Hoscar Bordeaux Workshop'13

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

INTERACTING WITH SCIENTIFIC WORKFLOWS FOR COMPUTATIONAL ANALYSES

Marta Mattoso, Patrick Valduriez (INRIA – Montpellier), Jonas Dias, Daniel de Oliveira, Kary Ocana, Eduardo Ogasawara, Flavio Costa, Felipe Horta, Vitor Silva and Igor Araujo.

Marta Mattoso - COPPE/Federal University of Rio de Janeiro

HOSCAR - Objectives

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- "…taking full benefits of the processing capabilities of future high performance massively parallel architectures in the framework of very large-scale datasets and numerical simulations…"

Computer Science contributions to

- Group 3 (HPC software systems): basis for everyone

- Intergroup collaboration Group 1 (numerical simulations) and Group 2 (large-scale datasets)

Managing a Scientific Experiment

- How to re-execute only part of a workflow ?
- What is the difference in execution time of the same program with different parameters
- What results are generated for particular sets of input values ?
- How to find previous results ?
- How can a user can trace the “process” that led to the aggregation of executions producing a particular output ?
- How to extract knowledge from previous experiments ?

SWfMS – support analysis AFTER execution

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Several SWfMS are available, being used on different apps

VisTrails

Kepler
Your Science. Enabled.

Trident

pegasus
Making Science Flow For You

swift

Taverna

- SWfMS keeps track of the execution through **provenance** support

SWfMS Workflow execution

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- SWfMS manages parameter exploration
- N algorithms,
  K parameters each,
  L values in each parameter ➔
  SWfMS manages the algorithms, parallel processing, provenance
- End workflow execution
- Results & provenace are analyzed

