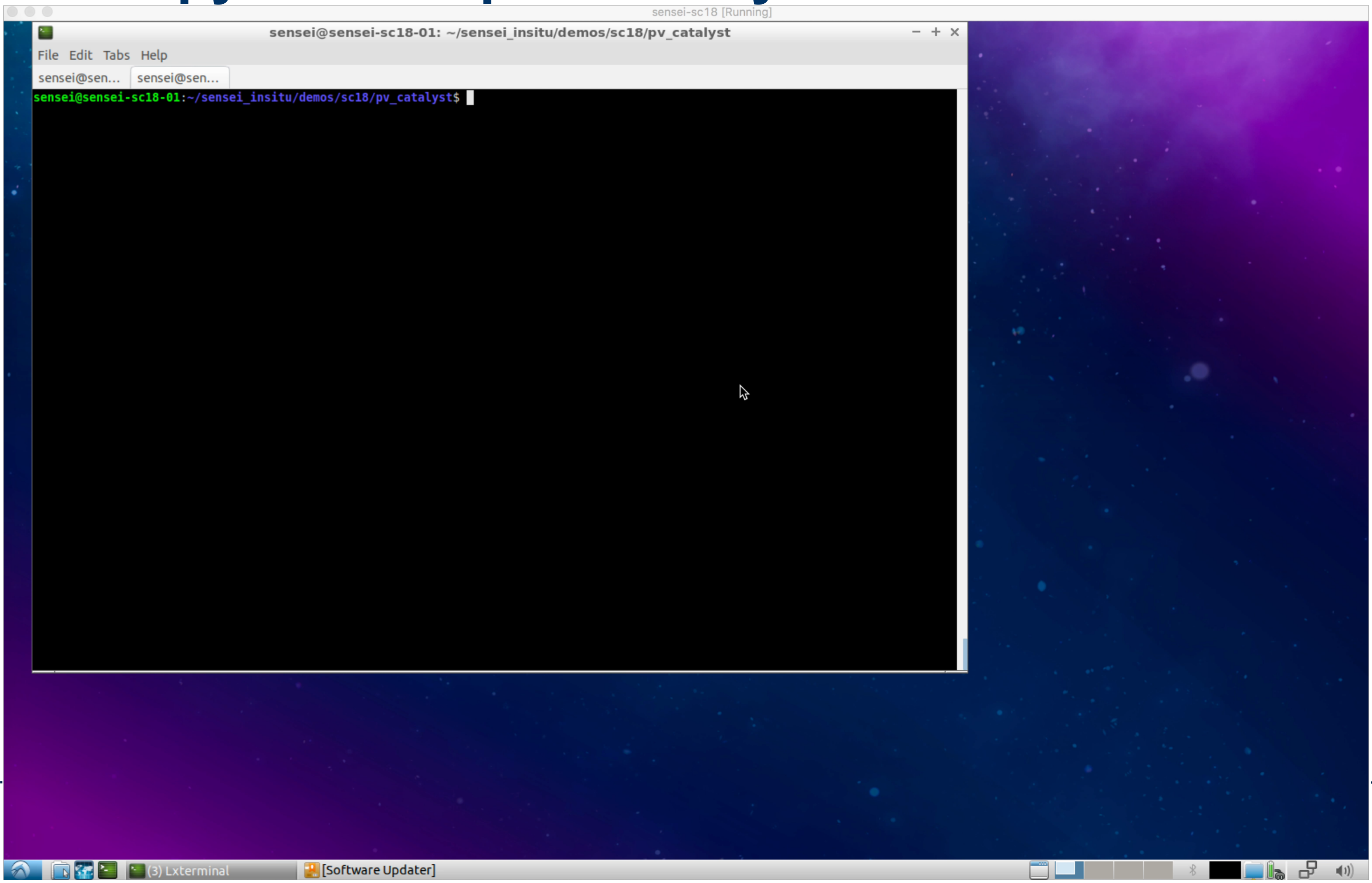
- MPI based C++ code that simulates a collection of periodic, damped, or decaying oscillators over a Cartesian grid.
- Unstructured grid also supported
- Each oscillator is convolved with a Gaussian of a prescribed width
- Can randomly place particles and advect them using an analytical velocity field
- Executable inputs are oscillator parameters, time resolution, length of the simulation, grid dimensions, grid partitioning, and number of random particles to generate



