Co-visualization of full data and in situ data extracts from unstructured grid CFD @ 160K cores

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Motivation - Outline

- Massively parallel solvers create data at ever increasing rates
- Our ability to write, store, and process the data has not kept pace
- Co-visualization seeks to resolve this dilemma
- Key components must be carefully combined
  - Solver: PHASTA CFD solver
  - Visualization tools: Paraview Coprocessing library, pvserver, and client GUI
  - I/O Acceleration: GLEAN
  - Hardware: Argonne ALCF (Intrepid/Eureka)

Live data visualization strategies

- Classical Co-Vis (CCV):

  Simulation data is sent to pvserver unfiltered,

  pvserver applies filters and renders on vis cluster

- In-situ data extracts (ISDE):

  Filters process simulation data on supercomputer,

  send extracts to pvserver for rendering on vis cluster

- Data transfer between supercomputer and vis cluster:

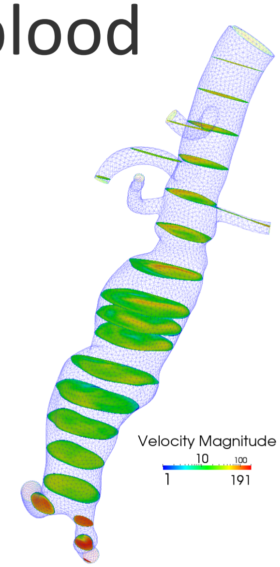
  - VTK Sockets: CCVS or ISDES

  - GLEAN: CCVG or ISDEG

PHASTA CFD solver

- Parallel Hierarchic Adaptive Stabilized Transient Analysis
- Models compressible or incompressible, Laminar or turbulent, steady or unsteady flows
- 3D finite elements discretization in space and fully implicit in time
- Used to model air flow over airplane wing, blood flow, two phase flow, etc
- Scaled to 288K cores (JUGENE - SC09)

$5B$ elements mesh (Jugene:IBM BG/P)		Eqn. form.		Eqn. soln.		Total	
num. of core	avg. elem./core	time	s-factor	time	s-factor	time	s-factor
65,536 (base)	76,480	119.64	1	162.59	1	288.23	1
131,072	38,240	59.69	1.00	84.09	0.97	143.78	0.98
262,144	19,120	30.02	1.00	43.24	0.94	73.26	0.96
294,912	16,995	26.71	1.00	39.15	0.92	65.86	0.95



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Analysis challenges posed by PHASTA scientists

- A "window to the simulation" to understand state and progress
- Extract continuous and reconfigurable insight from massively parallel simulations
- Enable interactive simulation / simulation steering
- Reduce the data being written to storage

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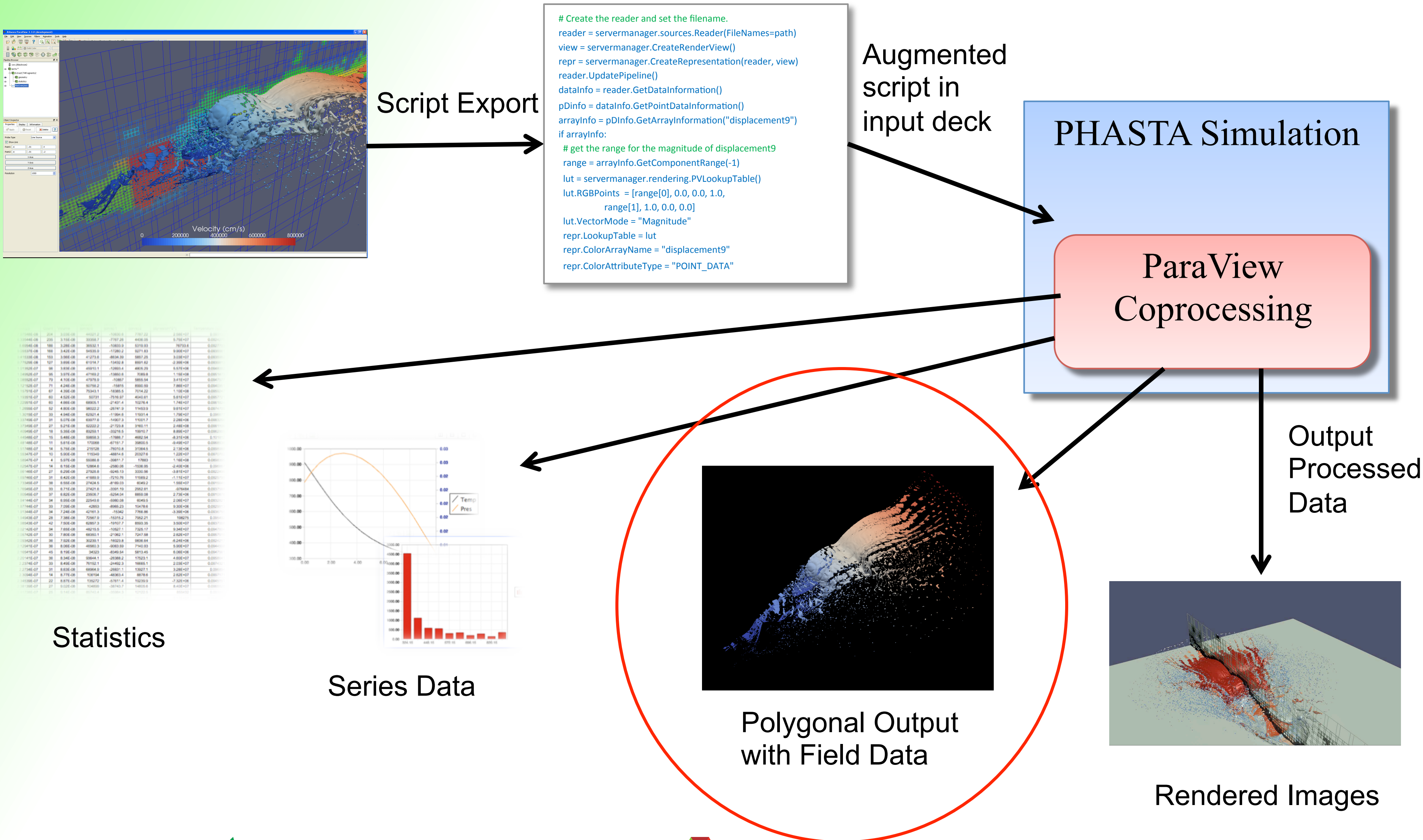
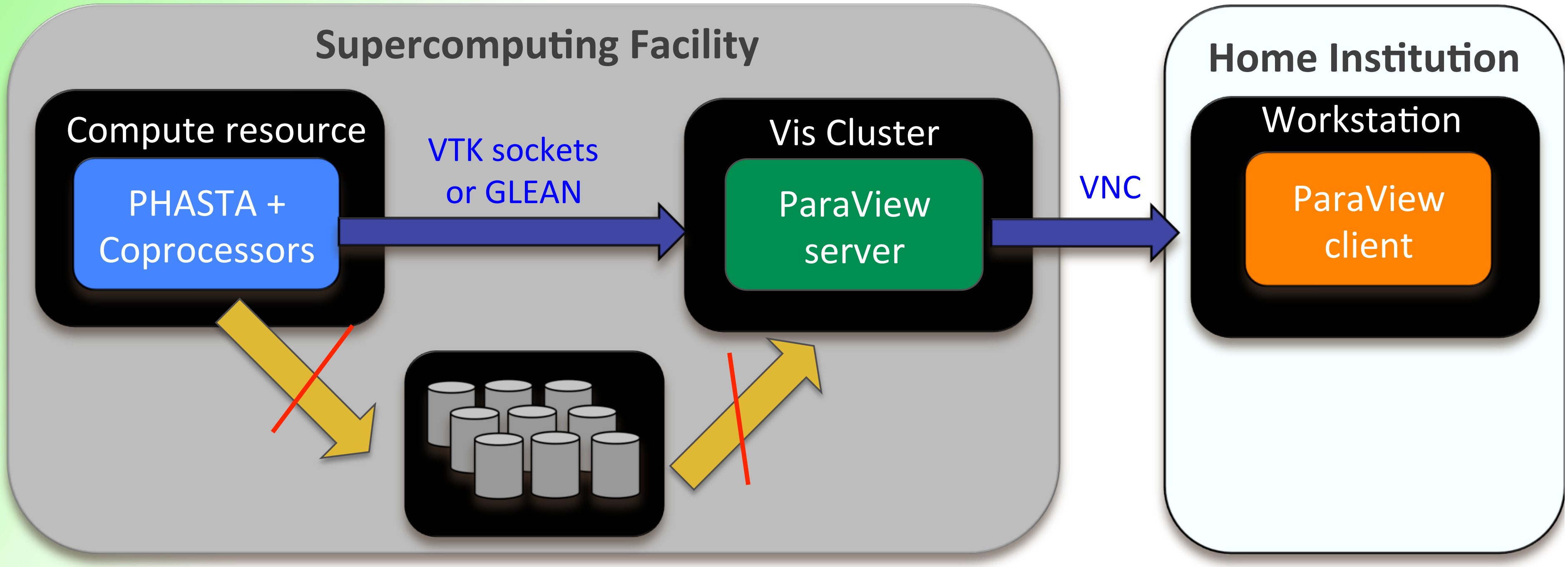
What is the ParaView Coprocessing Library?



