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Enabling In Situ Viz and Data Analysis with Provenance in libMesh

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HPC

Summary

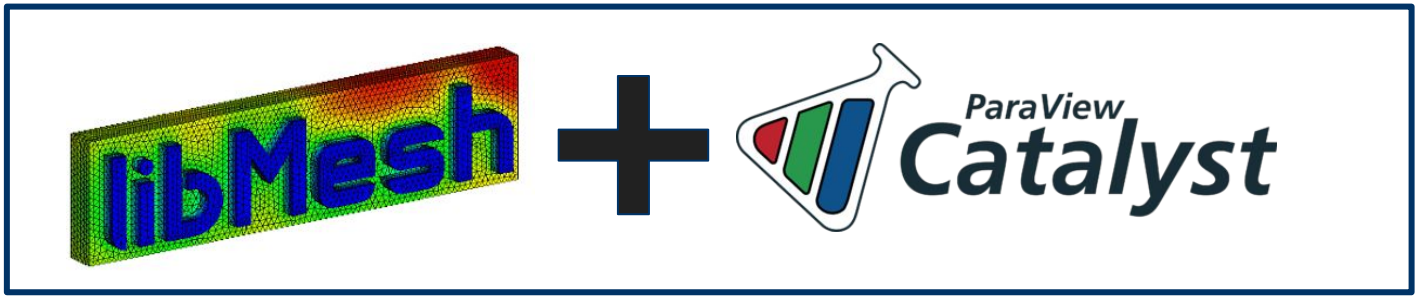
- Introduction
- libMesh Sedimentation Solver
- HPC Simulation Enhancements
  - In-Situ Viz and Raw Data Analysis
  - Provenance support
- Test Cases
  - de Rooij and Dalziel sedimentation tank
  - Real bed bathymetry
- Conclusions

Motivation

- In highly complex simulations, **data is efficiently managed in memory and stored in thousands of "isolated" files** (HDF5, XDMF, Exodus, NetCFD, Ensight, VTK, etc)
  - These data have to be related to enable viz and data analyses at runtime and, very often, after the simulation.
  - Track evolution of QoIs, associate simulation parameters and time steps to identify regions of interest spread among files: **provenance data**
- **Goal**:
  - Online analysis to detect outliers and dispensable input data to dynamically adapt the simulation
- **Challenge:**
  - ***no threat to solver's performance and scalability***

Objectives

- Provide In-Situ visualization capabilities to **libMesh**
  - libMesh is now Paraview-Catalyst enabled



- Introduce Dataflow Analysis tools (**DfAnalyzer**) based on data provenance
  - Tools enable **user steering**
- Show a cost analysis of In-Situ Viz and Dataflow Analysis tools in parallel simulations of sedimentation problems

Context: Sedimentation Simulation using libMesh

- **libMesh-sedimentation:** a sediment transport solver for simulating turbidity currents built upon **libMesh**, an open-source library with parallel adaptive mesh refinement and coarsening (AMR/C) support:
  - Employs a ***residual-based variational multiscale finite element method*** (Guerra et al, IJNMF, 2013)
  - AMR/C is an optimal strategy for large-scale sedimentation simulations

- The sediment transport due to fluid motion is described by a fully-Eulerian framework:
  - incompressible Navier-Stokes equation (fluid)
  - advection-dominated transport equations (sediment concentrations)