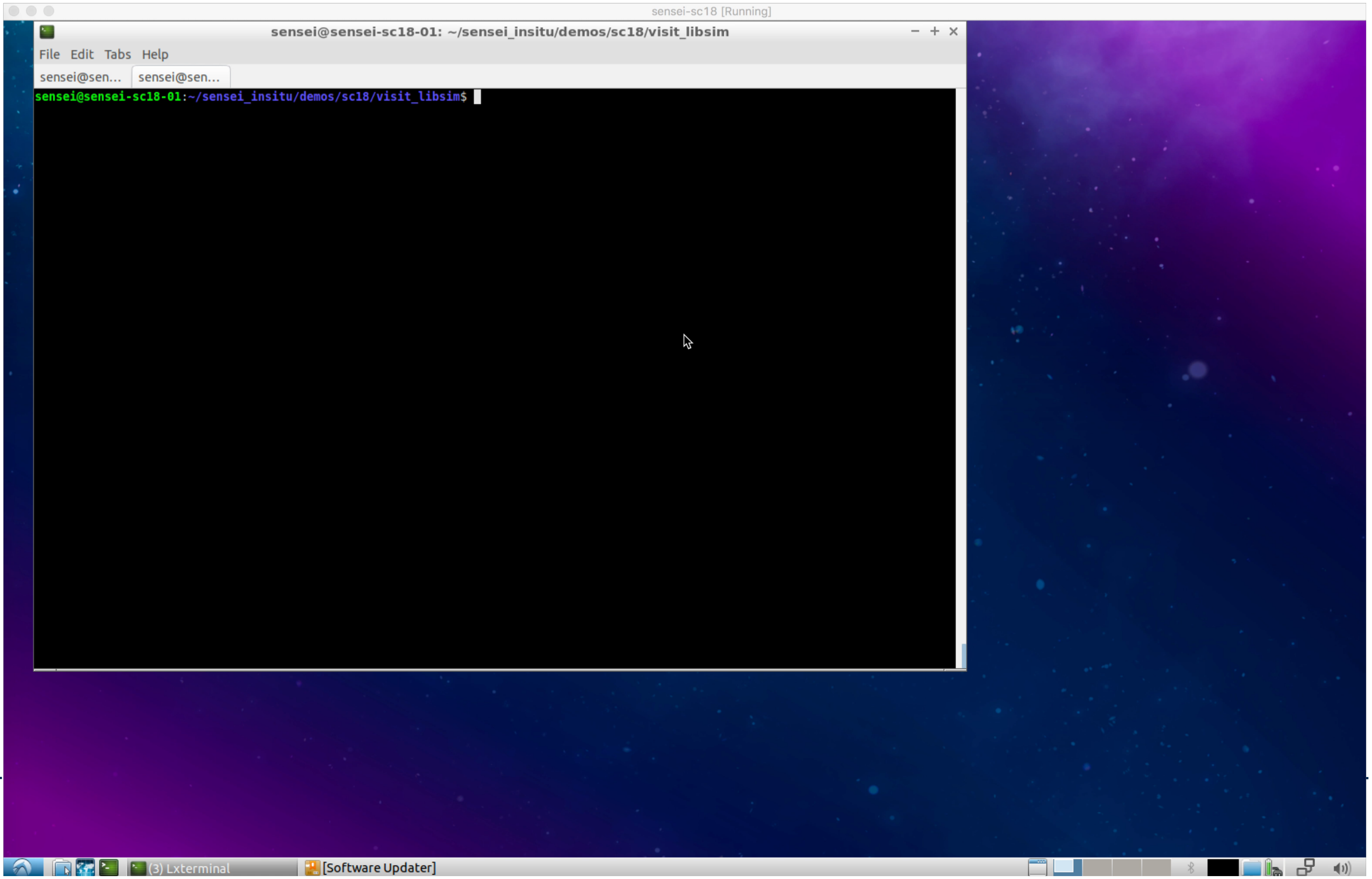
Demo 1: create slices with Catalyst in situ