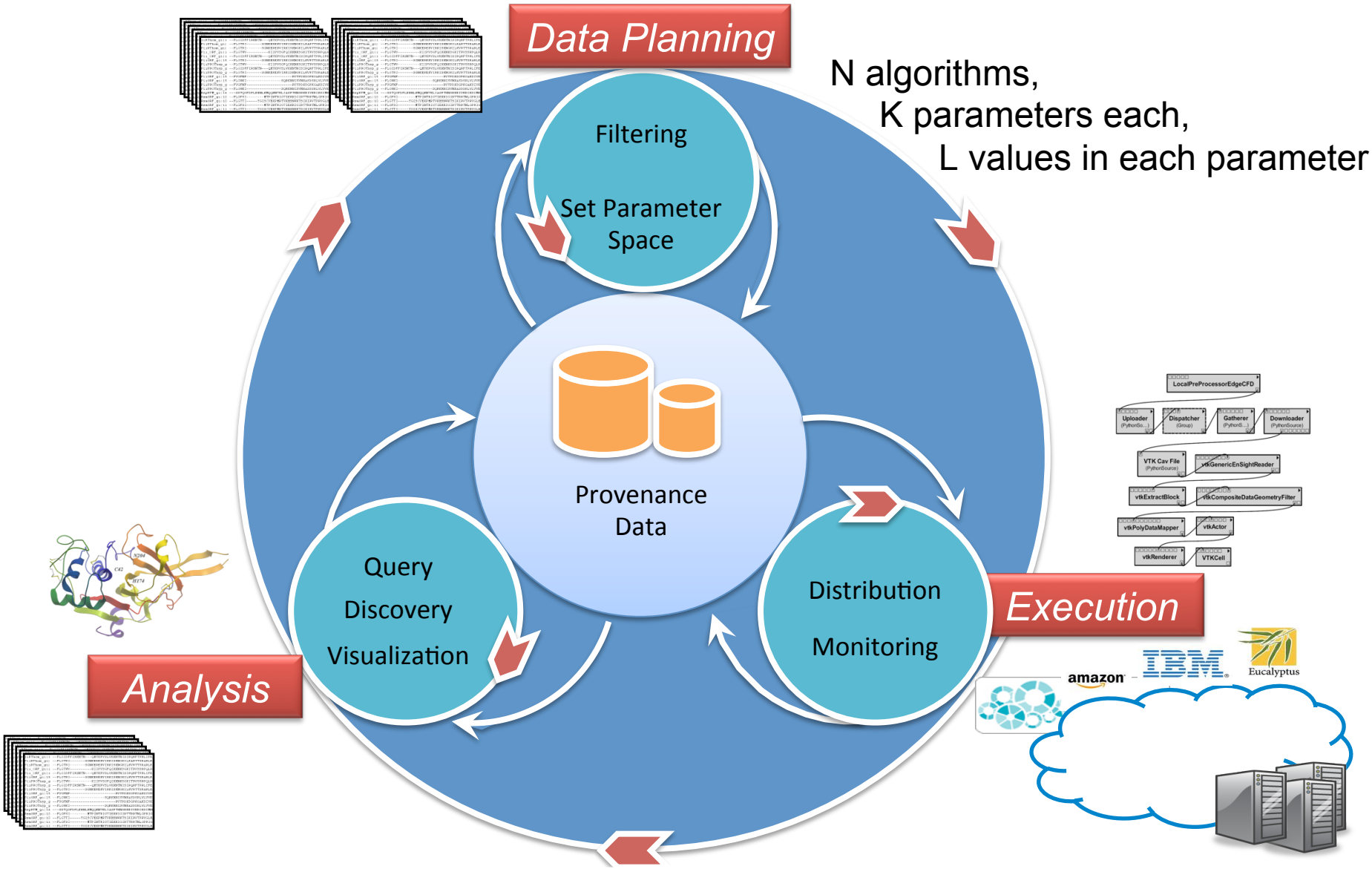
SWfMS execution life cycle

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- SWfMS manages parameter exploration
- N algorithms,
  - K parameters each,
    - L values in each parameter ➔
      - SWfMS manages the algorithms, parallel processing, provenance
- End workflow execution
- Results & provenace are analyzed

New parameters are defined

Workflow Execution Life Cycle



CFD analyses take several factors into consideration

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

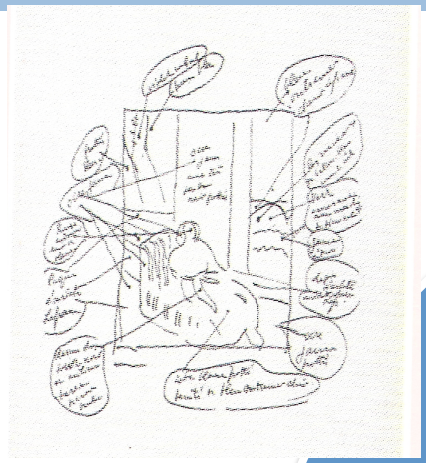
- geometry,
- material properties, e.g. viscosity,
- mesh partitioning,
- time step size,
- wall time
- the frequency at which the results are stored

Based on the produced outcome: explore the simulation differently

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- refine the mesh,
- change time step size
- store more or less results during specific simulation time intervals

Matisse's painting Life Cycle



Data Planning

Colours,
Texture,
Zooming

Filtering

Set Parameter Space

Provenance Data

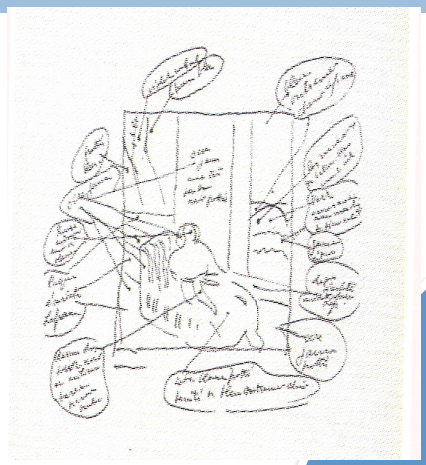
Analysis

Query
Discovery
Visualization

Distribution
Monitoring

Execution

Matisse's painting Life Cycle



Data Planning

Colours,
Texture,
Zooming

Filtering

Set Parameter Space

Provenance Data

Analysis

Query
Discovery
Visualization

Distribution
Monitoring

Execution

Workflow execution
Off-line (black-box) X On-line (steering)

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Only after the whole workflow execution :
  - Change parameters
  - Replace some algorithms
- Interrupt the execution

"Off-line"

During workflow execution

- Partial results & provenance are analyzed
- Fine tuning of parameters
- Skipping/replace some algorithms
- Skipping some parameter combinations

"On-line"

Workflow execution
Off-line (black-box) X On-line (steering)

