Addressing the Challenge of Exascale

European Exascale Software Initiative EESI

Towards Exascale roadmap implementation

EESI2 – Recommendations

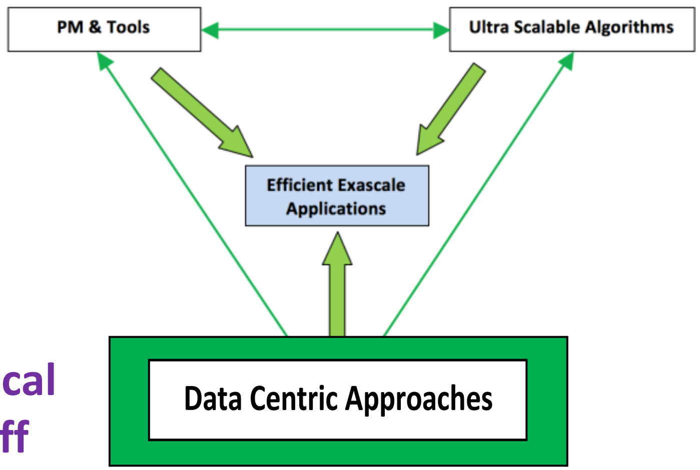
In situ Data Processing

Toward real time Extreme Data Processing
and better science through I/O avoidance
in High-Performance Computing systems

Philippe Ricoux (TOTAL, EESI2 Coordinator)

EESI2 recommendations

This recommendation is fully in the core of Exascale development, in the Data Centric Pillar, for the best compromise between Extreme Computing and Extreme Data .



Motivation

This approach is really disruptive by Changing the classical sequential paradigm which is: First Simulation ,Then "Off Line" post processing, Visualization and then feedback to new Simulations. This paradigm imposes to move data in memories and in storage.

New large simulations (Turbulence, Combustion, Oil & Gas Reservoir, Neutronics, Electromagnetism , Astrophysics, …) generate huge amount of simulated data

Combustion Turbulent : 1PB each 30 min
Giga Model Reservoir: 350 TB/Run

Impossible to move and store

⇒ Analysis, Reduction and Visualization on the Fly , In situ Data Processing

New Paradigm: In Parallel Compute and Analyse

Typical Reservoir simulations

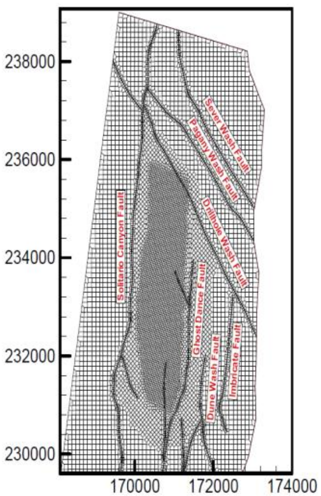


Figure 3 Plan view of the 3D simulation domain, gird and incorporated major faults

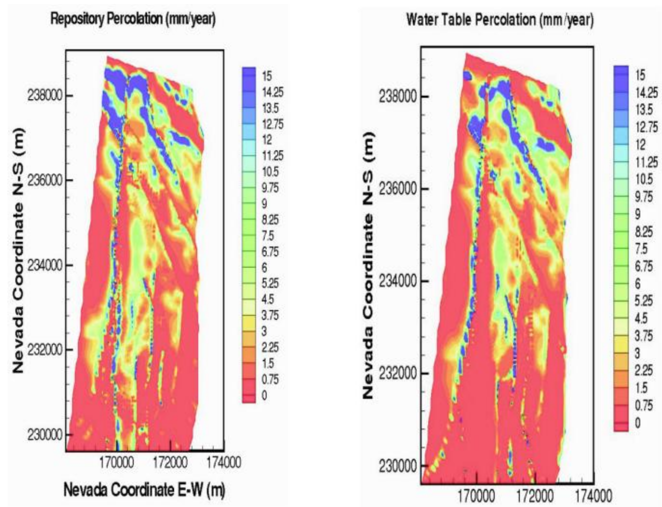


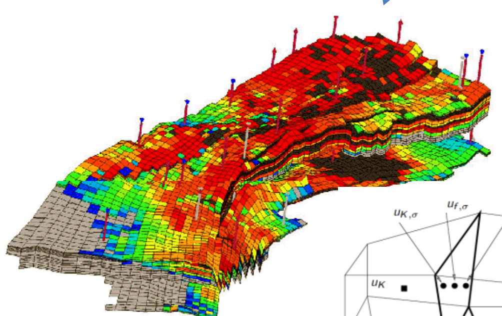
Figure 4 Simulated percolation fluxes at repository horizon