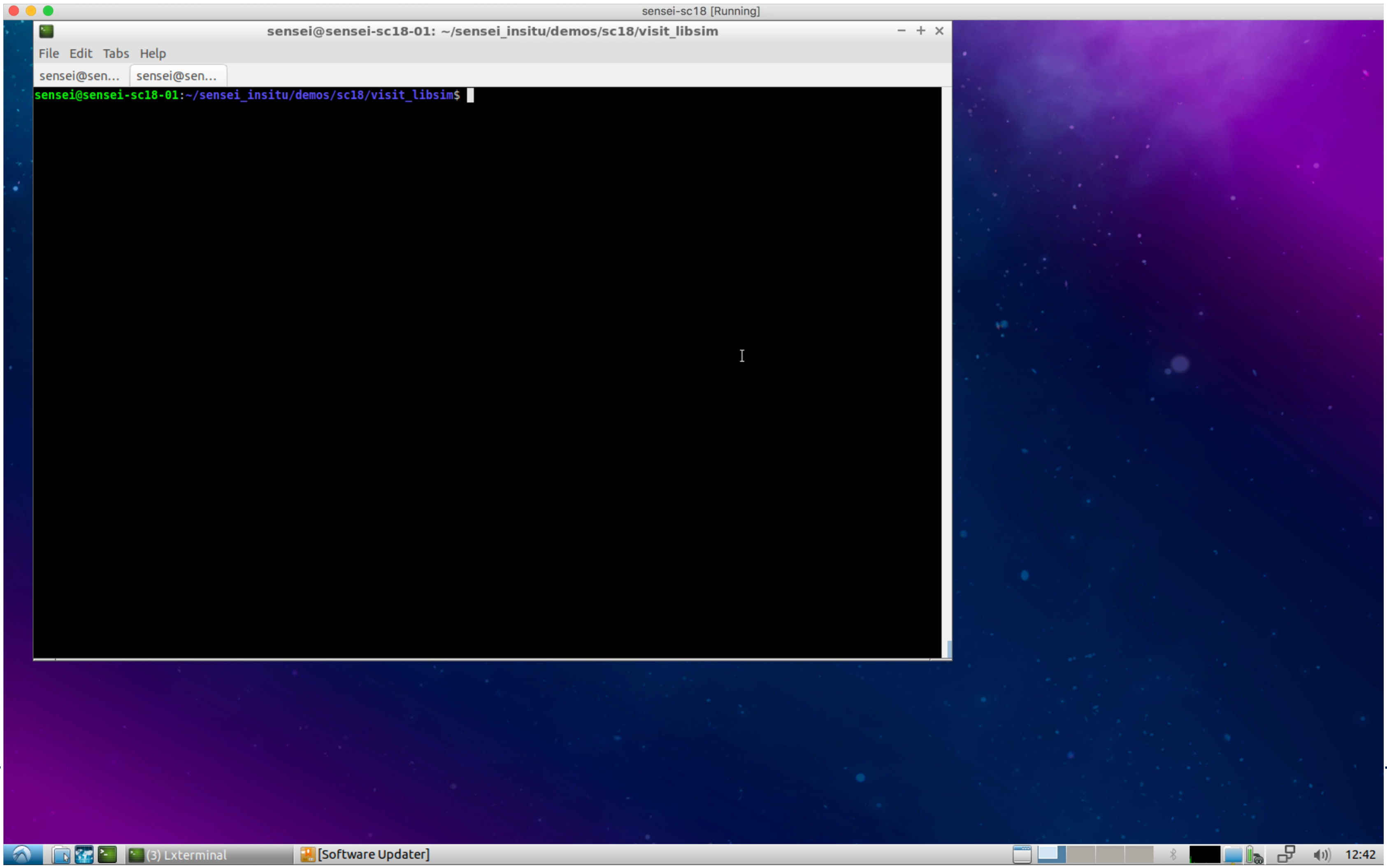
Demo 2: python script in Catalyst in situ