Run-Time visualization with PHASTA



- PHASTA simulation running on 160K cores of Intrepid BG/P
- ParaView server running on up to 100 Eureka nodes (800 cores)
- ParaView client running on Eureka head node and accessible via VNC
- VTK sockets or GLEAN for data transfer between Intrepid and Eureka

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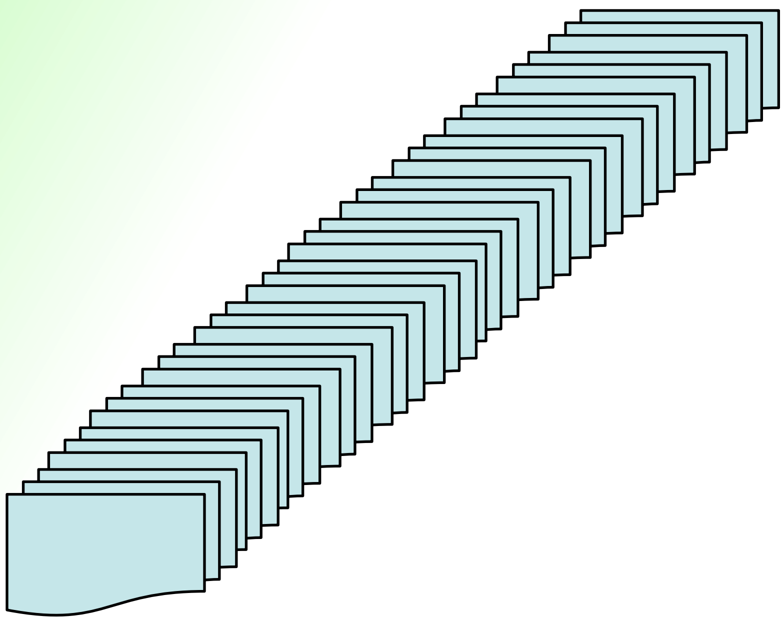
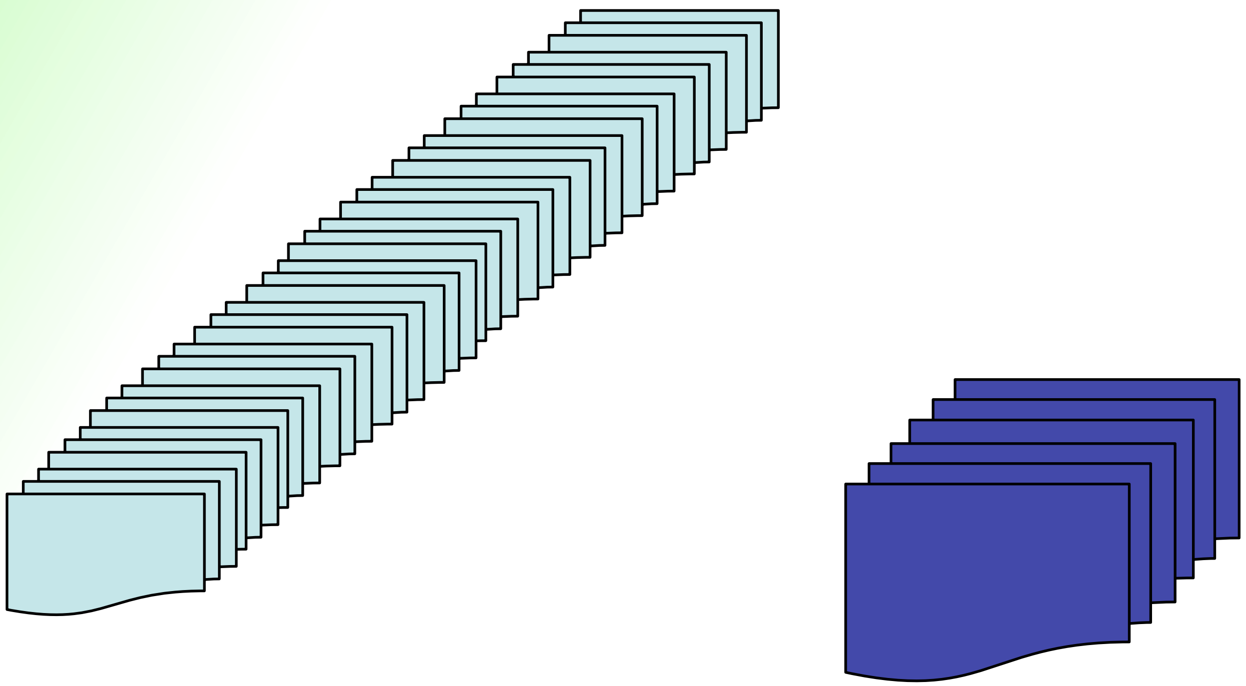
Procedure

