Data Visualization/Analysis and Performance Support In The XOLOTL Plasma Surface Interactions Model

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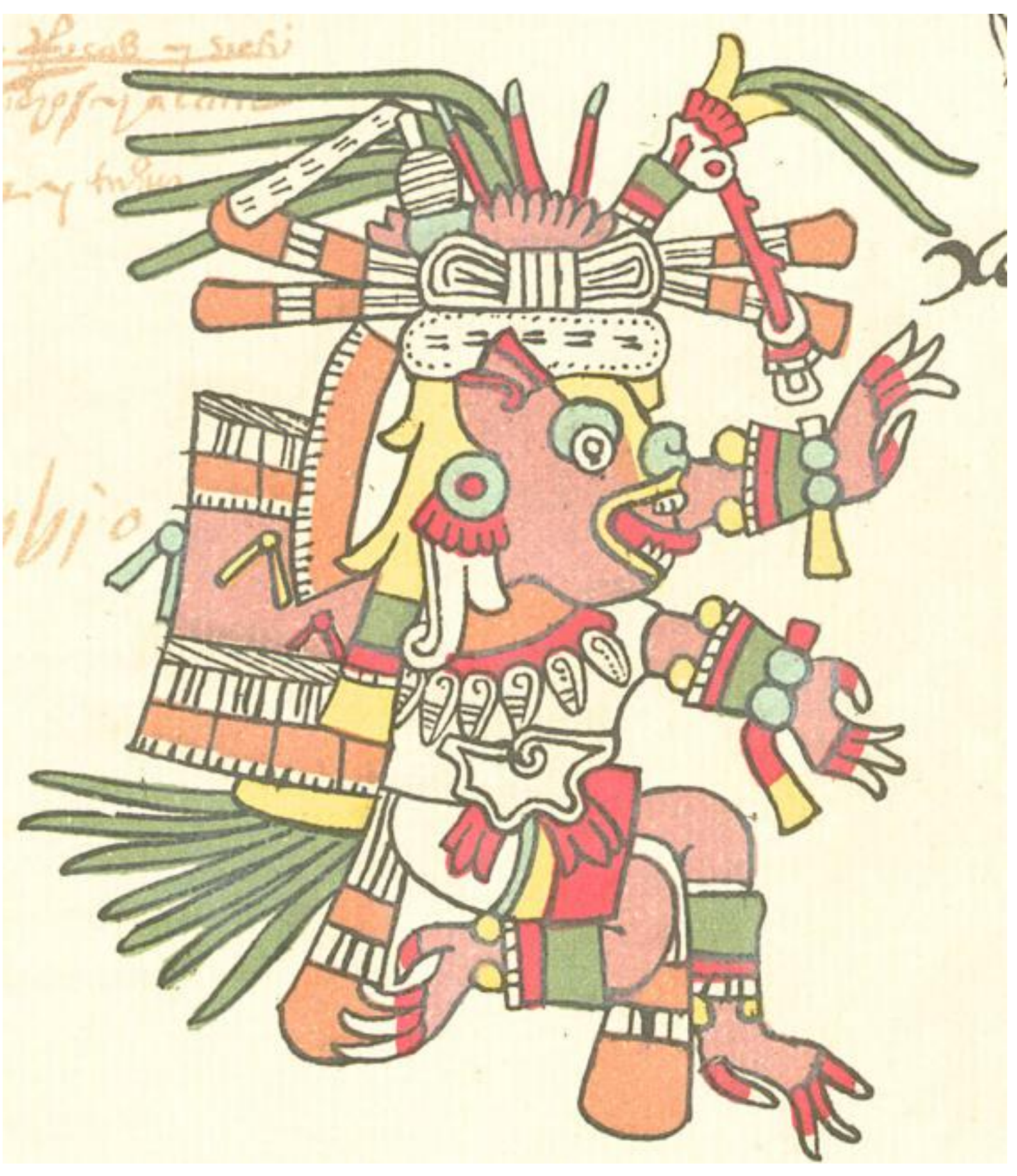
Background and Motivation