Demo 3: unstructured mesh with Libsim in situ



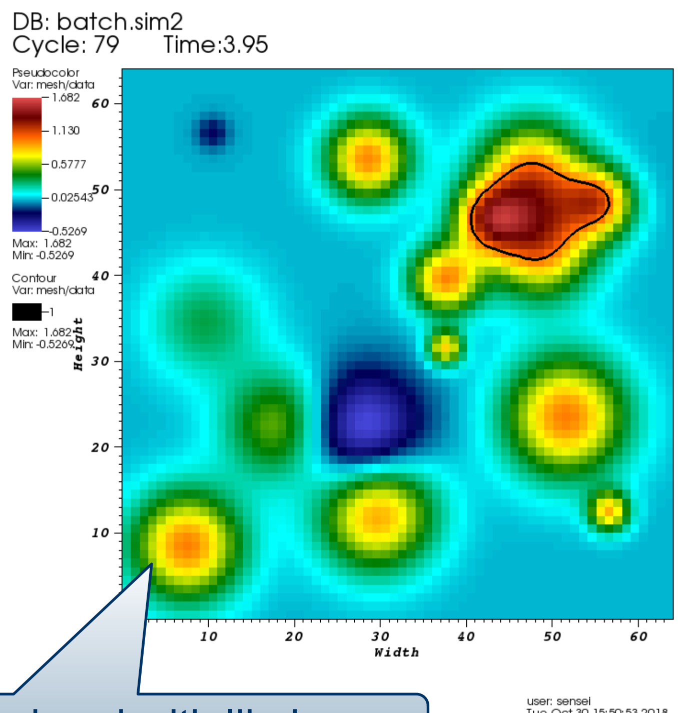
Demo 4: exploring Libsim extracts with Visit in situ



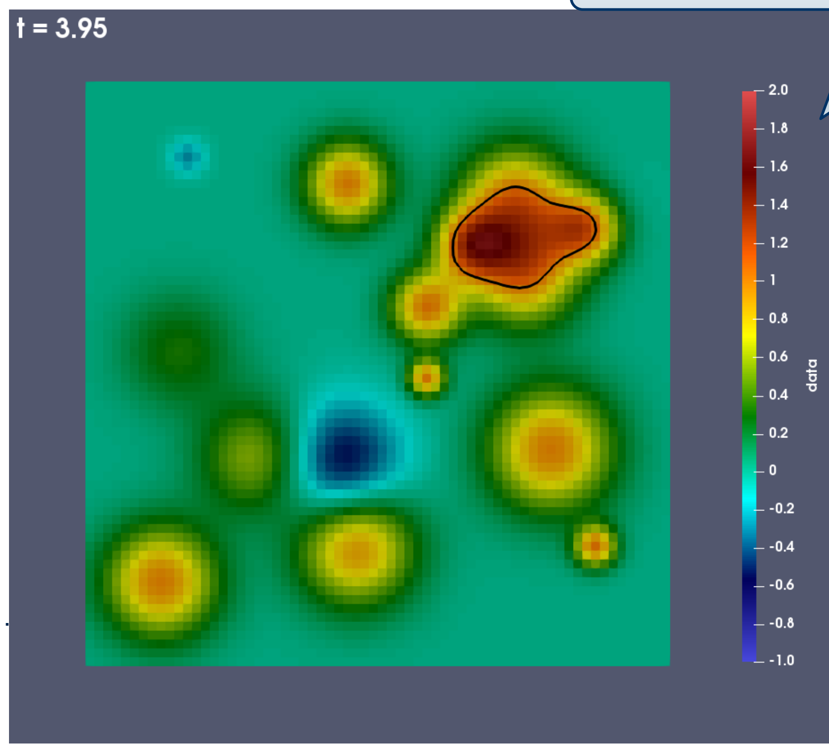
More demos in the SC18 tutorial

- ADIOS in transit demo
- Python mini app instrumented with SENSEI
- Catalyst, VTK-m, Haar wavelet, and Cinema databases