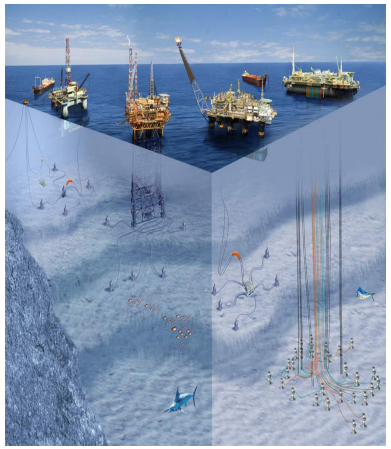
- ✓ **Hard to visualize partial results** "Off-line"
  - A lot of information to be filtered
  - Traceability of which input produces output
  - Some results may not be useful
    - Data and meta-data association
  - Fragmented Data
  - Relevance of data
    - Each analysis may focus on a subset of the obtained outputs
  - Time consuming data transfers

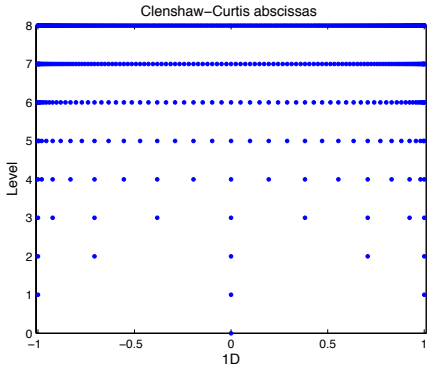
Some real examples that need “online”

- Bioinformatics
  - query and traverse partial results to change activities or parameters
- Oil & Gas
  - engineers need to explore the parameter space in slices skipping input data dynamically
- Numerical simulations, Uncertainty Quantification
  - snapshots of current simulation results to refine the model (iterations) during runtime

SciEvol

Evolutionary analysis





Why User Steering is still a challenge ? Provenance is distributed

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

Provenance database gathers data from the different environments

1.Data is generated and collected

Desktop

2. It is locally Evaluated

Provenance Data

3. Large volume of data produced ...

Storage

4. ...which need to be processed by a computing-intensive environment

Cloud

5. Final (?) results evaluated

Tyled wall display

Provenance is a key feature

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Keeps track of everything that happens during experiment execution
- A log that can be queried
- Allows for high-level and domain-specific queries
  - What are the maximum values for velocity and pressure on a given CFD simulation?
- A powerful association: Experiment meta-data with strategic experimental results
  - Runtime analysis
  - Good for time-consuming experiments
- User-steering for convergence analysis
  - User interacts with data of interest at runtime
  - Interfere in the workflow execution to adjust

Open issues

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Workflow execution monitoring
  - verifying the status of the execution at specific points
  - tools to handle data staging, consolidation, statistics and visualization
- Data analysis at runtime
  - discover if anything odd has happened
- Dynamic interference in the execution
  - change parameter values or even programs of the workflow during its execution
  - truncate the iteration based on the error

Current approaches: Data Analysis at Runtime

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

"access to preliminary results to analyze them empowered with data from provenance repositories and statistical and visualization tools" → N/A

- VisTrails- visualize results and compare them on a single screen or on tiled wall displays – **no HPC**
- Swift/Turbine or Pegasus
  - HPC in very large scale with provenance
  - No **runtime** provenance support
- ParaView- instruments the code and select produced results to be exported for visualization in their sw, **no SWfMS**

Dynamic Workflow Interference

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Needs monitoring and runtime analysis
- Simple interventions:
  - stopping a workflow, stopping an activity, or re-executing activities
- Complex interventions:
  - changing an activity of the workflow, interfering in the iterative process, changing the structure of the workflow and changing parameters or complete parameter sets

Current approaches: Dynamic Workflow Interference

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Pegasus - failure handling in scientific workflows
  - Regression trees to classify activity executions as failed or successful. Based on provenance data the framework learns activity execution behavior and predicts future failures.

- Dias *et al*. present dynamic parameter sweep in HPC workflows
  - Based on partial result data from runtime provenance scientists can decide when to stop a time dependent iteration (loop) of a scientific workflow.

Our experience with Chiron workflow engine

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Designed for HPC environments
- Algebraic engine based on relational algebra *
  - Runs legacy and third party applications
- SciCumulus in the Cloud
- Model to represent provenance data
  - PROV extension
  - Prospective and retrospective provenance
  - **Available for querying at runtime**

* Ogasawara et al., **An Algebraic Approach for Data-Centric Workflows**. *VLDB, 2011*

"*Algebraic engine and provenance oriented*"