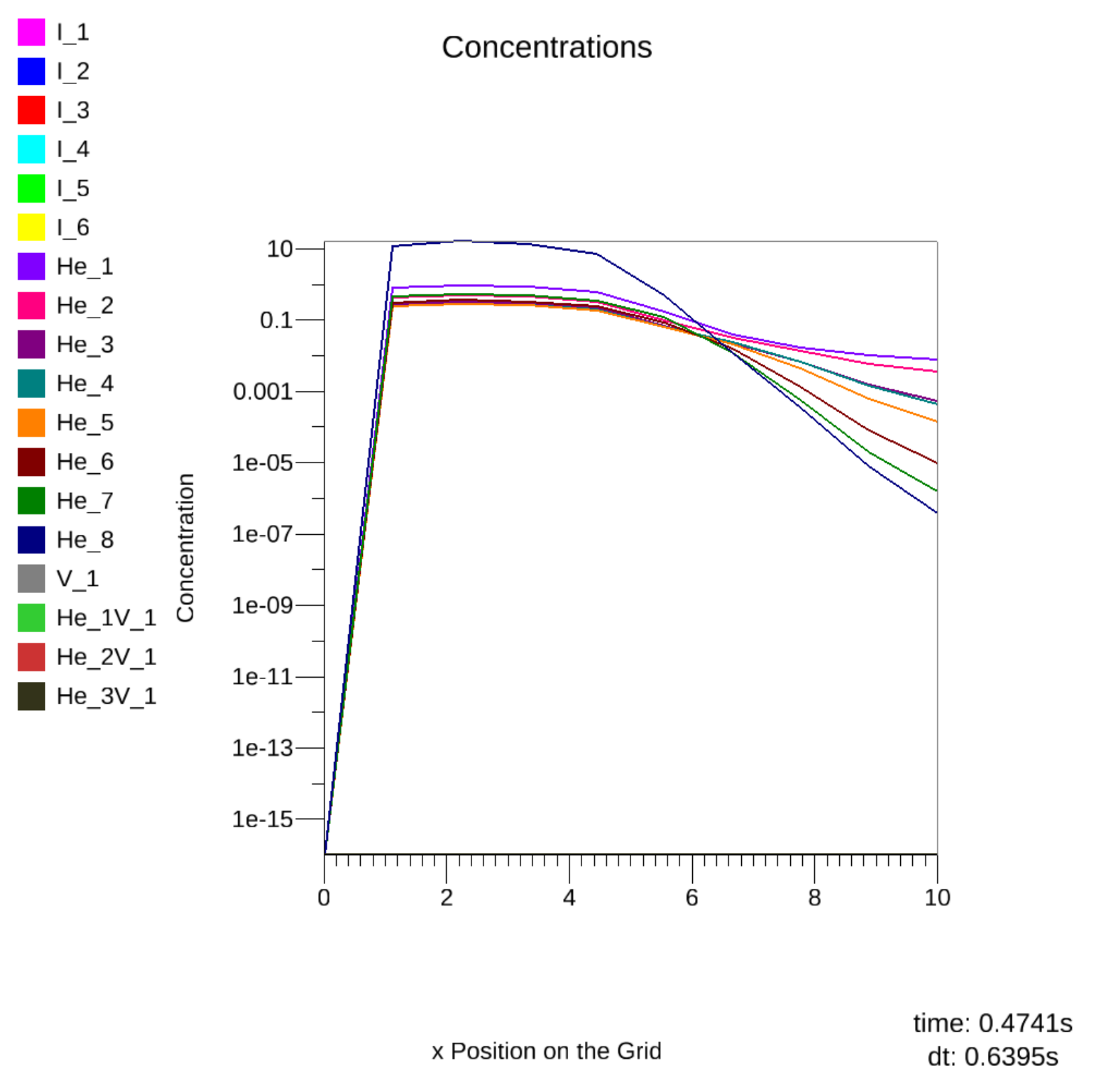
- XOLOTL model being developed as part of Plasma Surface Interactions SciDAC project
  - Intended for predictions of operating lifetime and performance of plasma facing components and bulk fusion materials
  - 3D, spatially discretized
  - Targeting range of computing systems from DOE Leadership Computing Facility (LCF) systems to traditional clusters to laptops and desktops
  - Targeting systems with traditional and heterogeneous architectures
- XOLOTL's rapidly changing code base creates challenges in understanding impact of code modifications on:
  - Quality of results
  - Performance and scalability
- Our response: build-in support for in-situ visualization/data analysis and lightweight performance data collection
  - Lightweight, "always on" data analysis and plotting for both performance and scientific data