rendered with catalyst



rendered with libsim

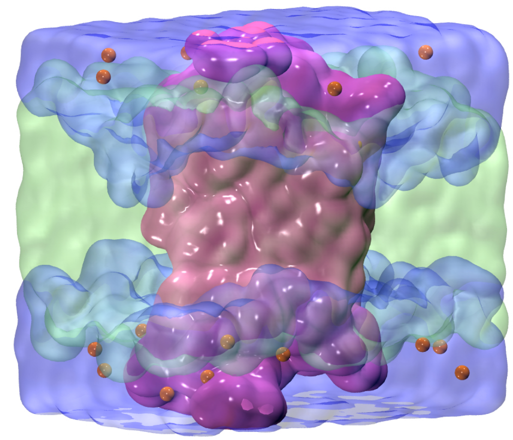


Instrumenting LAMMPS with SENSEI

LAMMPS

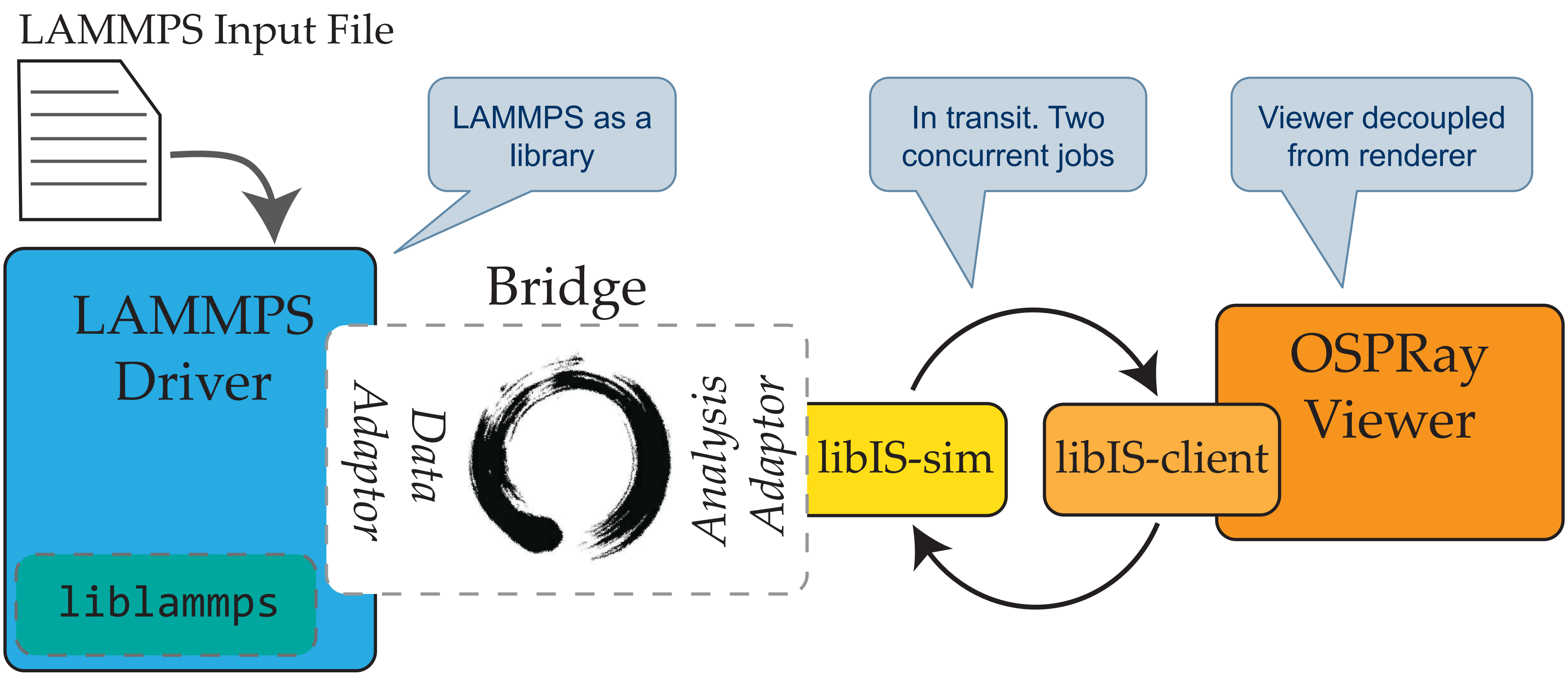
- Large-scale Atomic/Molecular Massively Parallel Simulator
- Classical molecular dynamics code
- Runs on single processors or in parallel using message-passing techniques and a spatial-decomposition of the simulation domain
- Accelerated performance on CPUs, GPUs, and Intel Xeon Phis
- Distributed by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