Trigger – Query

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

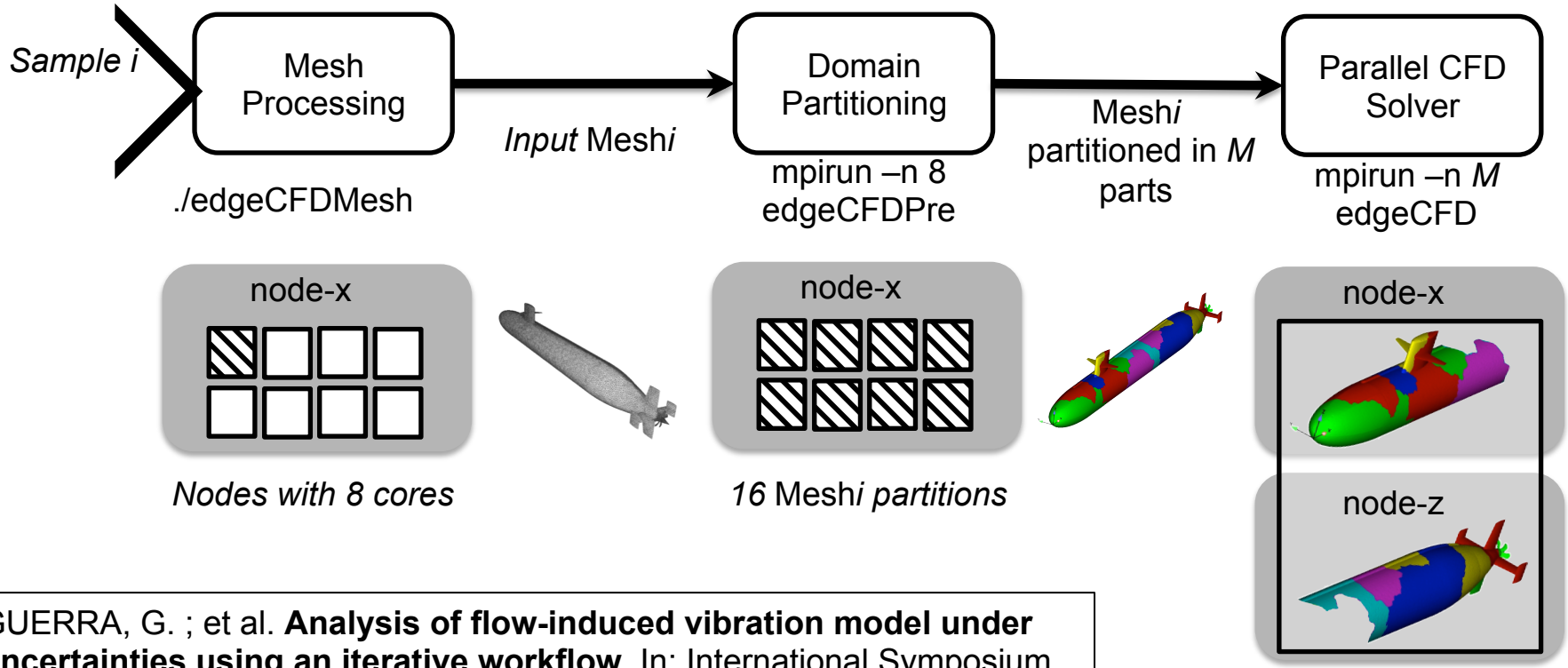
- Submit a query to the cloud (or cluster) to :
  - monitor the execution time of a specific activity execution and check if it is under or above the average time of previous executions of the same activity
  - obtain results from one specific parameter and do a visualization preview before the end of execution