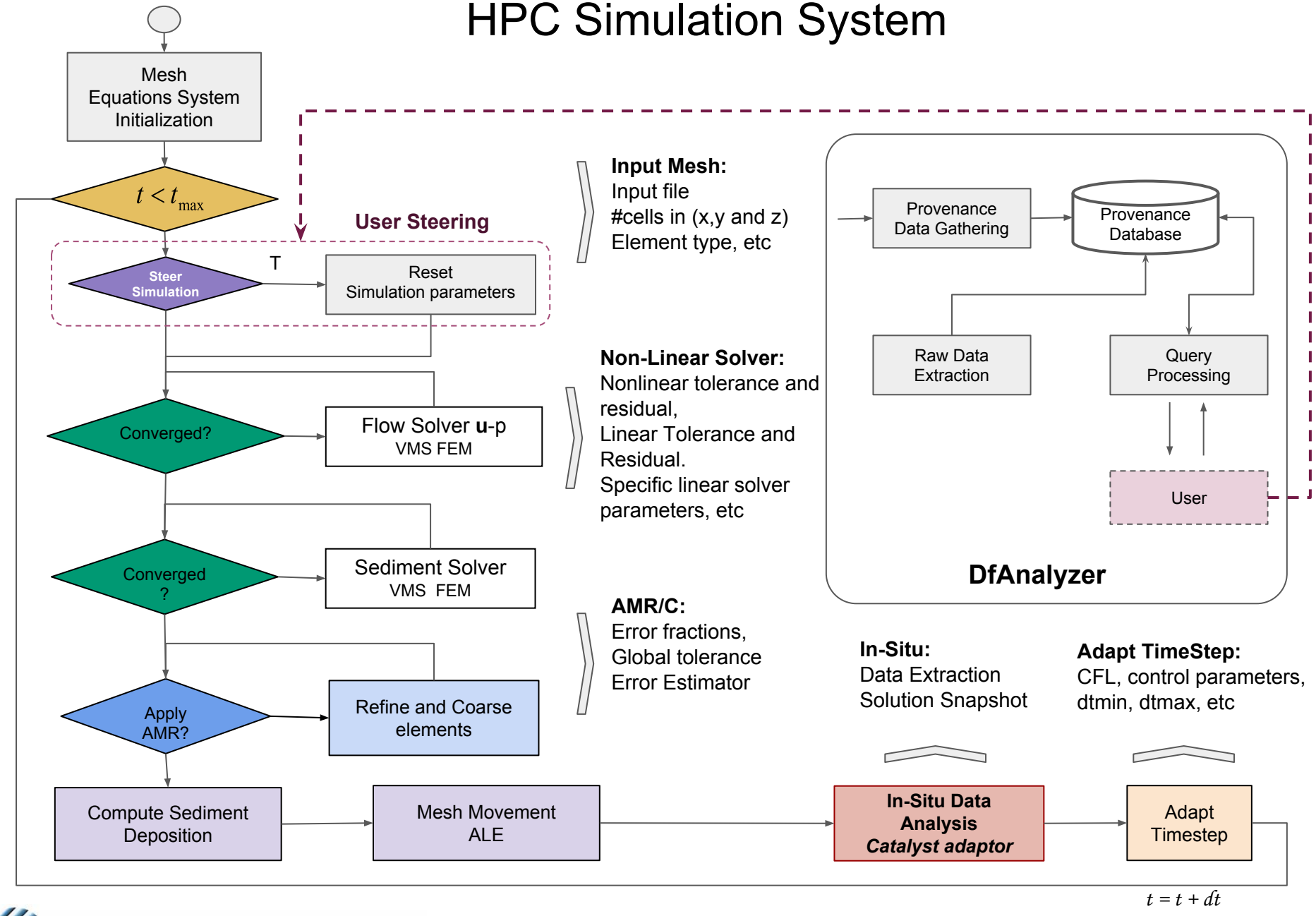
Provenance in Data Analysis

- In data-intensive high performance simulations, provenance data can help users to track all simulations parameters and relate thousands of raw data files
  - Allows reproducibility
  - Data analytical queries in these raw data files is challenging
    - Current solutions are independent and offline

- In our work, data analysis is improved combining provenance support and online queries on raw data file contents
  - Access to raw data files while they are generated
  - Parse raw data files to find useful info and extract relevant subsets of raw data
  - Index over data regions of interest
  - Prepare raw data for queries
  - Runtime queries relating raw data from different files, provenance data, and performance execution data