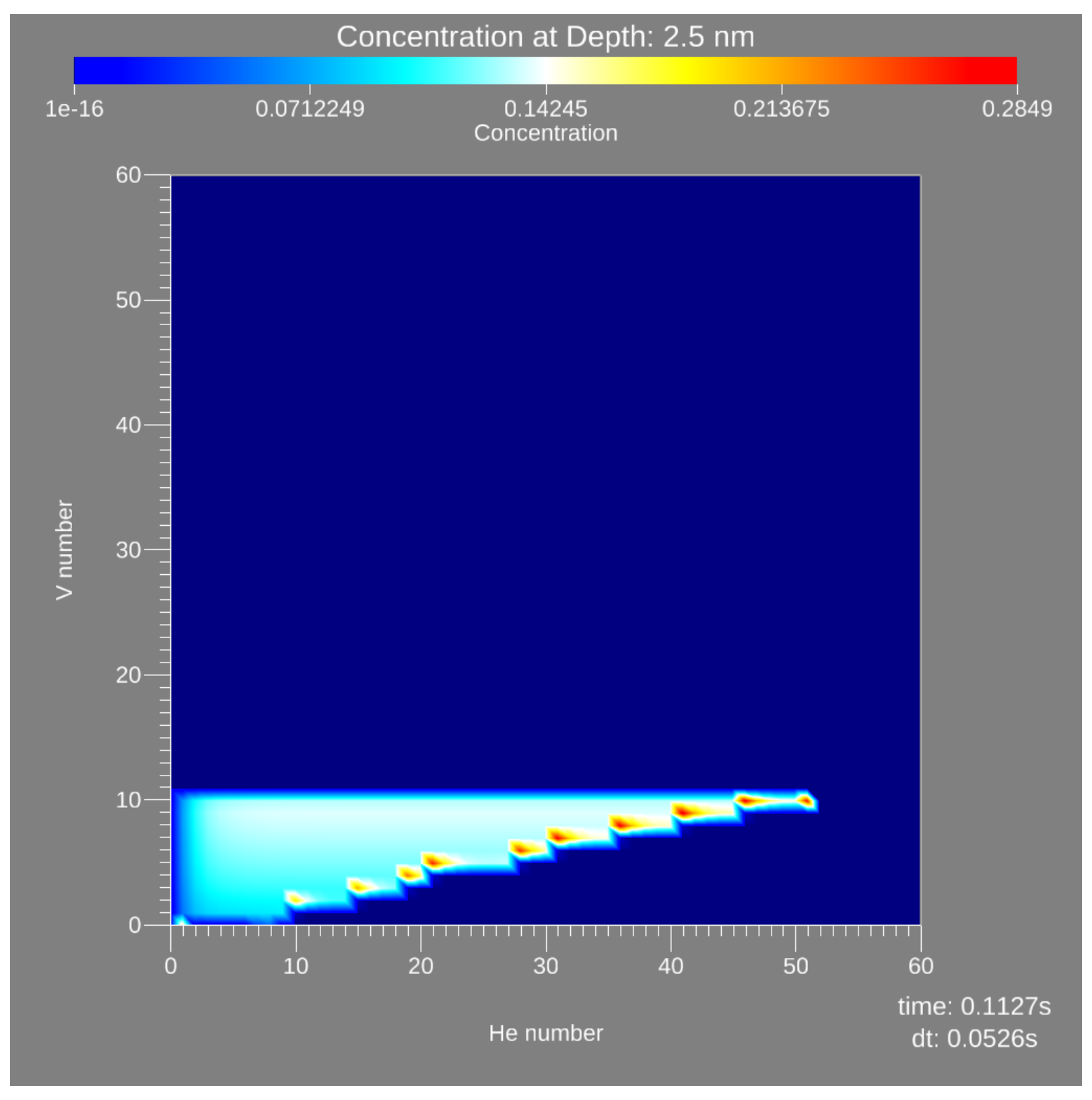
Data Visualization/Analysis

- C++ classes support collection and rendering of several types of scientific data:
  - Scatter plots show concentration along the grid
  - Series plots compare multiple species
  - Surface plots show range of cluster concentrations for each depth
- Uses Extreme-scale Analysis and Visualization Library (EAVL) for data analysis and rendering capabilities
  - lightweight, flexible, heterogeneous system support
- Controlled through command line switches
- Collaboration with **SDAV**, the SciDAC Institute for Scalable Data Management, Analysis, and Visualization