Turbulence UQ analysis on a submarine

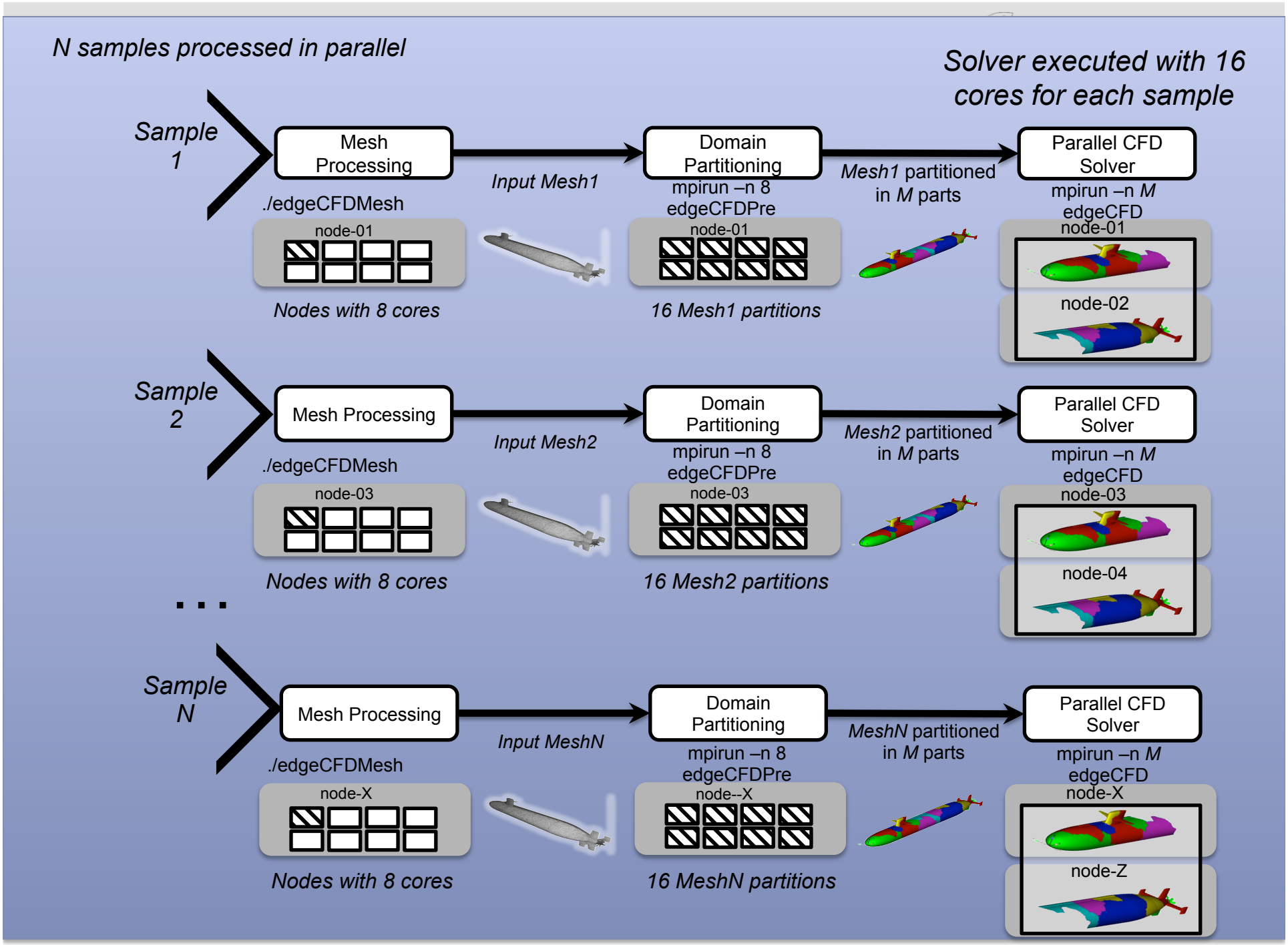
COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

Chiron is running in each core of each node:
managing scheduling, fault-tolerance, provenance data gathering, …
runtime provenance queries

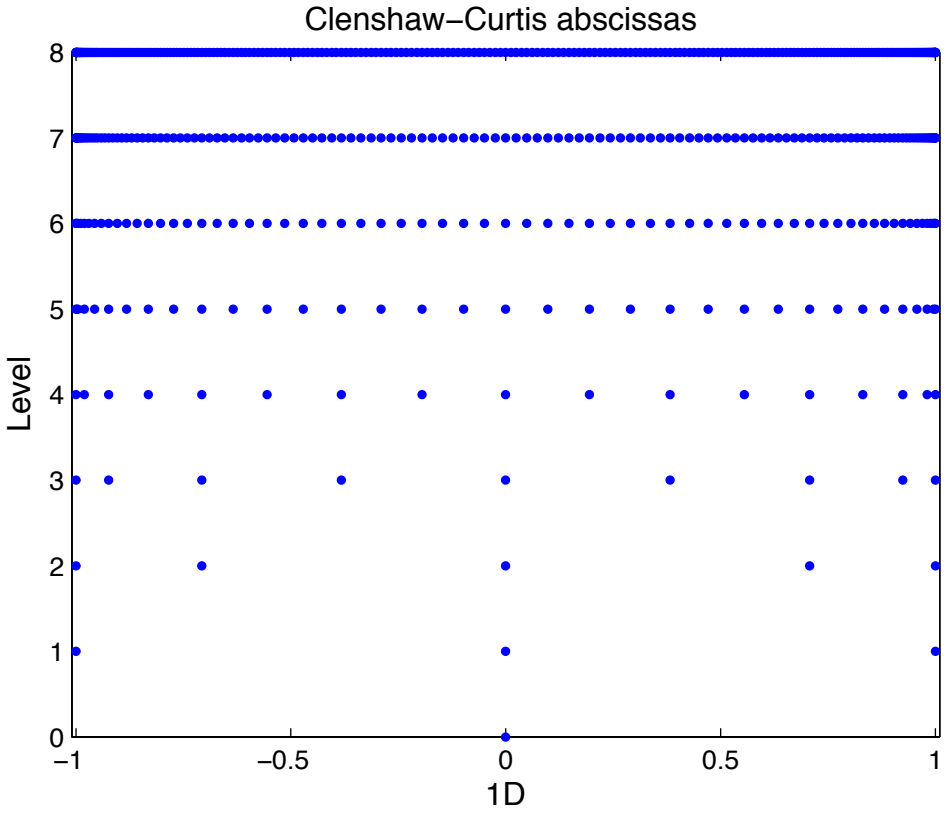
Solver executed with 16 cores for case i