LAMMPS instrumentation with SENSEI



Materials Science with LAMMPS

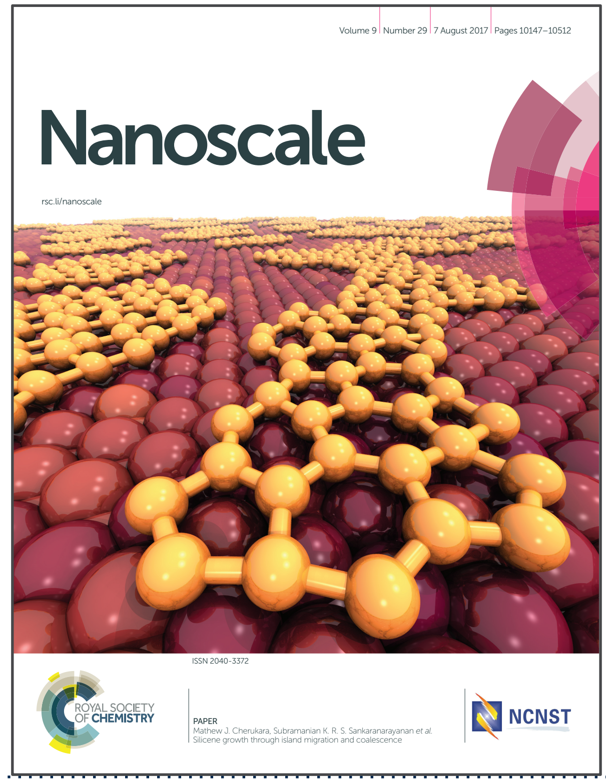
Silicene: Mono-layer Silicon / Iridium Substrate

- Massively-parallel classical molecular dynamics (MD) simulations with LAMMPS
- Various temperature conditions
- Varying rates of silicene deposition
- Characterize material structure and growth