- Query results can help the user to ***steer*** their simulations

HPC Simulation System



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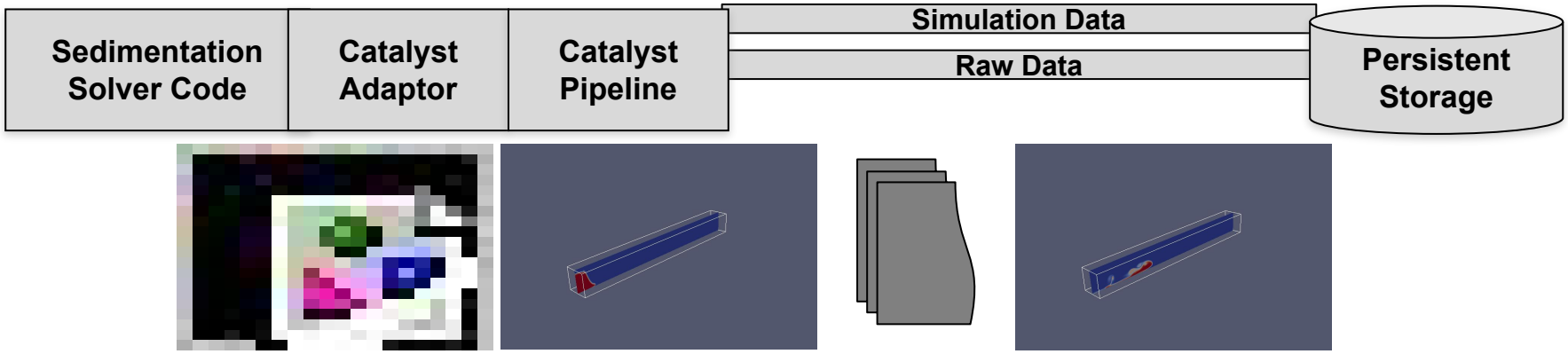
In-Situ Raw Data Analysis

- Integration between libMesh and Paraview Catalyst is provided by an ***adaptor*** (implemented in one of the Paraview Catalyst APIs)
  - Adaptor invokes Python scripts (exported from ParaView UI) for raw data analysis and visualization
  - Data structures from the simulation code accessed in memory (*in-situ*) are mapped into the adaptor using Paraview Catalyst API
    - Catalyst uses VTK's data model to perform the data structure mapping
    - *e.g.*, we map, mesh, velocity, pressure, sediment appearance, etc. from our sedimentation solver to VTK's data model

***In-situ* raw data analysis**



We can ALSO use this Paraview Catalyst adaptor for *in-transit* data analysis

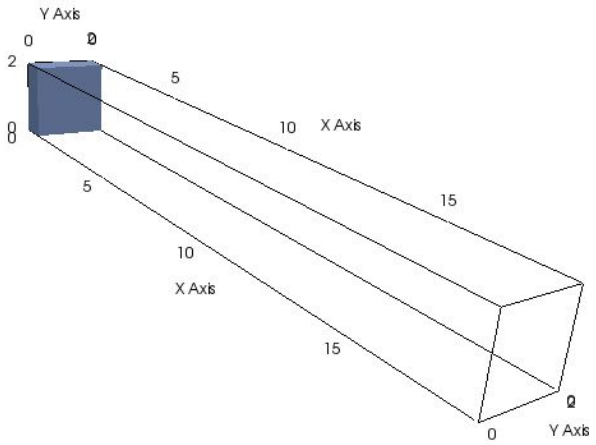
Computational Setup

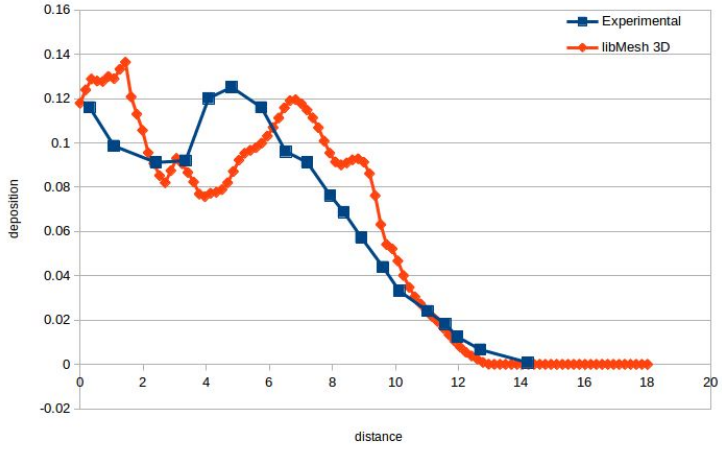
- Experiments were carried out on *Lobo Carneiro* machine at NACAD/COPPE/UFRJ[1]
  - SGI ICE-X 252 computer nodes
  - Each node with two Intel Xeon E5-2670v3 (Haswell)
  - 64GB of memory per node
  - Network: Infiniband FDR - 56Gb/s (Hypercube)
- libMesh-Sedimentation solver:
  - Intel Compilers (version 16.0) with -03 optimization flag
  - MPI Intel
  - Linked with Paraview Catalyst (v. 5.3) / Offscreen Rendering (Mesa 13.0 version)
  - Linked with Dataflow Analyzer (DfAnalyzer)
- Run configuration:
  - Standard nodes for libMesh and Paraview Catalyst
  - A dedicated node for simulation data management
    - Includes database component from DfAnalyzer