GUERRA, G. ; et al. **Analysis of flow-induced vibration model under uncertainties using an iterative workflow**. In: International Symposium on Uncertainty Quantification and Stochastic Modeling 2012


N samples processed in parallel
Solver executed with 16 cores for each sample
Sample 1
Mesh Processing
./edgeCFDMesh
node-01
Nodes with 8 cores
Input Mesh1
Domain Partitioning
mpirun –n 8 edgeCFDPre
node-01
16 Mesh1 partitions
Mesh1 partitioned in M parts
Parallel CFD Solver
mpirun –n M edgeCFD
node-01
node-02
Sample 2
Mesh Processing
./edgeCFDMesh
node-03
Nodes with 8 cores
Input Mesh2
Domain Partitioning
mpirun –n 8 edgeCFDPre
node-03
16 Mesh2 partitions
Mesh2 partitioned in M parts
Parallel CFD Solver
mpirun –n M edgeCFD
node-03
node-04
Sample N
Mesh Processing
./edgeCFDMesh
node-X
Nodes with 8 cores
Input MeshN
Domain Partitioning
mpirun –n 8 edgeCFDPre
node--X
16 MeshN partitions
MeshN partitioned in M parts
Parallel CFD Solver
mpirun –n M edgeCFD
node-X
node-Z