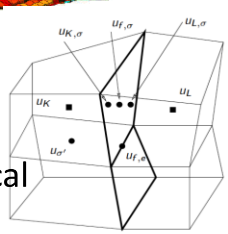
Case description

Matrix	N	NNZ	NNZ/ROW
SPE10-1	2,188,851	29,915,573	13.7
SPE10-2	2,188,851	29,915,573	13.7

57.7 GB IPARS (simulator) dataset distributed

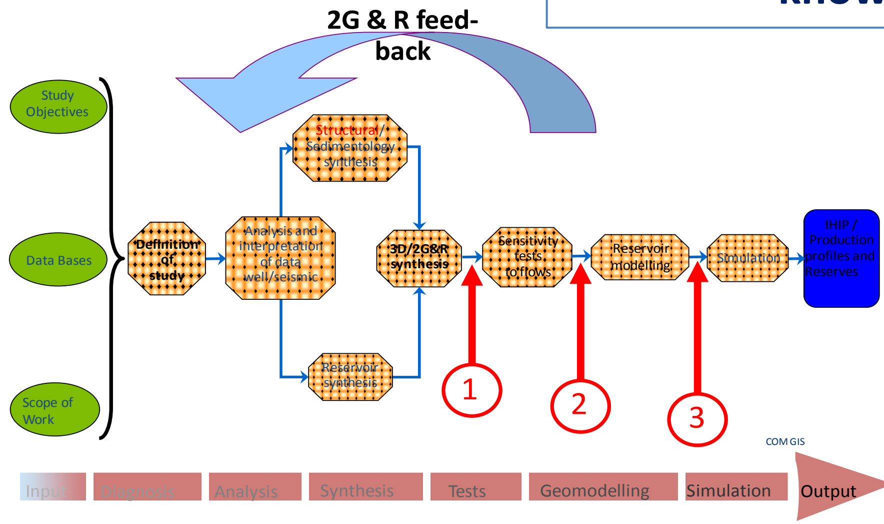
HPC allows to improve physical models increasing accuracy and knowledge





New Numerical Schema

Reservoir simulation workflow



N > 15 Millions
NNZ ≈10 Billions

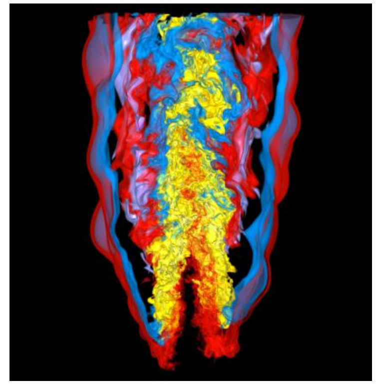
Generation of 350 TB / Run

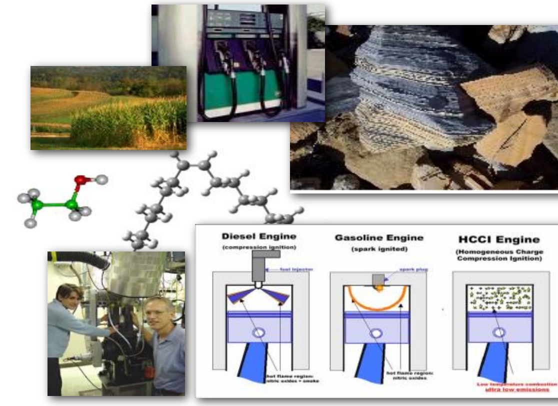
Exascale Combustion Turbulent

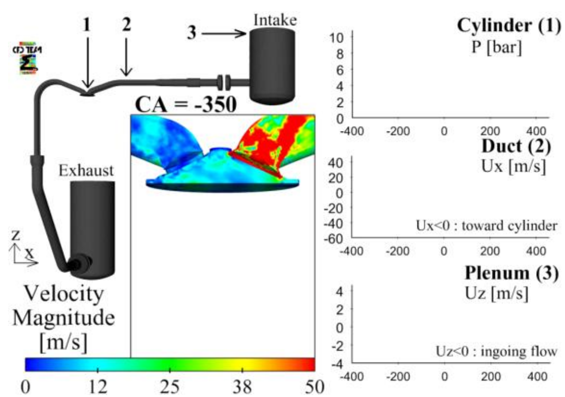
DNS of Autoigniting Jet Flames

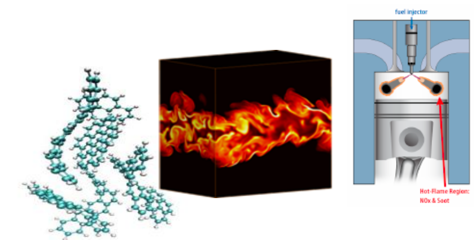
- **3D turbulence coupled with Chemistry (>100 species)**
- **Fundamental insights into stabilizing a lifted flame in hot ignitive environment**