[1]http://www.nacad.ufrj.br/en/recursos/sgiicex

Test Case: de Rooij and Dalziel Sedimentation Tank

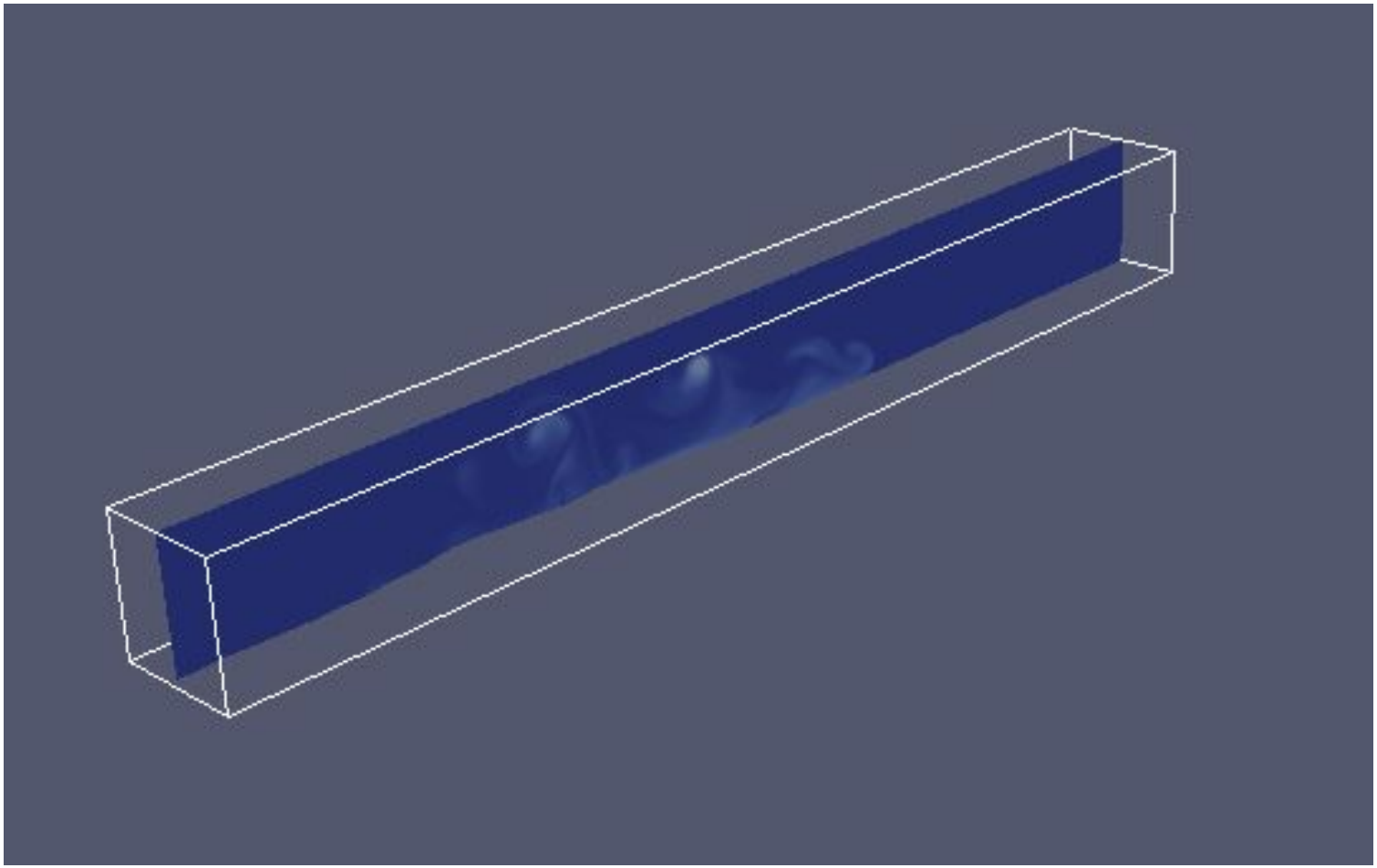
- Simulation Setup
  - Domain size: 20.0 x 2.0 x 2.0
  - Initial uniform grid in all directions, grid space 0.075
  - One initial uniform refinement, solution with max refine level=3
    - 1.5M HEX8 elements
  - Kelley's error estimator for **u** and c
  - The lock, in which the fluid initially is at rest, has dimensions 0.75 x 2.0 x 2.0
  - Reynolds number Re=5000
  - Run with 480 cores at Lobo Carneiro
- Simulation Management
  - Raw data files are written each 50 time steps
  - In-situ data extraction are called each 50 time steps
  - In-situ visualization generates pngs files each 50 timesteps
  - Catalyst data extraction: plot over line filter
  - Catalyst viz: slice filter