Uncertainty Quantification using Adaptive Sparse Grid Collocation

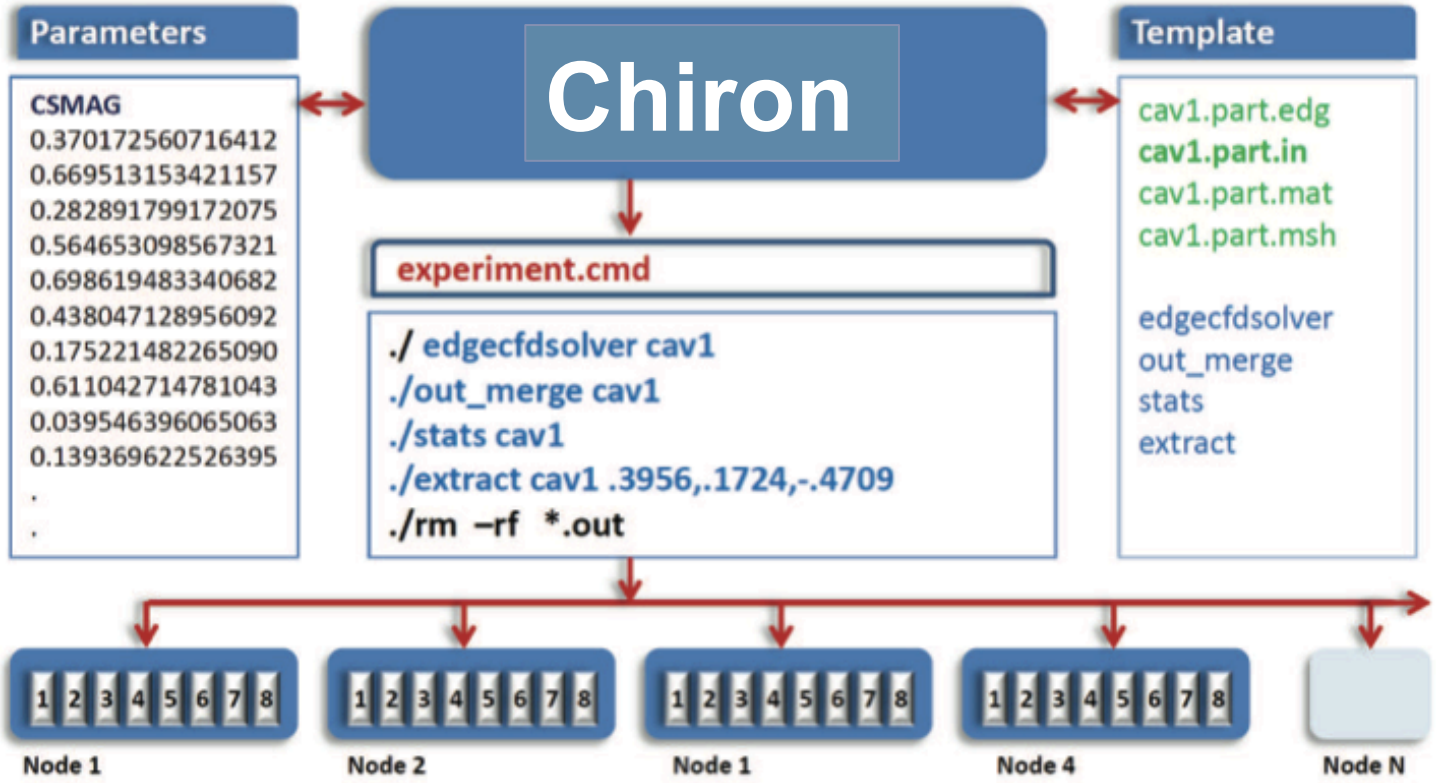


1D sparse grid for increasing interpolation level

- MC reference solution with 1,000 samples, 126hs in 32 cores
- ASGC with 8 approximation levels, 257 support nodes, 39hs (32 cores)

Guerra, G. et al., **Uncertainty Quantification in Computational Predictive Models for Fluid Dynamics Using Workflow Management Engine**. International Journal for Uncertainty Quantification, , v. 2(1) 2012

Large Eddy Simulation Workflow Parallel Execution in Chiron



- Provenance gathers data to be used to evaluate statistical moments
- We can track the error between MC and ASGC and determine an interpolation level to satisfy a minimum error
- Provenance capabilities in Chiron can automatically increase the interpolation level and resubmit the experiment to obtain statistical moments with a prefixed error

Visualization and User-Steering

- **Go fast to the results you need to analyze**
  - ✓ Navigation over data results (partial) added by provenance (log)
  - ✓ Filter results and stage out only the data you need to analyze
  - ✓ Interact with a web-based user interface
- **Export and analyze partial results to take decisions**
  - ✓ Efficient data consolidation and data staging features to aggregate and stage out only relevant information
  - ✓ Use statistical and visualization tools empowered by provenance data
  - ✓ Draw preliminary conclusions

Visualization and User-Steering

- **Monitor and Analyze workflow execution**
  - ✓ Awareness of the current workflow status
  - ✓ Identify and solve problems during execution
  - ✓ Recover from failures and misconceptions
  - ✓ Reduce time spent in processing low-quality data
  - ✓ Cut execution time and reduce financial costs
    - Stage data out can be costly!
    - Remote clusters

Visualization and User-Steering

- **Use high-resolution display environments**
  - ✓ Visualize multiple results to establish comparisons
    - On parameters exploration scenarios
  - ✓ Analyze detailed images and simulations
  - ✓ Can take advantage of available tiled display technologies such as TACC DisplayCluster, SAGE, CGLX, and Paraview

Large-Scale Scientific Data Visualization using Provenance

- **Web interface connected to Provenance Database and visualization environment**
  - ✓ Interactive interface
  - ✓ Navigate through its activities and i/o data
  - ✓ Filtering options to select the desired results
  - ✓ Stage data out of the execution environment
  - ✓ Text, images, PDF, video and Paraview visualization