Example showing multiple species concentrations across grid points

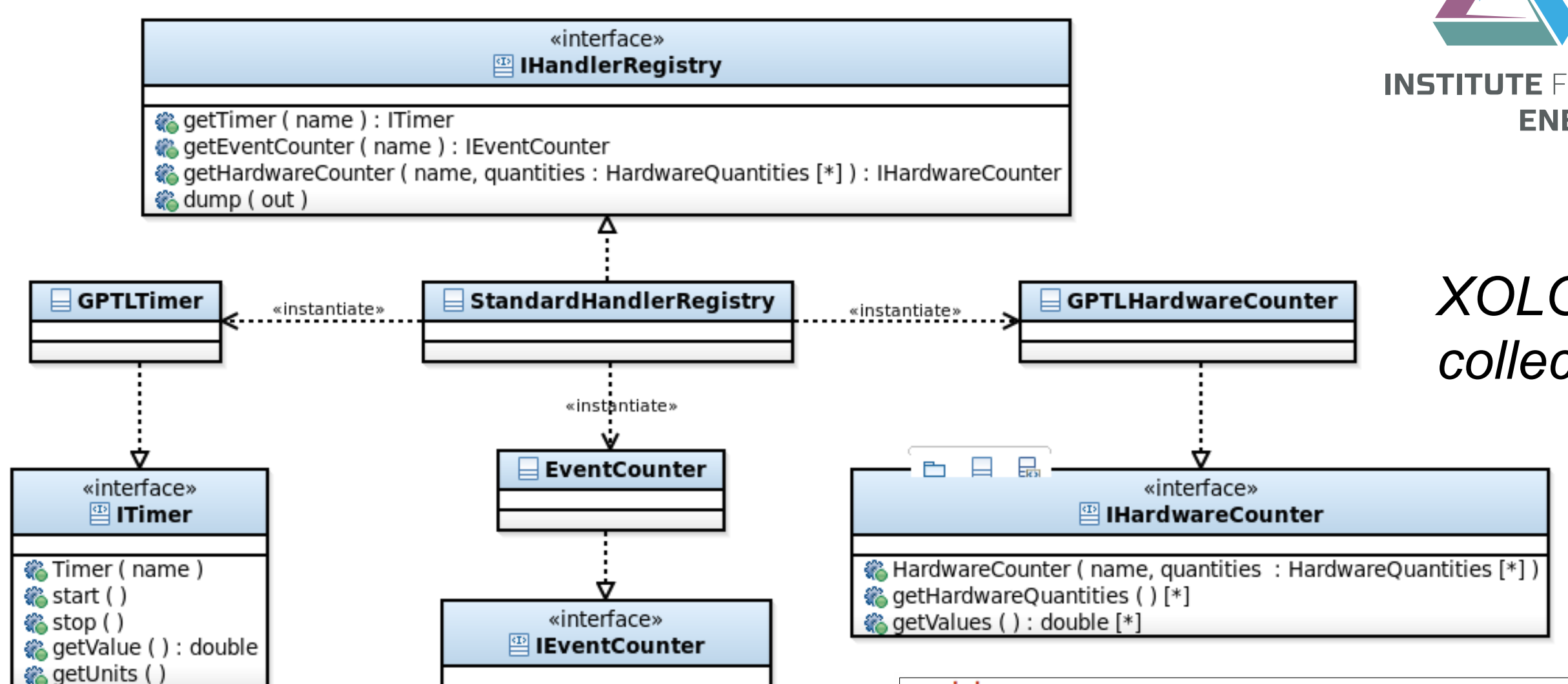


Example showing concentration for each cluster type at 2.5mm



Performance

- C++ classes support collection and analysis of several kinds of performance data:
  - Timers: measure wall-clock time required to execute a specific part of the code
  - Event counters: count the number of times an event of interest occurs
  - Hardware counters: provide access to processor hardware counters
- Uses General Purpose Timing Library (GPTL) with optional Performance Application Programming Interface (PAPI) integration
- Can be disabled with command line switch for lowest overhead