- Start simulation + coprocessor on supercomputer



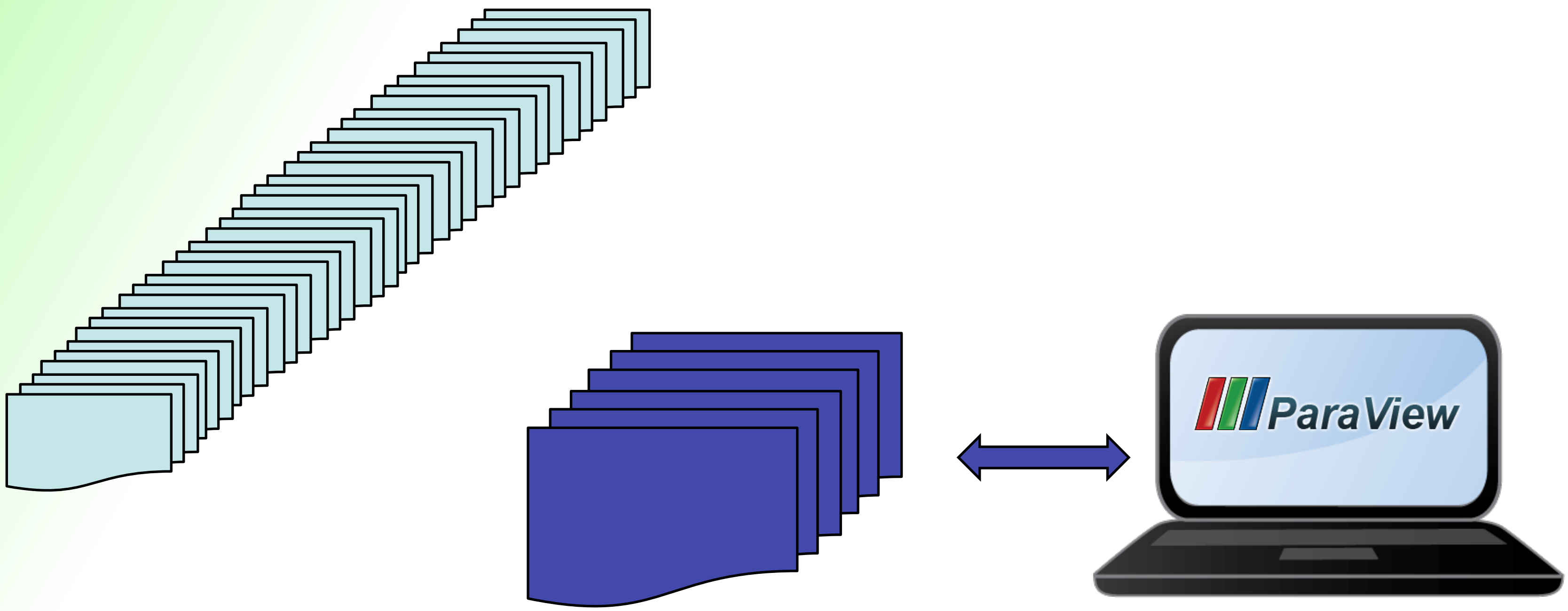
Procedure

- Start ParaView server (pvserver) on vis cluster



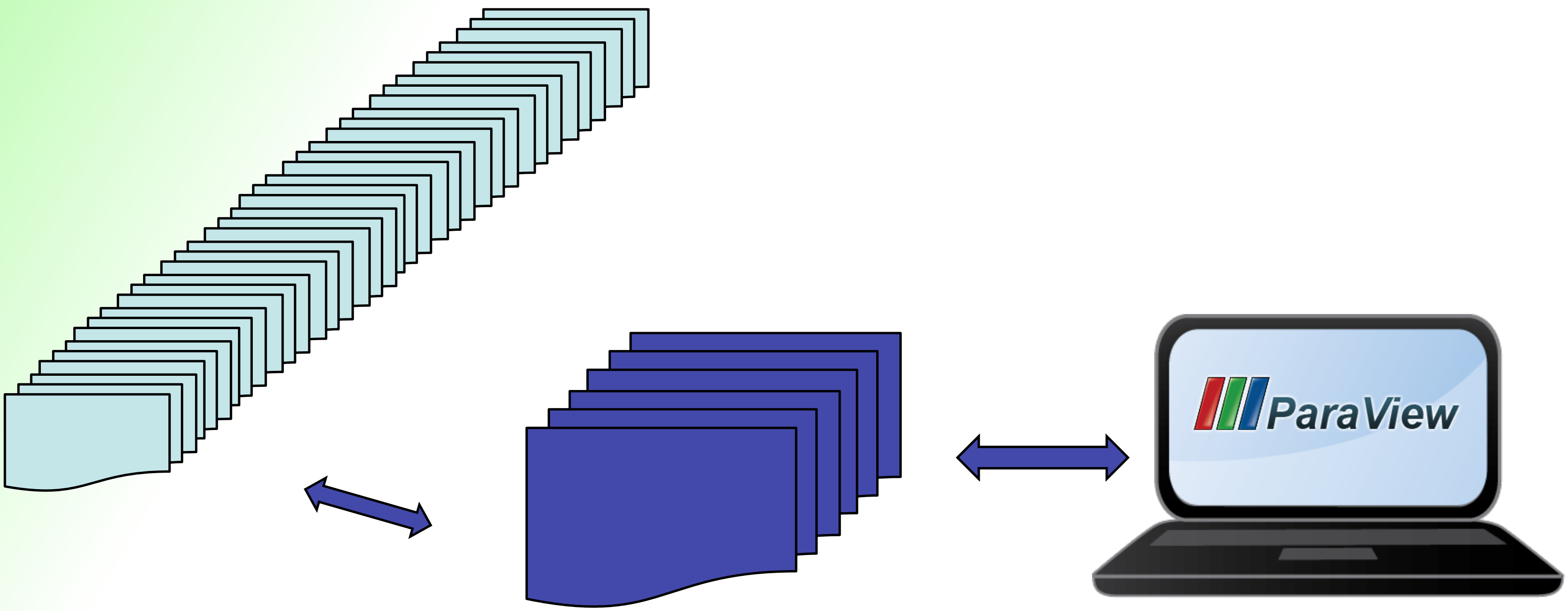
Procedure

- Launch ParaView client, connect to pvserver



Procedure

- Create Live Data Source filter
- pvserver now communicates with the coprocessor



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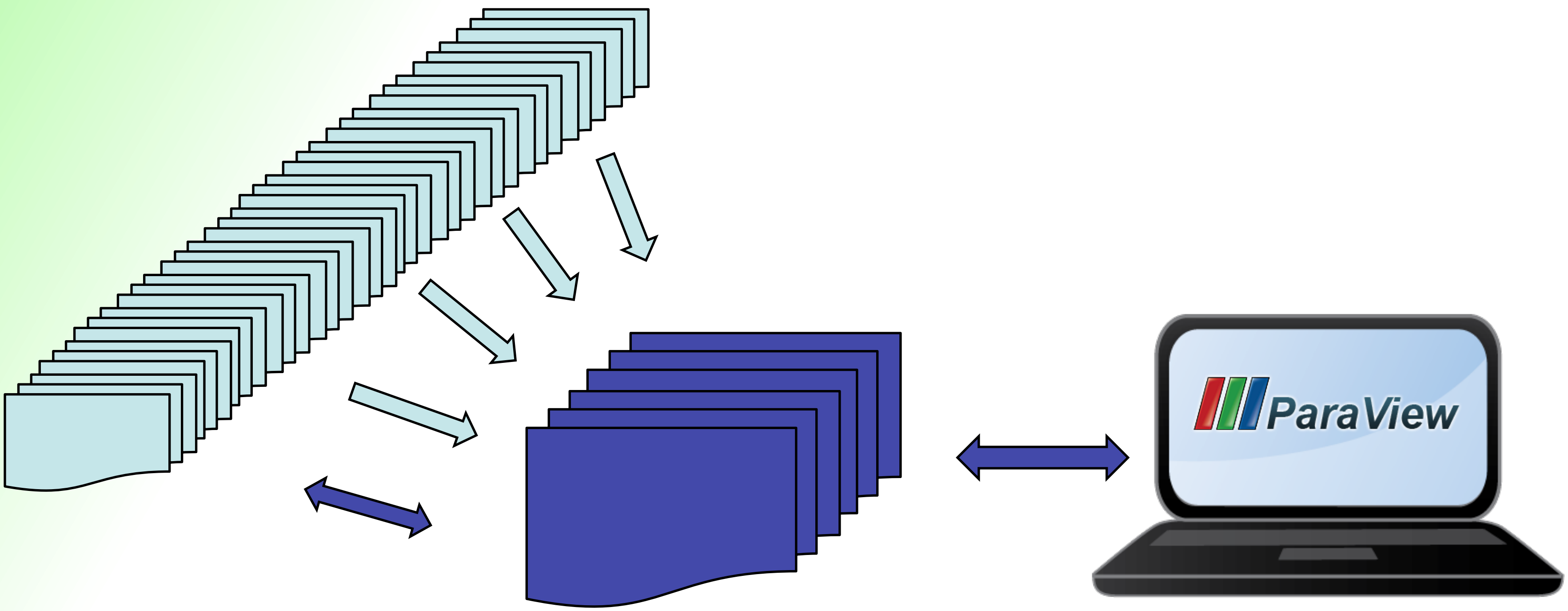