Simulations were run on Mira at Argonne

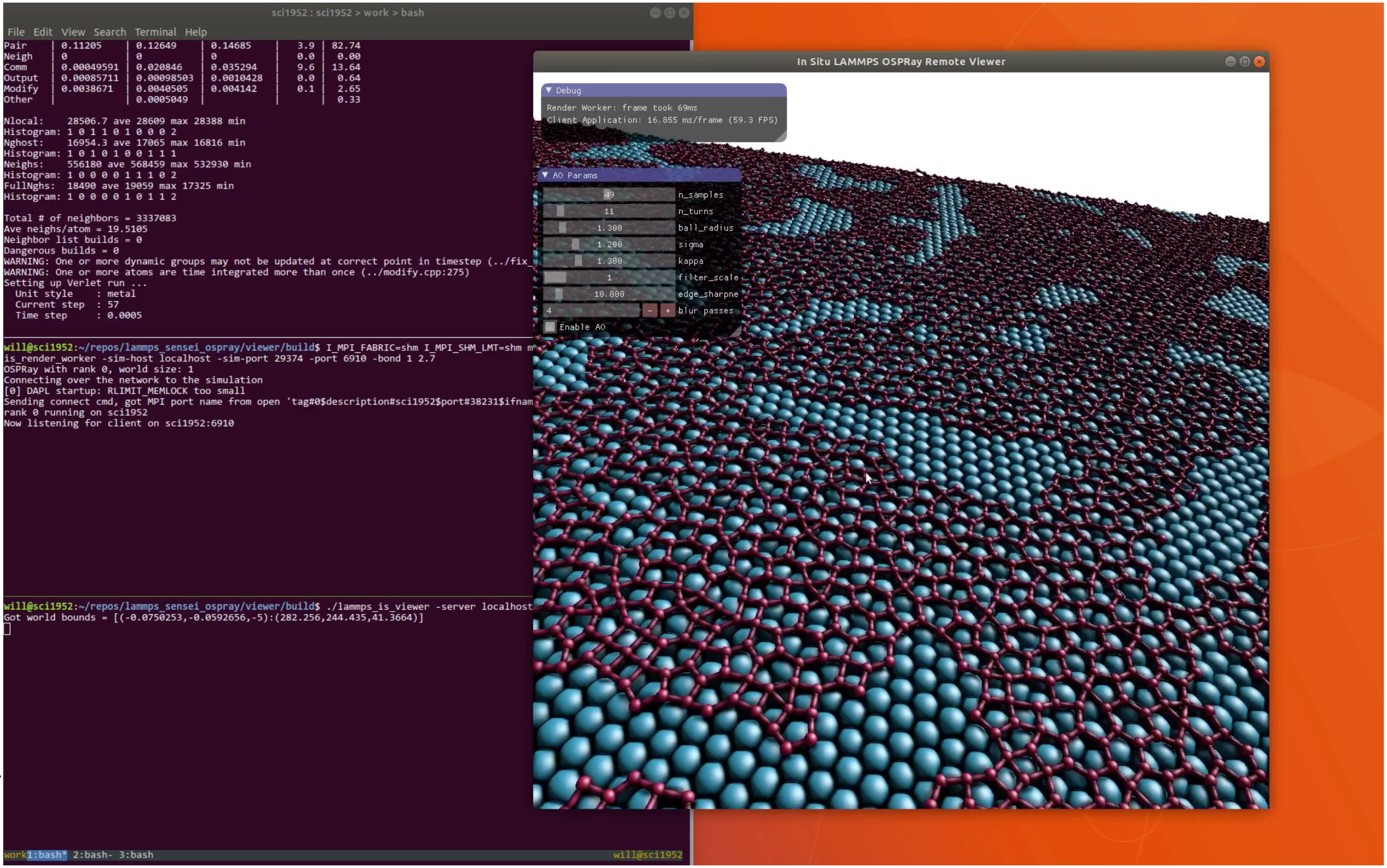
162,000 iridium atoms

~6 Million total compute hours



Cherukara, Mathew J., Badri Narayanan, Henry Chan, and Subramanian Sankaranarayanan. "Silicene growth through island migration and coalescence." Nanoscale 9, no. 29 (2017)

Slide courtesy Joe Insley, Argonne National Laboratory


sci1952 : sci1952 > work > bash
File Edit View Search Terminal Help
Pair | 0.11205 | 0.12649 | 0.14685 | 3.9 | 82.74
Neigh | 0 | 0 | 0 | 0.0 | 0.00
Comm | 0.00049591 | 0.020846 | 0.035294 | 9.6 | 13.64
Output | 0.00085711 | 0.00098503 | 0.0010428 | 0.0 | 0.64
Modify | 0.0038671 | 0.0040505 | 0.004142 | 0.1 | 2.65
Other | | 0.0005049 | | | 0.33
Nlocal: 28506.7 ave 28609 max 28388 min
Histogram: 1 0 1 1 0 1 0 0 0 2
Nghost: 16954.3 ave 17065 max 16816 min
Histogram: 1 0 1 0 1 0 0 1 1 1
Neighs: 556180 ave 568459 max 532930 min
Histogram: 1 0 0 0 0 1 1 1 0 2
FullNghs: 18490 ave 19059 max 17325 min
Histogram: 1 0 0 0 0 1 0 1 1 2
Total # of neighbors = 3337083
Ave neighs/atom = 19.5105
Neighbor list builds = 0
Dangerous builds = 0
WARNING: One or more dynamic groups may not be updated at correct point in timestep (../fix_
WARNING: One or more atoms are time integrated more than once (../modify.cpp:275)
Setting up Verlet run ...
Unit style : metal
Current step : 57
Time step : 0.0005
will@sci1952:~/repos/lammps_sensei_ospray/viewer/build$ I_MPI_FABRIC=shm I_MPI_SHM_LMT=shm m
is_render_worker -sim-host localhost -sim-port 29374 -port 6910 -bond 1 2.7
OSPRay with rank 0, world size: 1
Connecting over the network to the simulation
[0] DAPL startup: RLIMIT_MEMLOCK too small
Sending connect cmd, got MPI port name from open 'tag#0$description#sci1952$port#38231$ifnam
rank 0 running on sci1952
Now listening for client on sci1952:6910
will@sci1952:~/repos/lammps_sensei_ospray/viewer/build$ ./lammps_is_viewer -server localhost
Got world bounds = [(-0.0750253,-0.0592656,-5):(282.256,244.435,41.3664)]
work 1:bash* 2:bash- 3:bash
will@sci1952
In Situ LAMMPS OSPRay Remote Viewer
Debug
Render Worker: frame took 69ms
Client Application: 16.855 ms/frame (59.3 FPS)
AO Params
49 n_samples
11 n_turns
1.300 ball_radius
1.200 sigma
1.300 kappa
1 filter_scale
10.000 edge_sharpne
4 - + blur passes
Enable AO

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QUESTIONS ?

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https://sensei-insitu.org/

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