- Collaboration with **SUPER**, the SciDAC Institute for Sustained Performance, Energy and Resilience



«interface»
IHandlerRegistry
getTimer (name) : ITimer
getEventCounter (name) : IEventCounter
getHardwareCounter (name, quantities : HardwareQuantities [*]) : IHardwareCounter
dump (out)

GPTLTimer

«instantiate»

StandardHandlerRegistry

«instantiate»

GPTLHardwareCounter

«instantiate»

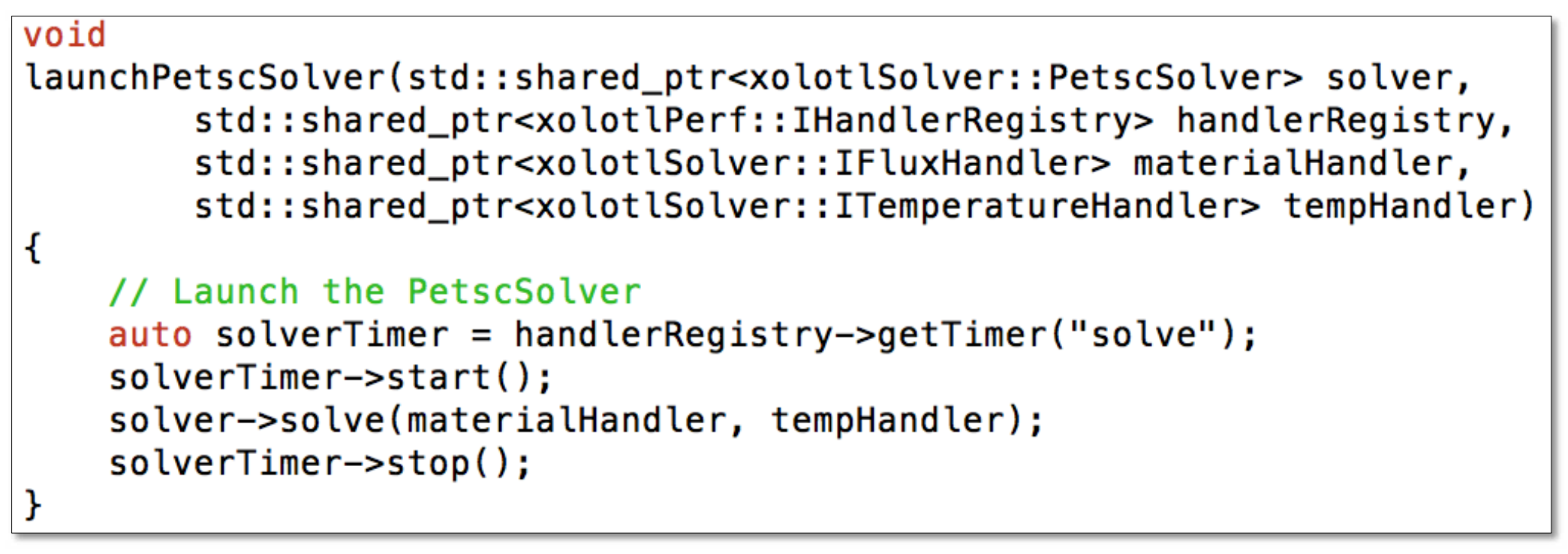
«interface»
ITimer
Timer (name)
start ( )
stop ( )
getValue ( ) : double
getUnits ( )

EventCounter

«interface»
IHardwareCounter
HardwareCounter (name, quantities : HardwareQuantities [*])
getHardwareQuantities ( ) [*]
getValues ( ) : double [*]