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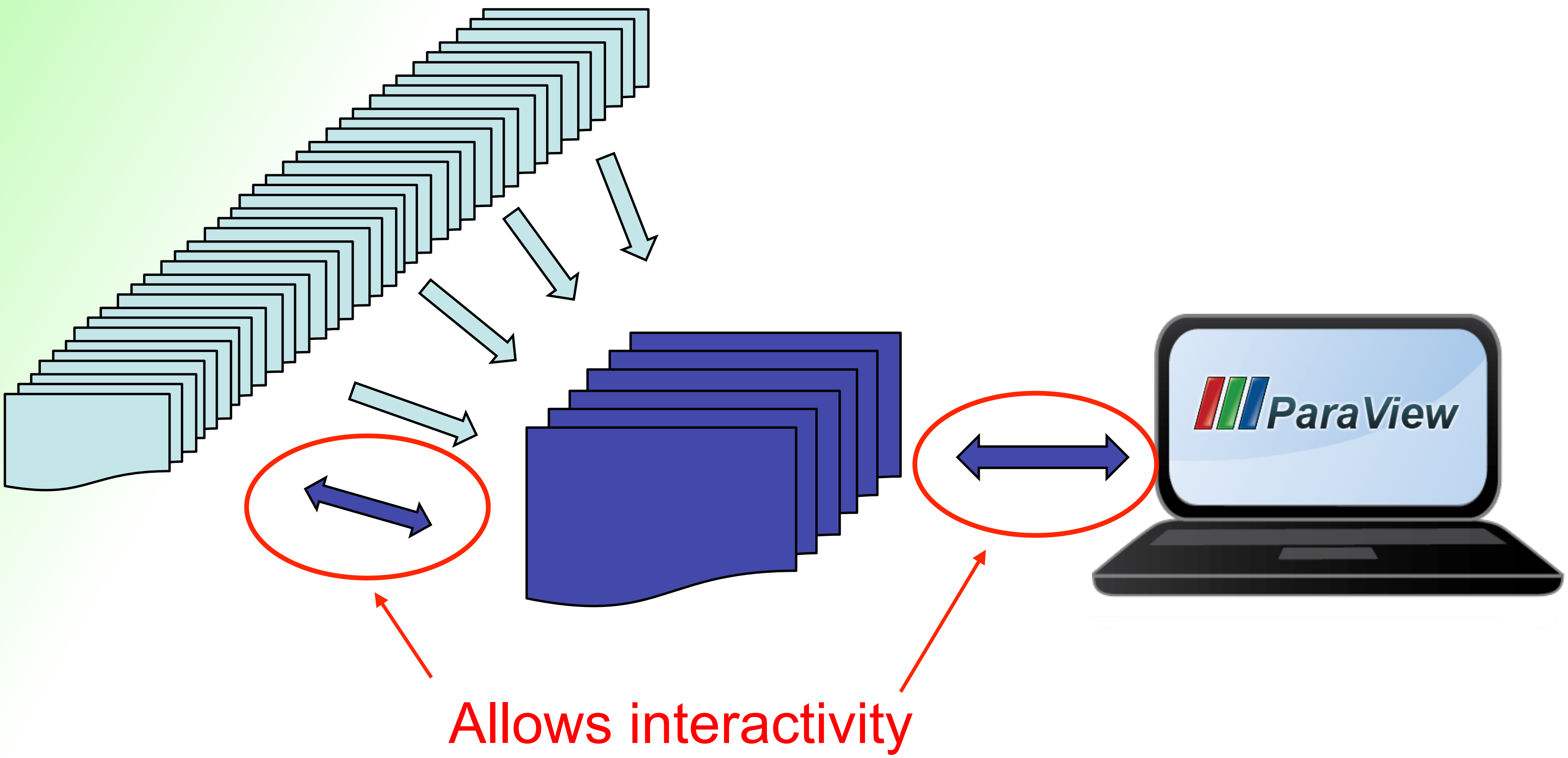
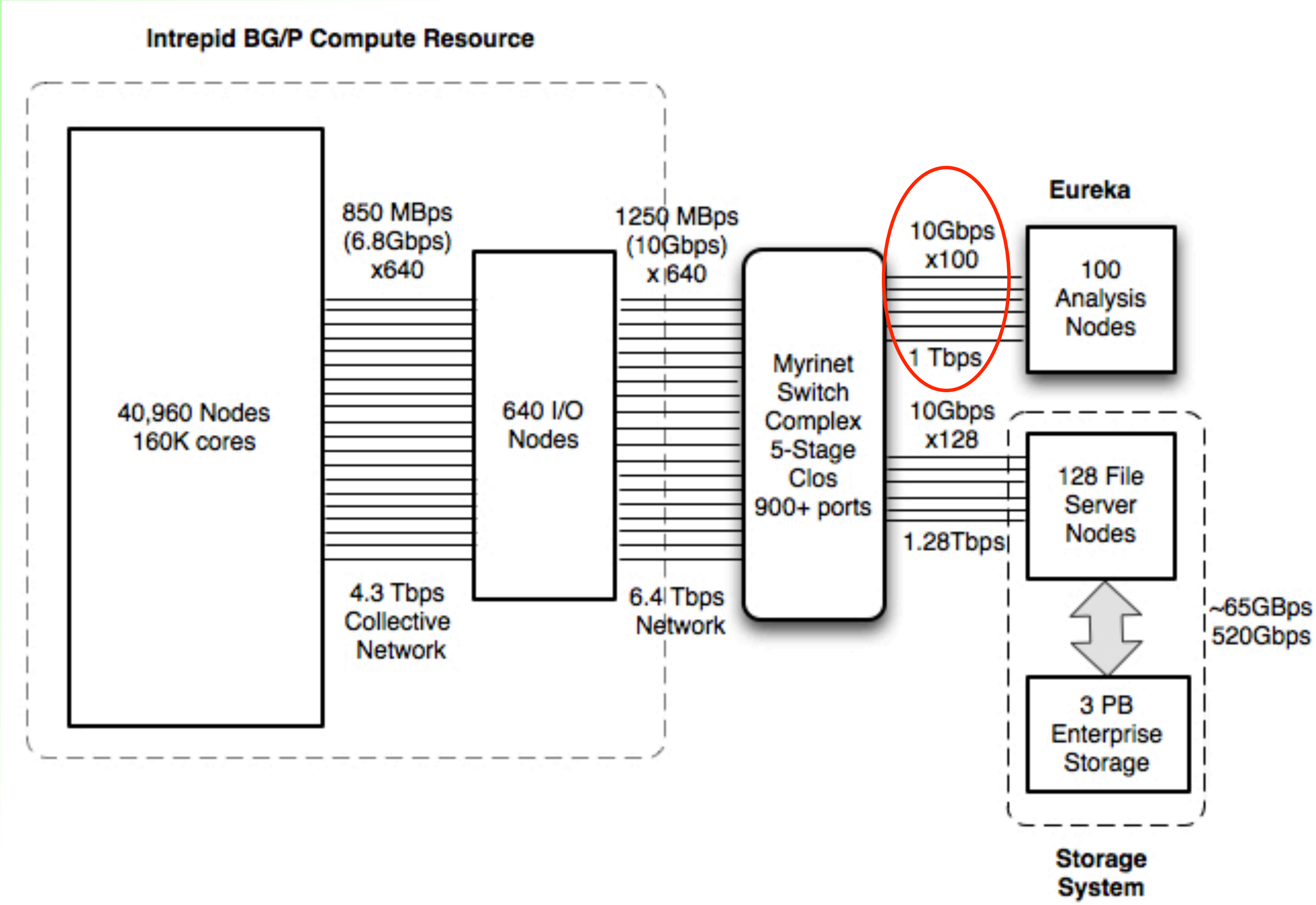
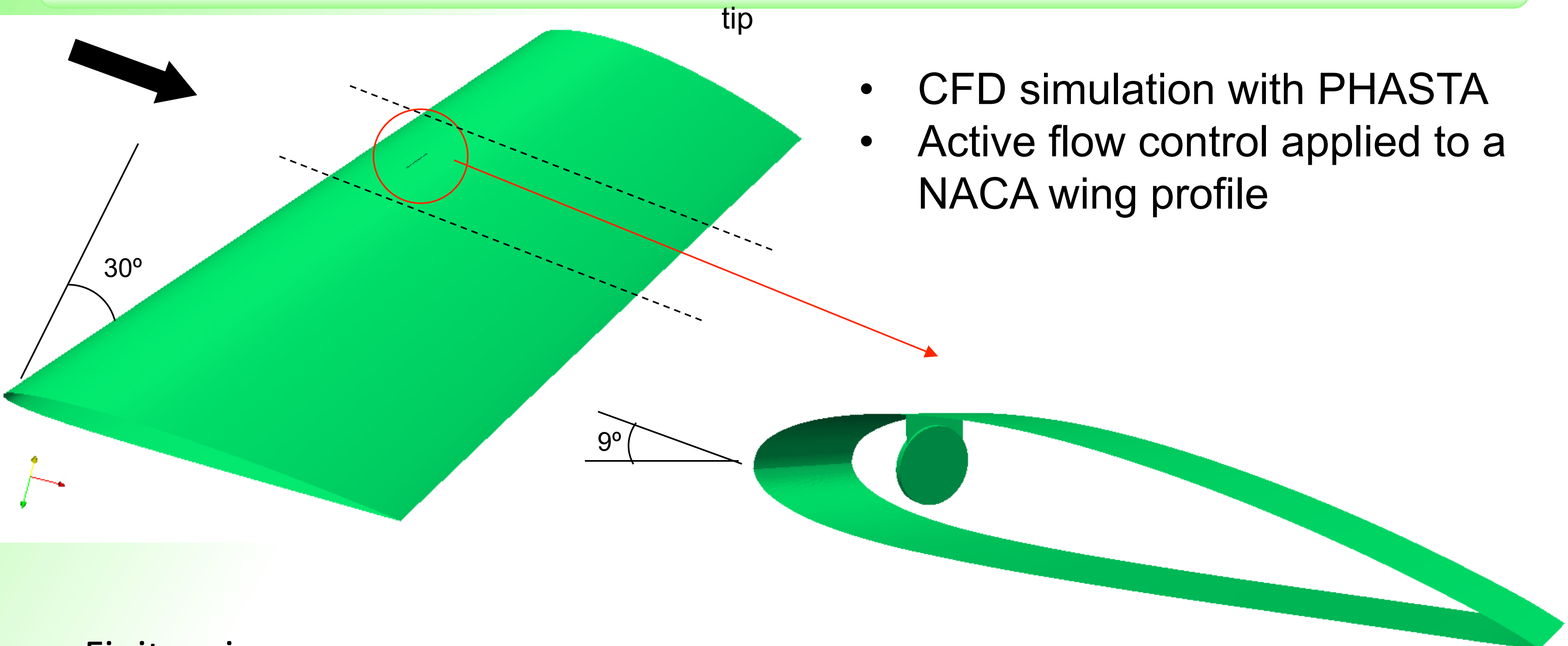


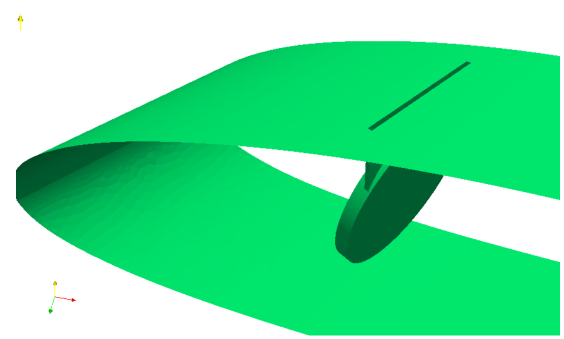
Resources - ALCF



Problem Description



- CFD simulation with PHASTA
- Active flow control applied to a NACA wing profile



- Finite wing
- Angle of attack $\alpha = 9^0$
- Swept angle 30^0
- Re = 100,000
- Synthetic jet with blowing coefficient C_b = 1.2 and f_{act} = 1,750Hz