In-Situ Catalyst data extraction plot over line filter

Test Case: de Rooij and Dalziel Sedimentation Tank



In-Situ Catalyst viz: slice filter

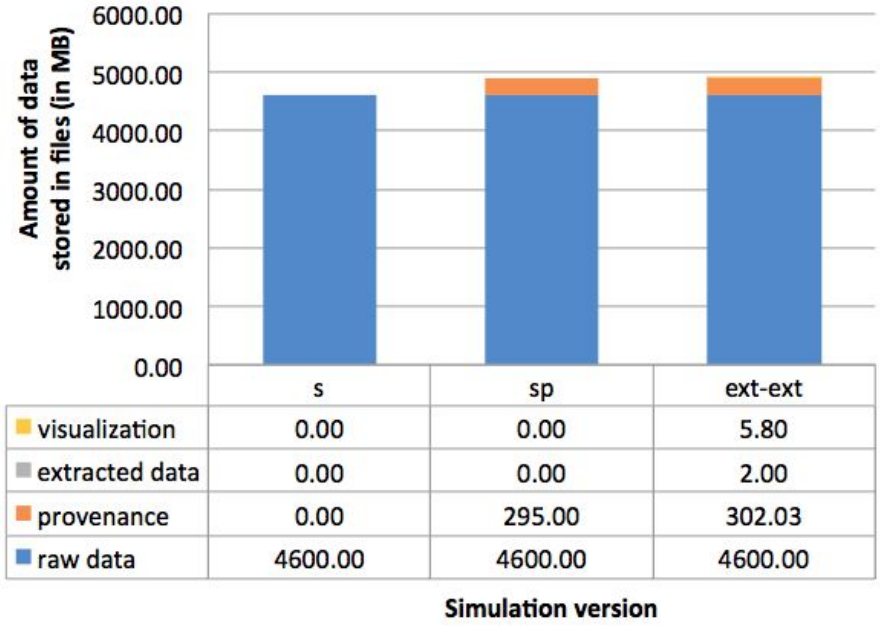
Sedimentation Tank: Computation Cost - CPU Time

TABLE 1: Elapsed time for different stages on libMesh-Sedimentation - Sedimentation Tank

Time Contribution	CPU Time (in s)	cost/call	%cost
Flow Solver	23533.21	1.26	**37.85%**
AMR/C	13122.20	93.73	**21.11%**
Sediment Solver	4941.66	0.27	**7.95%**
InSitu Catalyst Viz+Extraction	2065.08	22.45	**3.32%**
XDMF/HDF5 Raw Data	1329.21	14.45	**2.14%**
Provenance (DfAnalyzer)	83.38	0.01	**0.13%**
Others (libMesh)	17096.26		**27.5%**
Total	62171.00		