«interface»
IEventCounter
EventCounter (name)
getValue ( ) : unsigned long
increment ( )

XOLOTL performance data collection class model



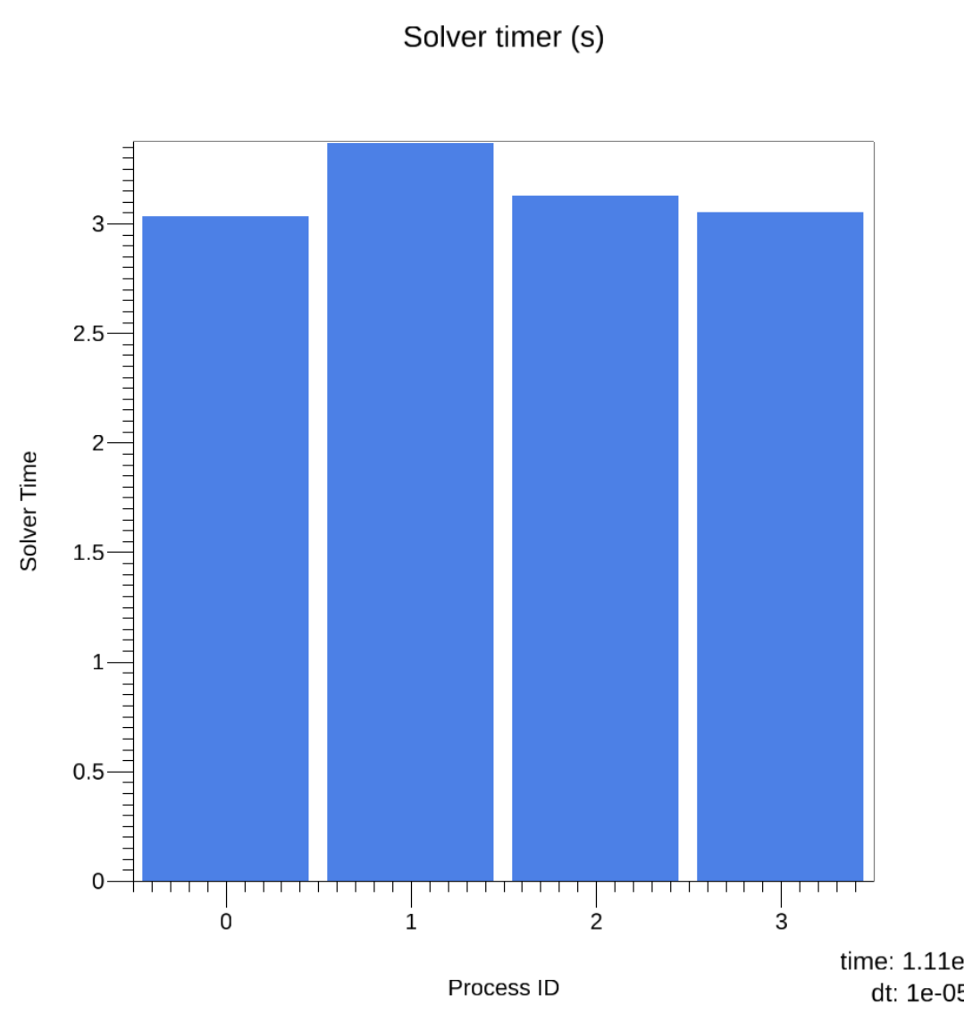
```
void
launchPetscSolver(std::shared_ptr<xolotlSolver::PetscSolver> solver,
        std::shared_ptr<xolotlPerf::IHandlerRegistry> handlerRegistry,
        std::shared_ptr<xolotlSolver::IFluxHandler> materialHandler,
        std::shared_ptr<xolotlSolver::ITemperatureHandler> tempHandler)
{
    // Launch the PetscSolver
    auto solverTimer = handlerRegistry->getTimer("solve");
    solverTimer->start();
    solver->solve(materialHandler, tempHandler);
    solverTimer->stop();
}
```