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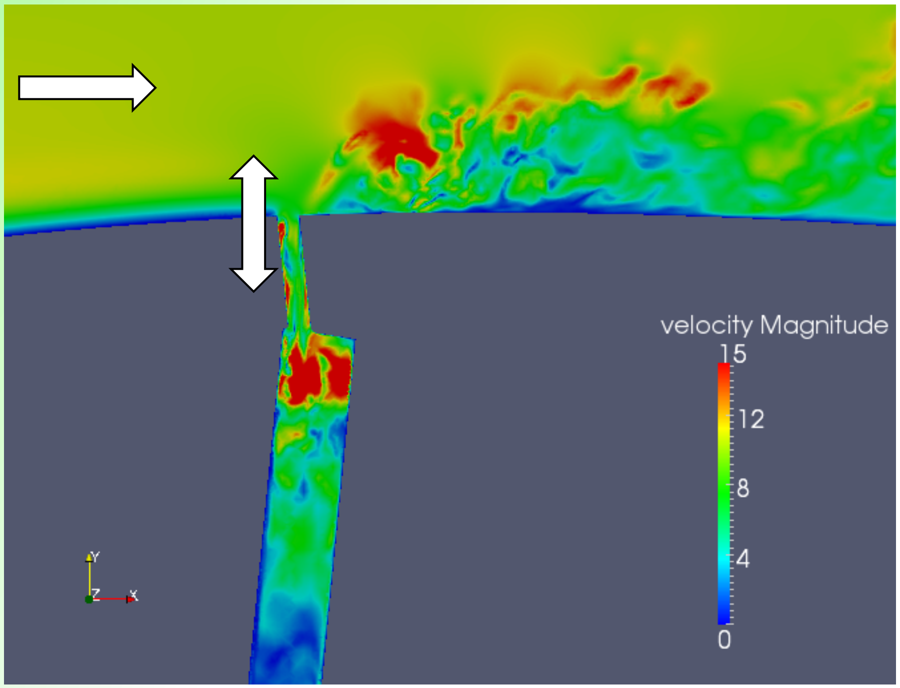
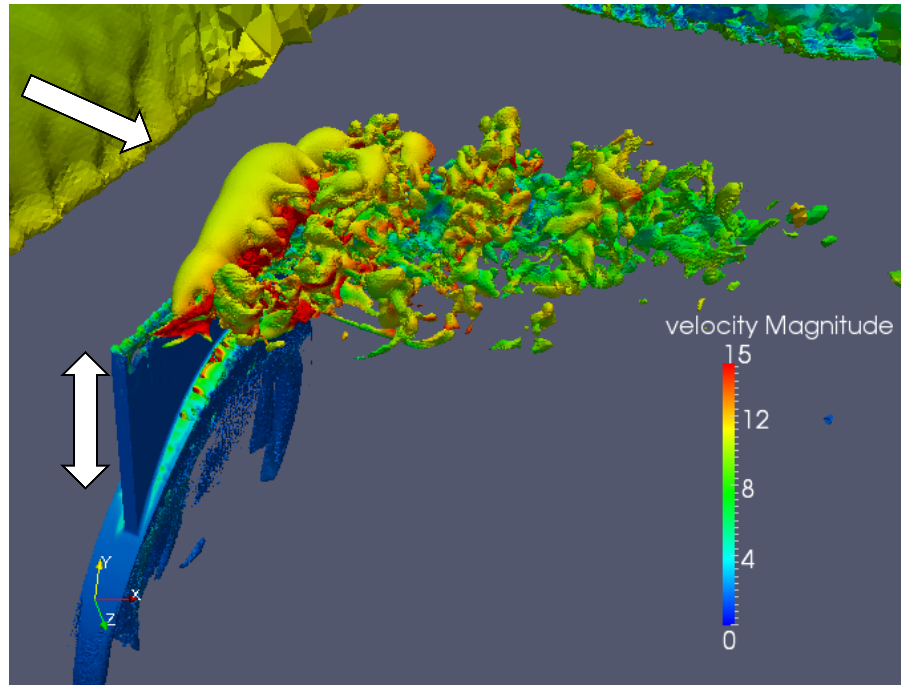
Problem Description

Flow control applied to a NACA wing profile (3.3 Billion elements)



Cut plane through a synthetic jet and velocity magnitude



Isosurface of vertical velocity colored by velocity magnitude near the slit of a synthetic jet

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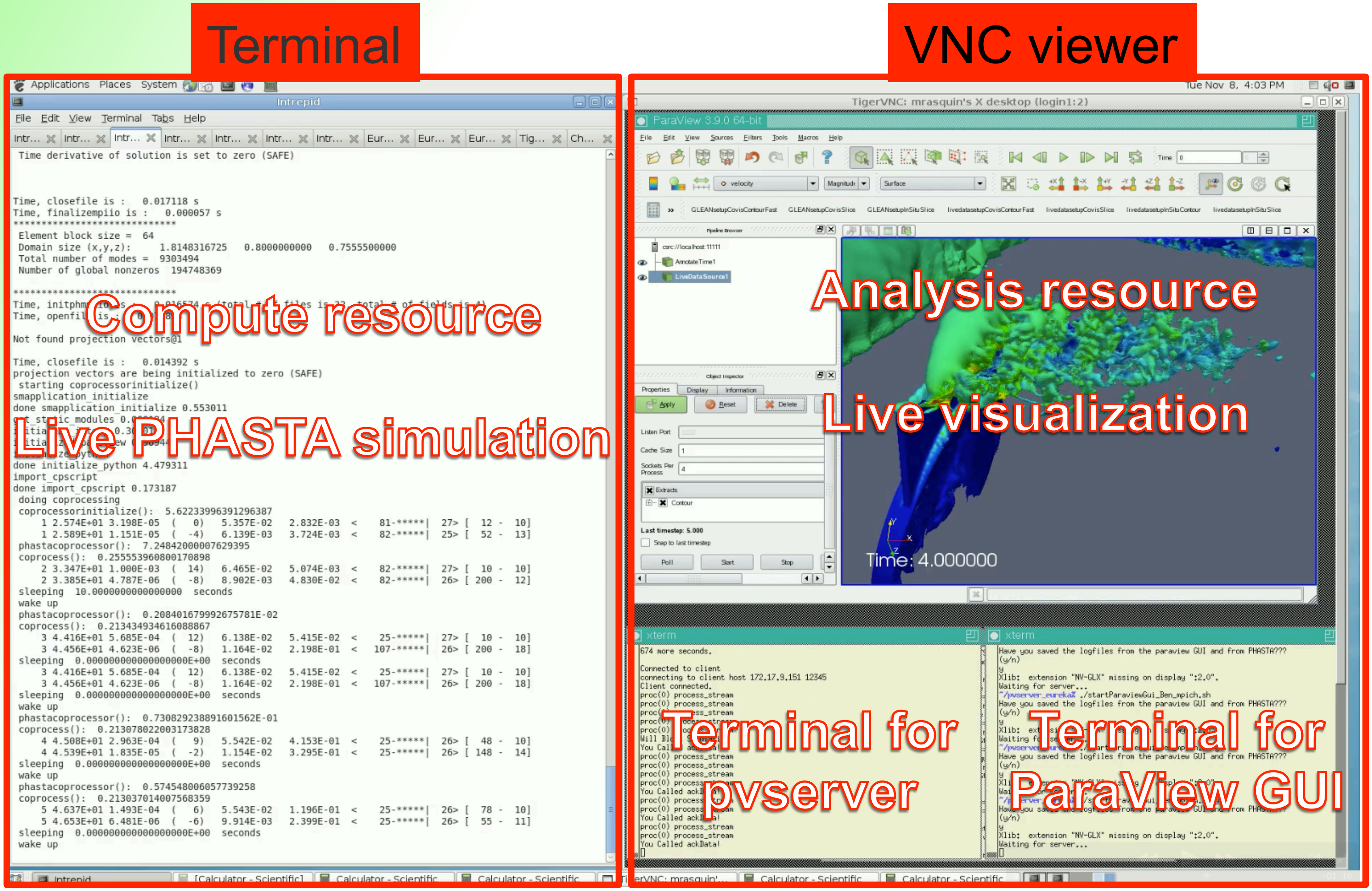
Covis Demonstration



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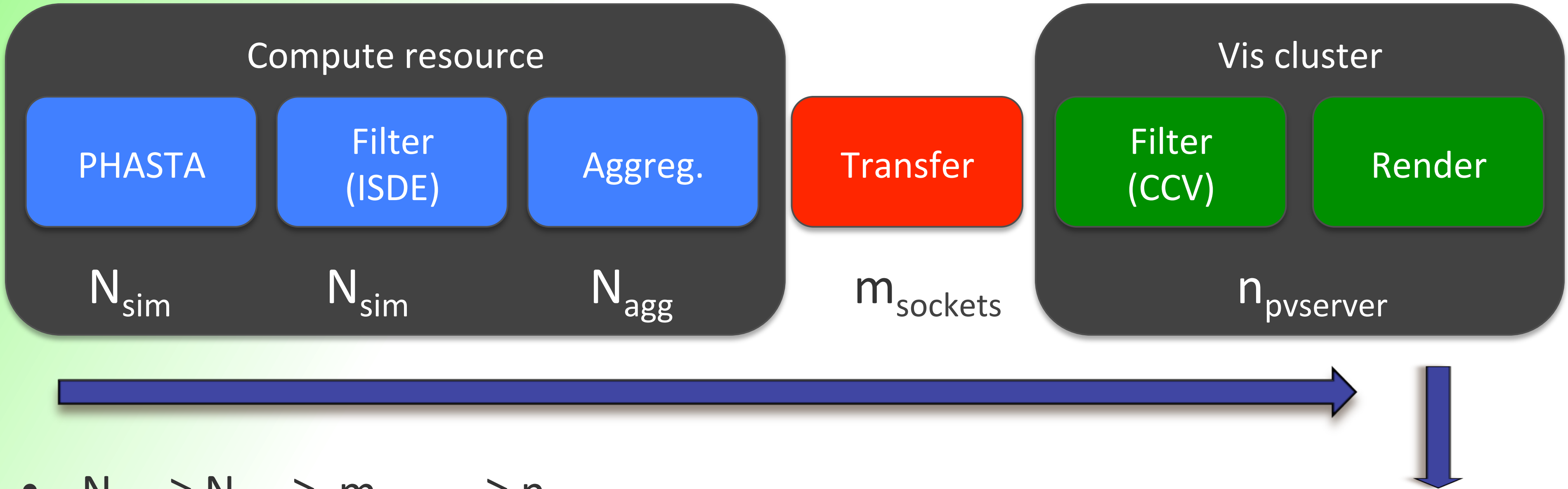
Data Reduction