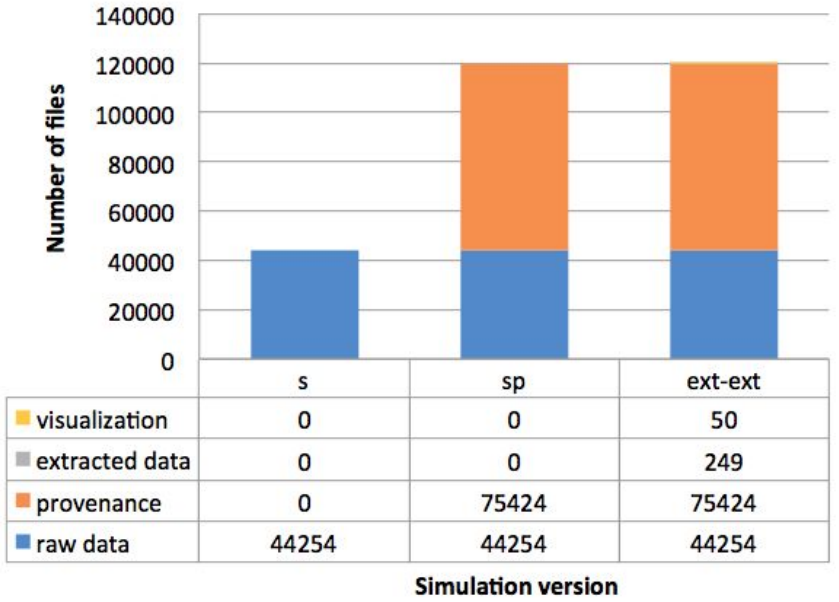
- **Remarks:**
  - Provenance adds low overhead to overall simulation costs.
  - In-Situ Viz + extraction cost in relation to Raw data Writer could be offset by disk bandwidth constraints as well as limited disk capacity.
  - CPU time spent in In-Situ Catalyst depends how many filters are applied.

Sedimentation Tank Computation Cost: Raw Data vs. In-Situ and Provenance Data Storage



	s	sp	ext-ext
visualization	0.00	0.00	5.80
extracted data	0.00	0.00	2.00
provenance	0.00	295.00	302.03
raw data	4600.00	4600.00	4600.00

Simulation version



	s	sp	ext-ext
visualization	0	0	50
extracted data	0	0	249
provenance	0	75424	75424
raw data	44254	44254	44254

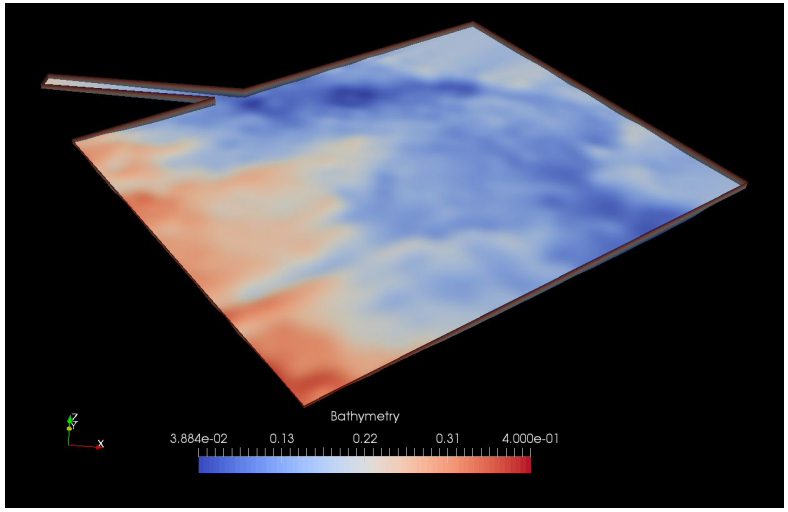
Simulation version

Legend:
s:: Solver
sp: Solver with Provenance
ext-ext: Solver + Provenance + In-situ

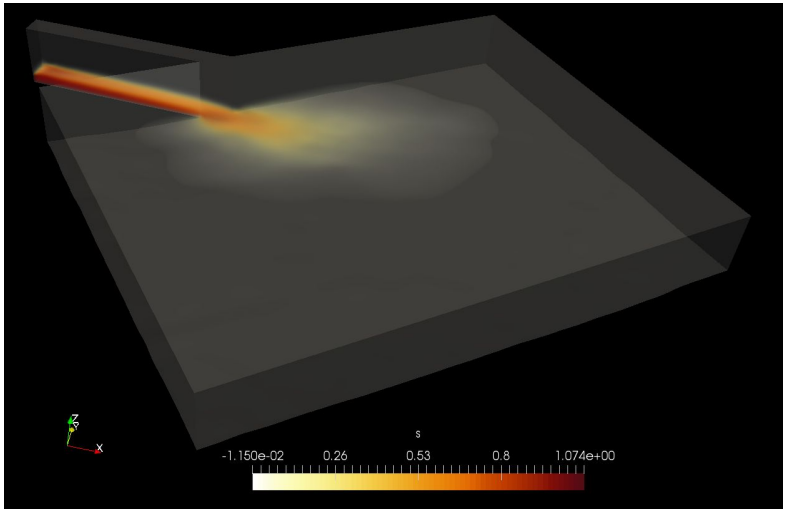
Provenance Data: 6%
In-Situ Visualization : 0.12%
Data Extraction: 0.04%
% in relation of raw data stored