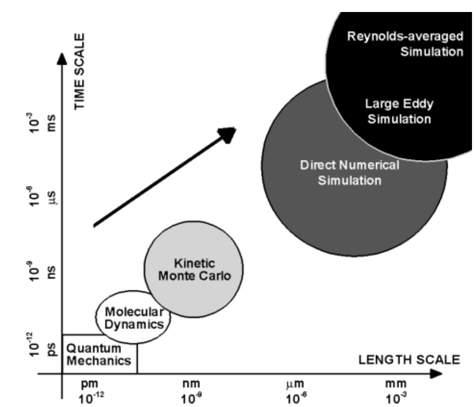
- Predict behavior of new fuels in different combustion scenarios **at realistic pressure and turbulence conditions**
  - Develop new combustor concepts
  - Design new fuels
- Co-design center is focusing **on high-fidelity direct numerical simulation methodologies**
  - Need to perform simulations with sufficient chemical fidelity to **differentiate effects of fuels** where there is strong coupling with **turbulence**
  - Need to **address uncertainties in thermo-chemical properties**







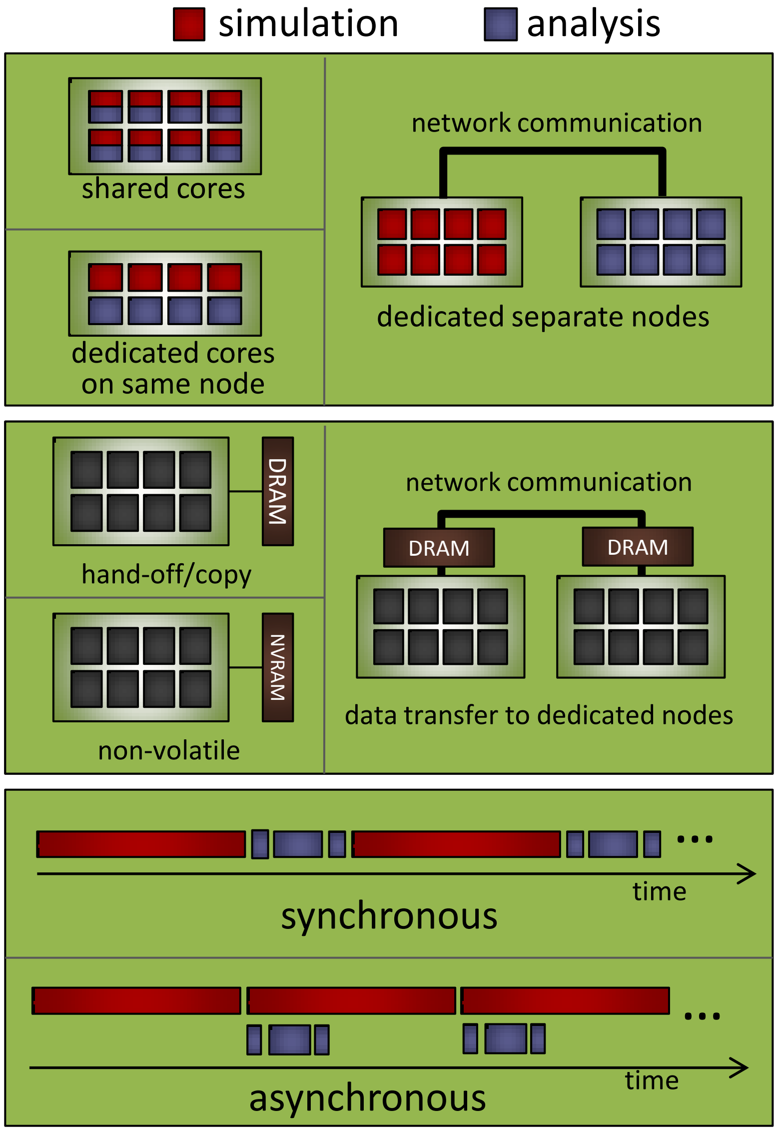




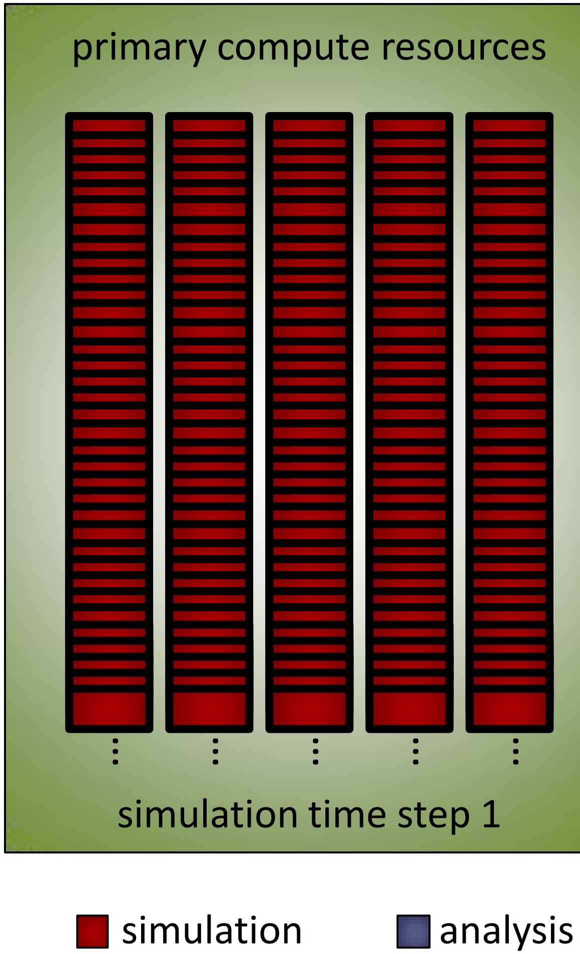
Full DNS with coupling all physics and chemistry generates PB of data

Exploring the design space of new workflows

- Location of analysis compute resources