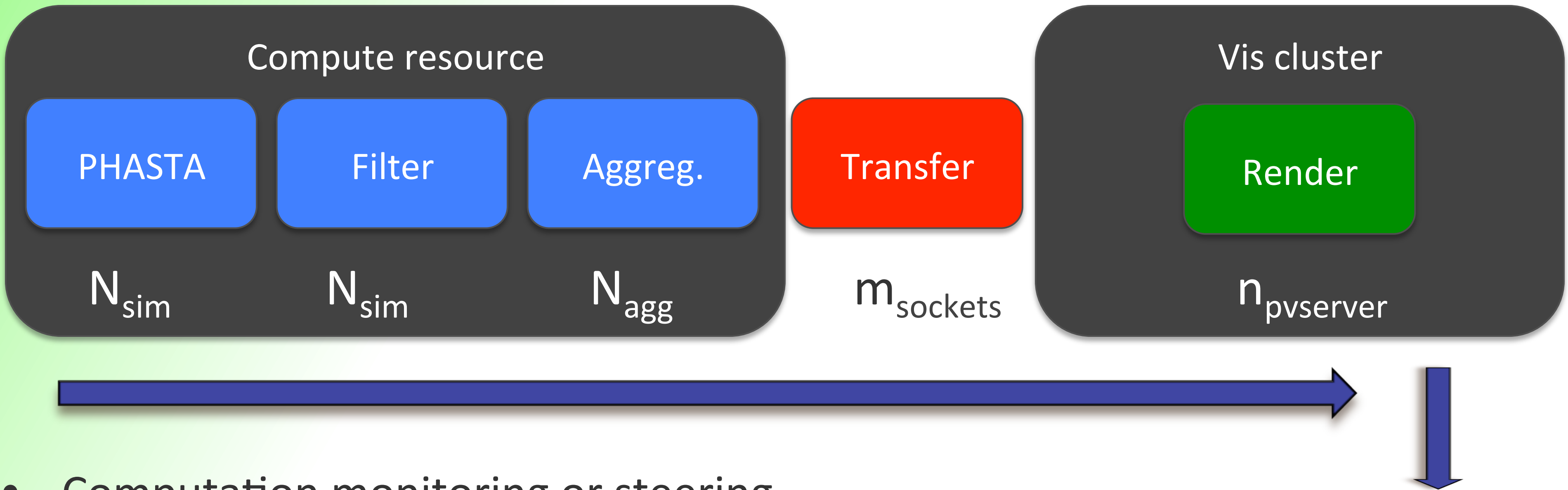


- $N_{sim} \geq N_{agg} \geq m_{sockets} \geq n_{pvserver}$
- N_{sim} = 160K; $N_{agg} = m_{sockets}$; npvserver $\in$ [5 - 800]
- if N_{agg} increases, - reduction in layers of aggregation

  - but more and more smaller packets
- Possible issue: - aggregation can overflow core memory

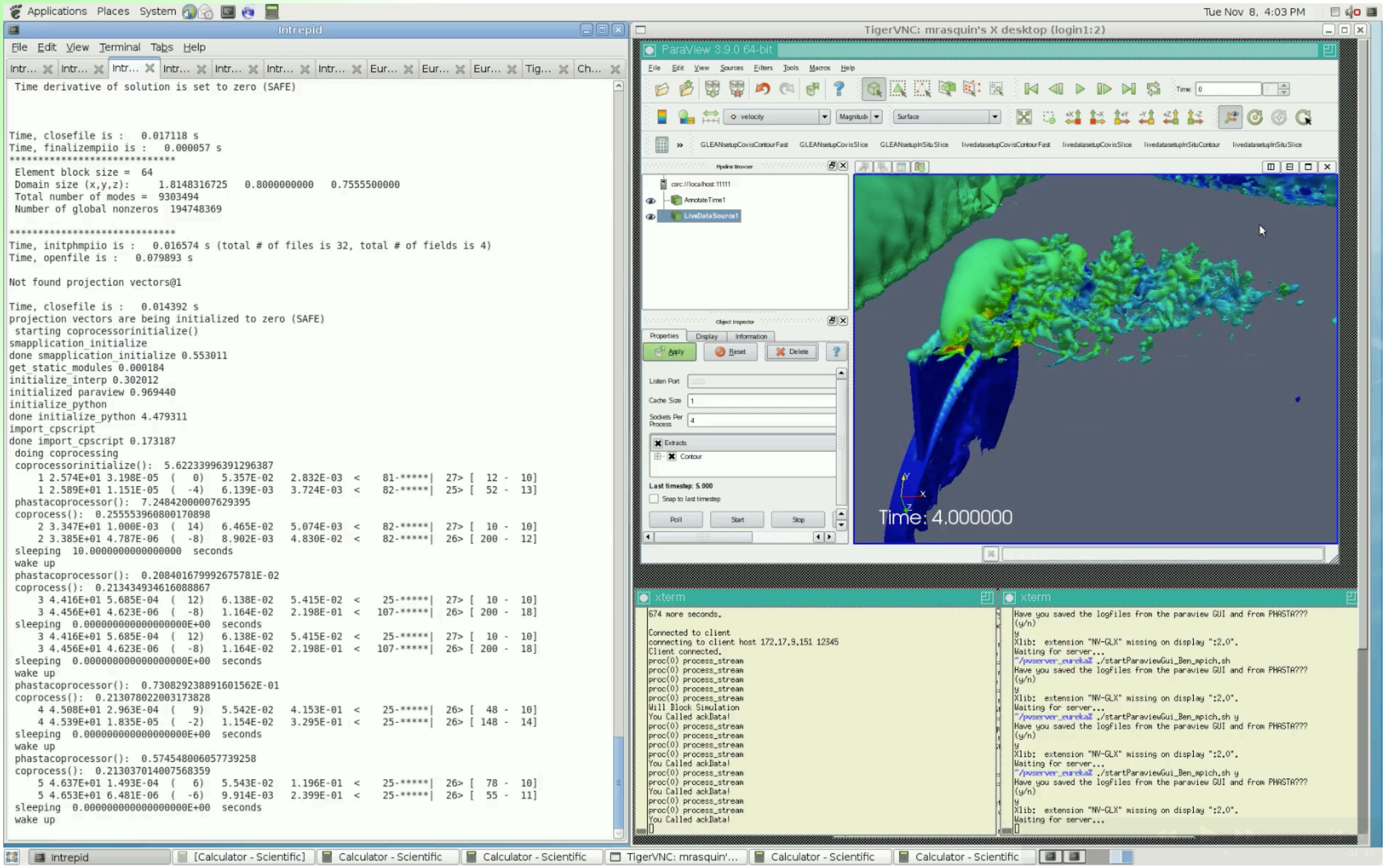
  - limitation in the number of sockets open