Example showing use of a Timer from XOLOTL's main.cpp

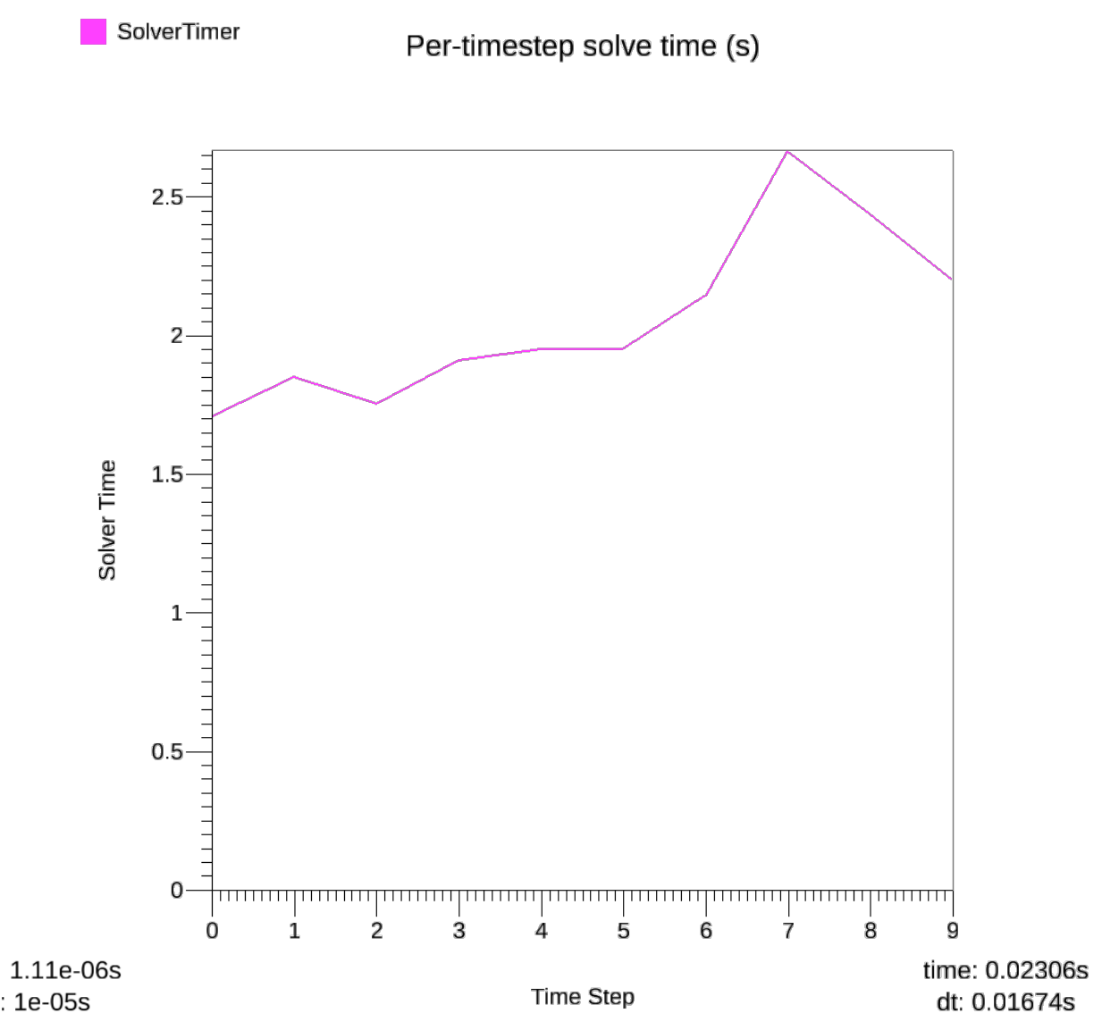
Integration

- Combining in situ performance analysis with scientific visualization and rendering capabilities
- Plot types showing key performance metrics over tasks and over time

Example showing cumulative time per MPI task



Example showing runtime for each timestep



Next Steps

- Data Visualization/Analysis
  - Additional in situ analysis, including temporal data
  - Detailed performance data visualization
- Performance
  - Deployment of a performance database to collect XOLOTL performance results over time
  - Determine regimes where XOLOTL is compute-bound and communication-bound

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