Real Case: Sedimentation and Deposition with Real Bed Bathymetry

- **Run on 480 cores at Lobo Carneiro**
- **Domain Size:**
  - Tank: 14 x 12 x 2
- **Fixed Unstructured mesh:**
  - 7.6M linear tetrahedral elements
  - 1.4M nodes
- **Dimensionless Parameters:**
  - Grashof: 10^6 (Reynolds approx. 2000)
  - Monodisperse:
    - Settling velocity: 5.6651E-03
- **Boundaries conditions:**
  - **Flow:**
    - no slip is applied at bottom and channel walls
    - Prescribed velocity at front wall channel
    - Free slip at top
  - **Sediment:**
    - Concentration prescribed at front channel wall
- **Data Analysis**
  - In-Situ visualization of sediment deposition
  - Data Extraction: sediments profile over lines



Bed bathymetry



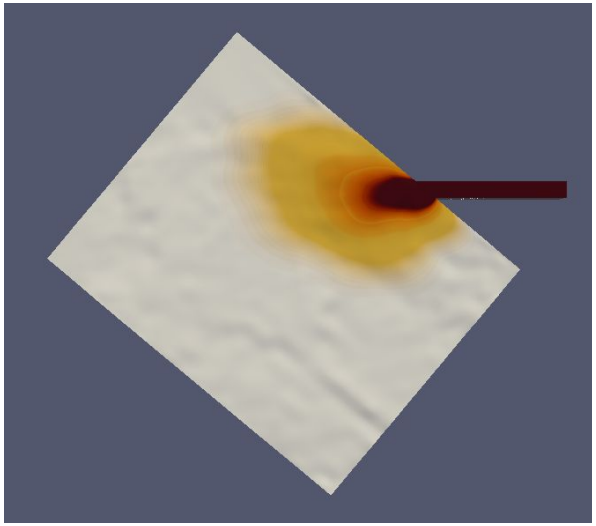
Sediment concentration at t=200

Real Bed Bathymetry Case: Computation Cost

TABLE 2: Elapsed time for different stages - Real Bed Bathymetry Case - Simulation final time t=100

Time Contribution	Elapsed Time	%Cost
Flow Solver	72523.49	50.71%
Concentration Solver	28000.50	19.58%
In-Situ Viz + Extraction	2175.16	1.52%
XDMF/HDF5 Raw data	421.23	0.29%
Provenance	451.70	0.32%
Total	143029.00	

Storage Requirements	Size (in GB)	% Raw Data
XDMF/HDF5 Raw data	23.44	
Provenance + Data Extraction	0.38	1.60%
In-Situ Viz + Extraction	0.28	1.21%



Sedimentation map generated by In-Situ Catalyst ⇨

Conclusions

- In this work we have shown the integration of In-Situ Visualization and Dataflow Analysis in libMesh
- We have used ParaView Catalyst and DfAnalyzer, openly available
- Performance measurements in representative sedimentation test cases show low overhead for both In-Situ Visualization and Dataflow Analysis tools
- What we have gained?
  - Parallel runtime interaction with simulation parameters: reset tolerances, solvers, etc, querying the provenance database from DfAnalyzer
  - Tracking QoIs at runtime through visual information provided by Paraview Catalyst/DfAnalyzer
  - Registry of computational set-up for complex multiphysics analysis for further simulations: increases reproducibility
  - Possible reduction of data stored in persistent file systems
- Want to see more?
  - Steering UQ: Dias *et al.*, FGCS, 2015
  - UQ-support in sedimentation simulations: Guerra *et al.*, Computational Geosciences, 2016
  - Dataflow Analysis in CFD, Silva *et al.*, FGCS, 2017
- Future work: scalability at higher core counts

Thanks