Scenario 1: In Situ Data Extract

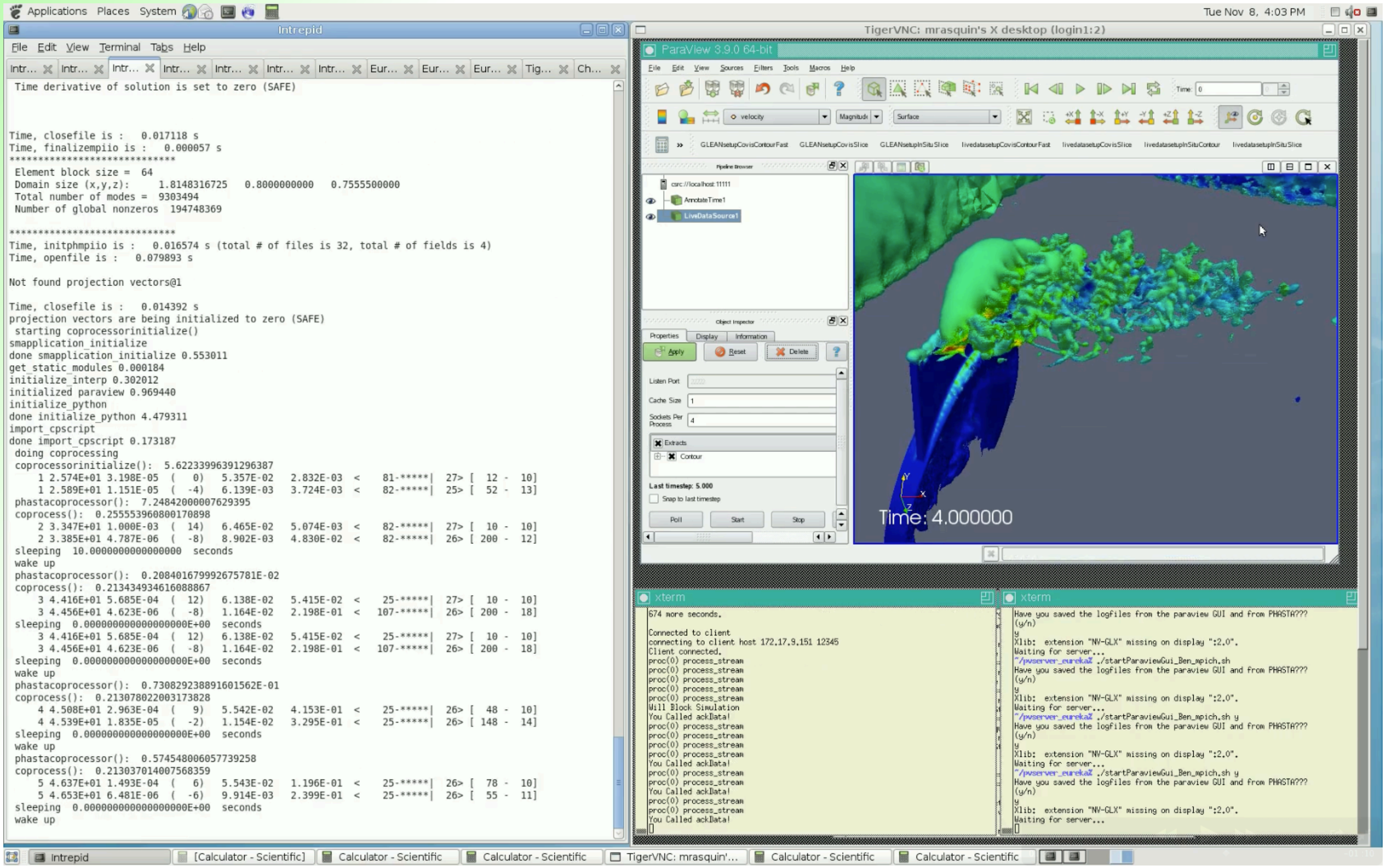


- Computation monitoring or steering
- Mainly interested in streaming a live filter pipeline's evolution in time (not replaying different filters on a given time window)
- Size of the data extract limited (data compression realized)
- In Situ Data Extract likely to provide the lowest tax on the solver

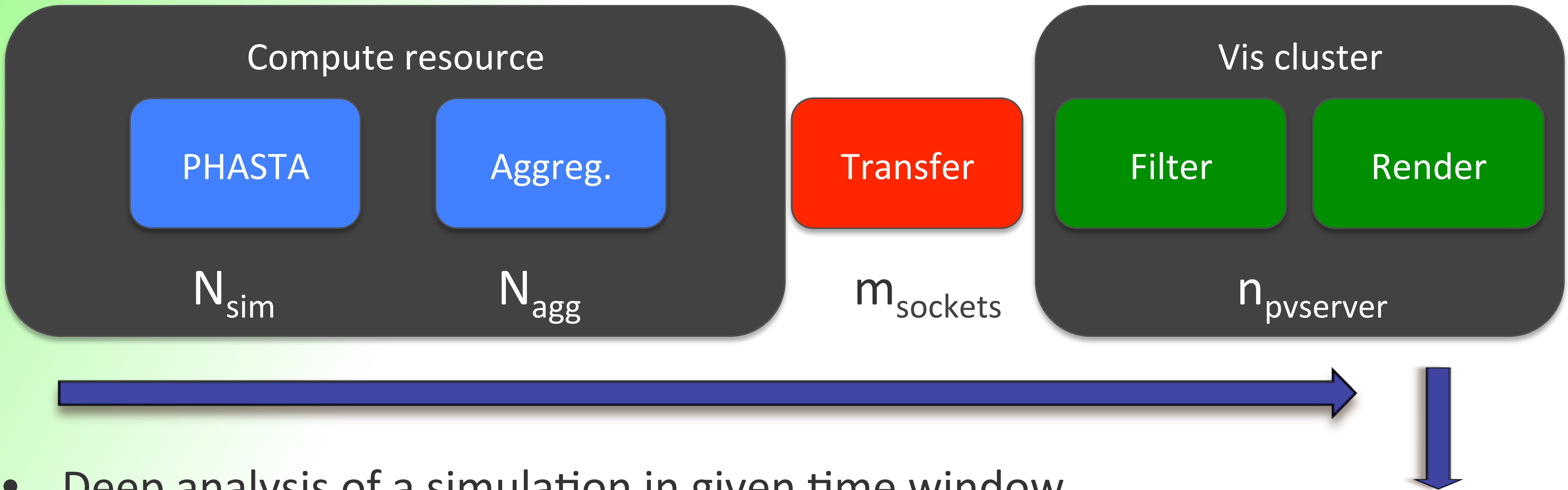
Demonstration – In Situ Data Extract



Demonstration – In Situ Data Extract

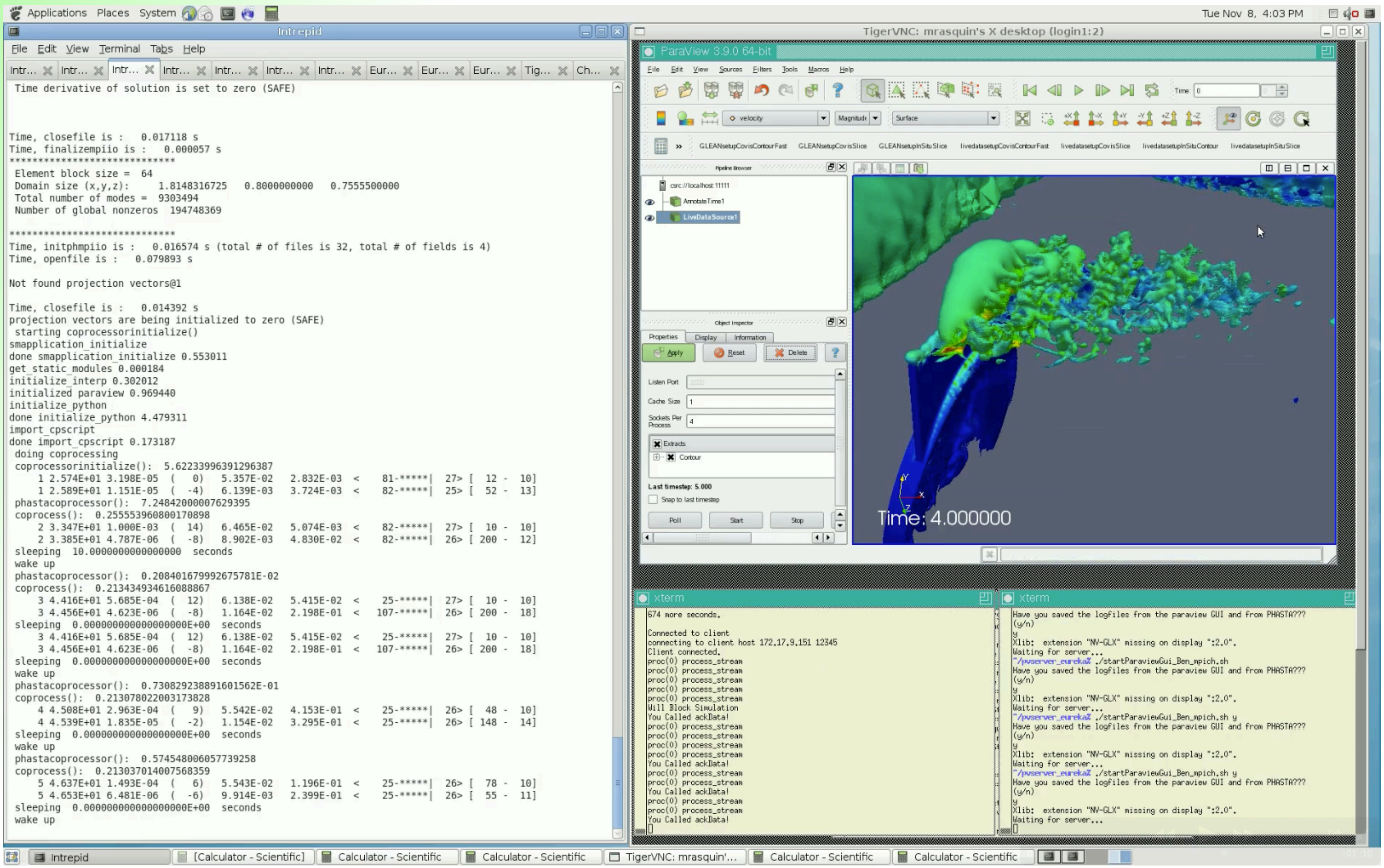


Scenario 2: Classical CoVis



- Deep analysis of a simulation in given time window
- Capacity to roll forward and backward in time, changing filters
- Uncertainty on the filters needed
- Size of the data extract significant compared to the size of the solution itself
- Poorly scalable filter (particle tracer)