Large-Scale Scientific Data Visualization using Provenance

COPPE UFRJ

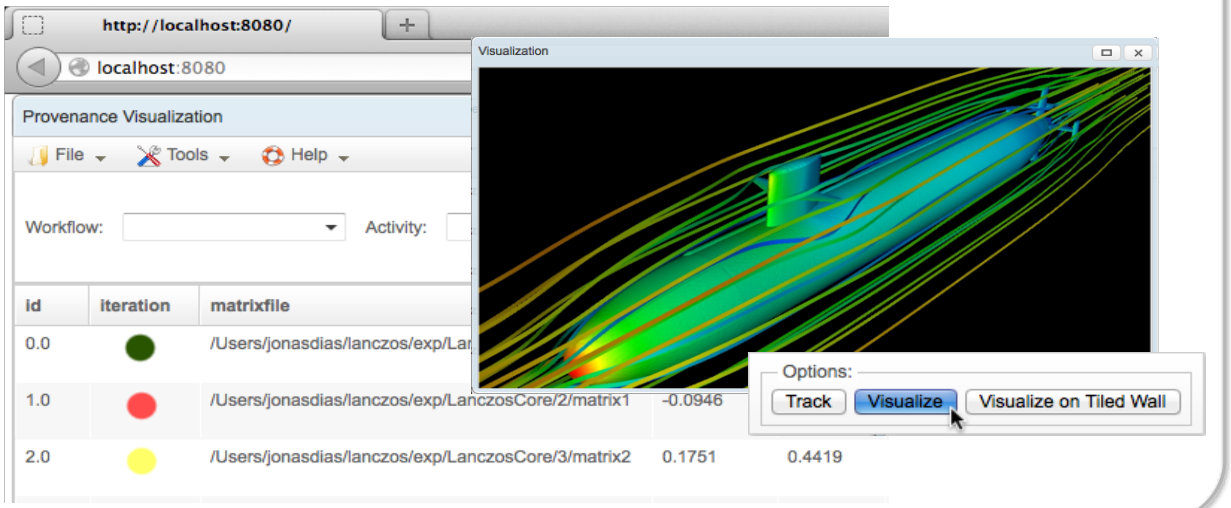
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- **Web service in the visualization cluster to display staged out data in the Tiled Wall Display**
  - ✓ Implemented as a Web Service
  - ✓ Interface accessed by the web module in runtime
  - ✓ Can also stage data out of the execution environment
  - ✓ Pluggable to support different tiled wall displays middlewares.

Steering in HPC – ProVis visualization

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

Web Client



- Exploration 1
- Exploration 2
- Exploration 3
- ...
- Exploration N

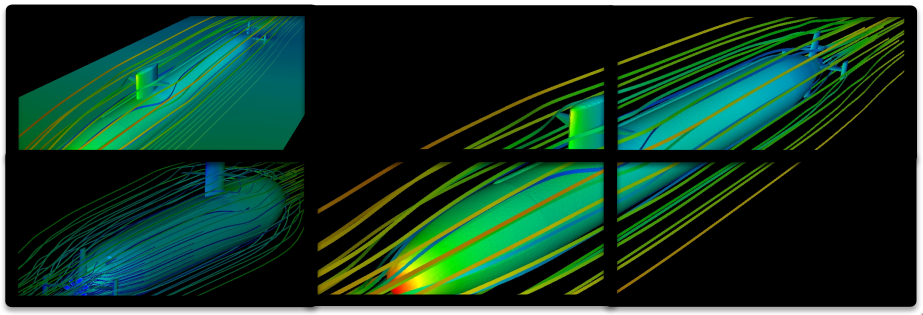
Remote Application

Tiled Wall Display

TACC DisplayCluster

SAGE

ParaView



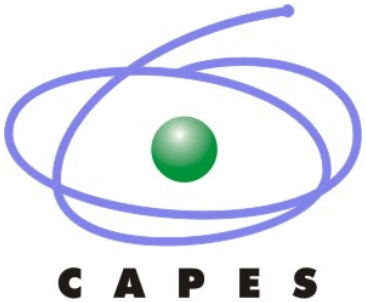
Action in tags can be one of paraview's recorded scripts that reads the experiment results and produces a video, for example.

Conclusions

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia

- Traces of a real-time provenance database
  - It is possible to take more advantage of experiment's provenance data
- Real-time provenance offers valuable information to help scientists
  - Monitor, analysis, steering, interference …
- Effort to follow PROV recommendation
  - How to define stereotypes for HPC in PROV
    - Considering hybrid workflows
    - Running in the cluster or Cloud with distinct systems

Acknowledgements



Hoscar Bordeaux Workshop'13

Thank you!

- Chiron workflow engine
  - http://sourceforge.net/projects/chironengine/

- SciCumulus in the Cloud
  - http://sourceforge.net/projects/scicumulus/

Marta Mattoso
Federal Univ Rio de Janeiro

COPPE UFRJ
Instituto Alberto Luiz Coimbra de Pós-Graduação e Pesquisa de Engenharia