Demonstration – Classical CoVis



Parameters study

- Visualization of every time step
- CCV (Classical Co-Viz) or ISDE (In Situ Data Extract)
- Data transport: GLEAN or VTK sockets
- Pvserver configuration: number of Eureka nodes and number of pvserver per node (1, 2, 4 and 8)
- VTK sockets: number of sockets per pvserver -> number of aggregators
- Filter pipeline: slice or contour
- Mesh size: 52 M, 416 M or 3.32 B elements (all tets)

# elements	Whole mesh + solution	Contour filter	Slice filter
52 M	1.98 GB	276.4 MB	18.5 MB
416 M	13.4 GB	1006 MB	64.8 MB
3.32 B	98.6 GB	3796 MB	240 MB

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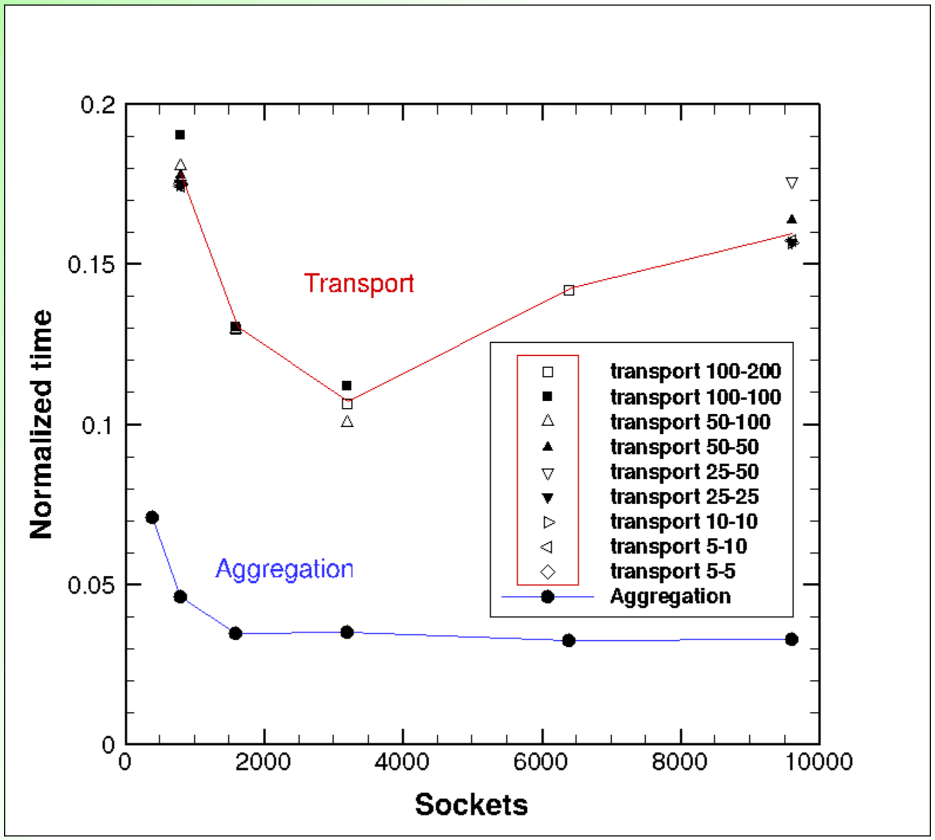
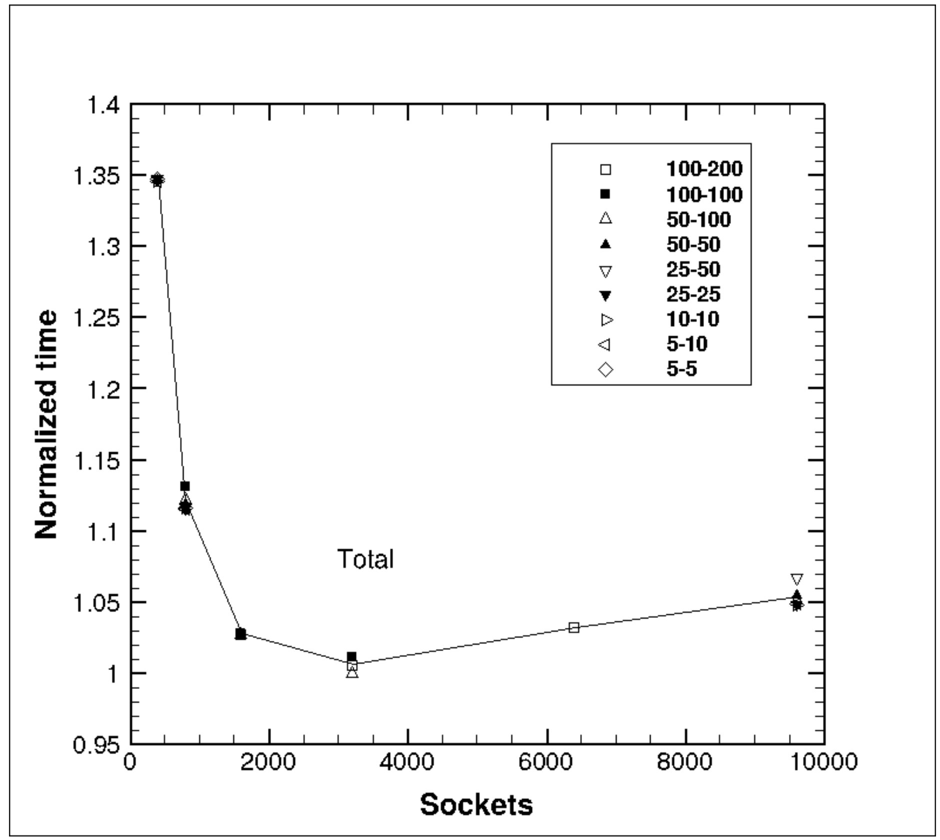
ISDES - Data aggregation and transfer

Contour filter, 416M elts, 1006 MB, VTK sockets
Different combinations of Eureka nodes - pvservers
$N_{agg} = m_{sockets}$





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In-Situ Data Extract

Percentages = PHASTA delay over original PHASTA time (“vis tax”)

# elements	Flow solve w/o filter	Filter	Total Blocking Time (Filtering + aggregation + transfer time)		
			Current		After ongoing improvement
3.32 B	14.3 s	Slice	0.200 s	1.4 %	0.63 %
		Contour	0.586 s	4.1 %	3.0 %
416 M	1.84 s	Slice	0.175 s	9.5 %	3.4 %
		Contour	0.269 s	14.6 %	6.6 %
52 M	0.474 s	Slice	0.158 s	33.3 %	9.9 %
		Contour	0.215 s	45.4 %	22.0 %

- Ongoing improvement: Initialization and cleaning of the pipeline performed only at the 1st and last time step (or when pipeline is updated)
- Above performance unchanged down to 1/10 of Eureka resource

Classical CoVis

Percentages = PHASTA delay over original PHASTA time ("vis tax")

# elements	Flow solve w/o filter	Transfer method	Total Blocking Time (Aggregation + transfer time)	
			Current	
3.32 B	14.3 s	VTK Sockets	13.9 s	97.2 %
		GLEAN	2.02 s	14.1 %
416 M	1.84 s	VTK Sockets	0.207 s	11.2 %
		GLEAN	0.360 s	19.5 %
52 M	0.474 s	VTK Sockets	0.100 s	21.1 %
		GLEAN	N/A yet	N/A yet

- Ongoing improvement: Transfer the connectivity and coordinates only when the mesh changes and reduce the volume of data transfer 10 times
- ParaView server able to filter and render the full data set every time step before the next one is computed; More cpu helps for the filters

Conclusions

- Live data analysis of a CFD simulation with 160K cores BG/P and up to 800 pvservers on 100 vis nodes @ ALCF
- ParaView Copressing Library: provides continuous and reconfigurable insight into massively parallel simulations at a low tax (~ 5-10 %)
- GLEAN: allows a ~50 GB/s data transfer between supercomputer and vis cluster @ ALCF
- In Situ Data Extract or Classical Co-Vis? It depends upon:
  - Computation monitoring and steering? Deeper analysis?
  - Visualization frequency
  - Size of the full data or data extract (choice of filters)
  - Future development for both ISDE and CCV
  - Future ratio between available compute and vis resources

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Thank You