  - **Same cores as the simulation (in-situ)**
  - Dedicated cores on the same node (in-situ)
  - **Dedicated nodes on the same machine (in-transit)**
  - Dedicated nodes on external resource (in-transit)
- Data access, placement, and persistence
  - **Shared memory access via hand-off / copy**
  - Shared memory access via non-volatile near node storage (NVRAM)
  - **Data transfer to dedicated nodes or external resources**
- Synchronization and scheduling
  - **Execute synchronously with simulation every n^{th} simulation time step**
  - **Execute asynchronously**



Exploring the design space of workflows:
In-situ workflow performed synchronously with simulation



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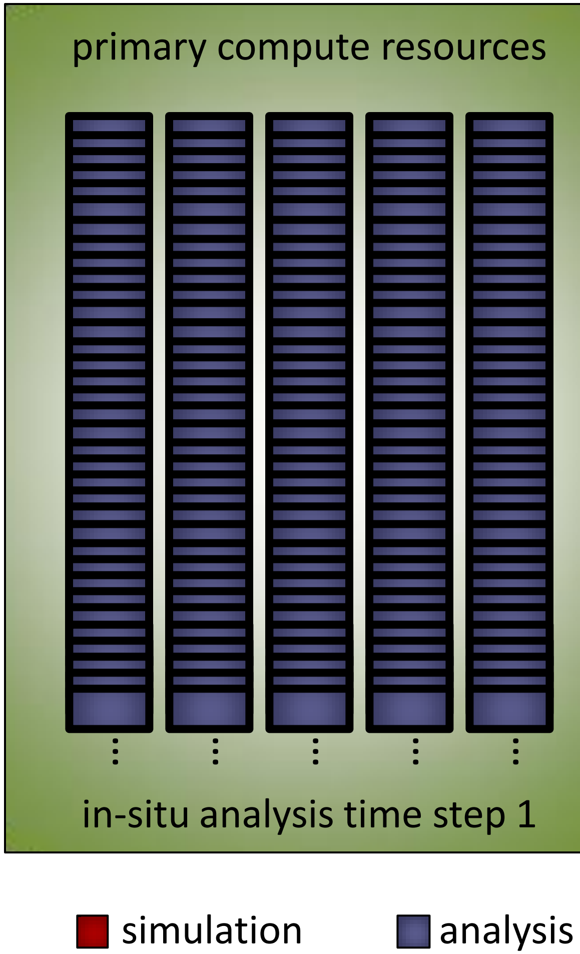

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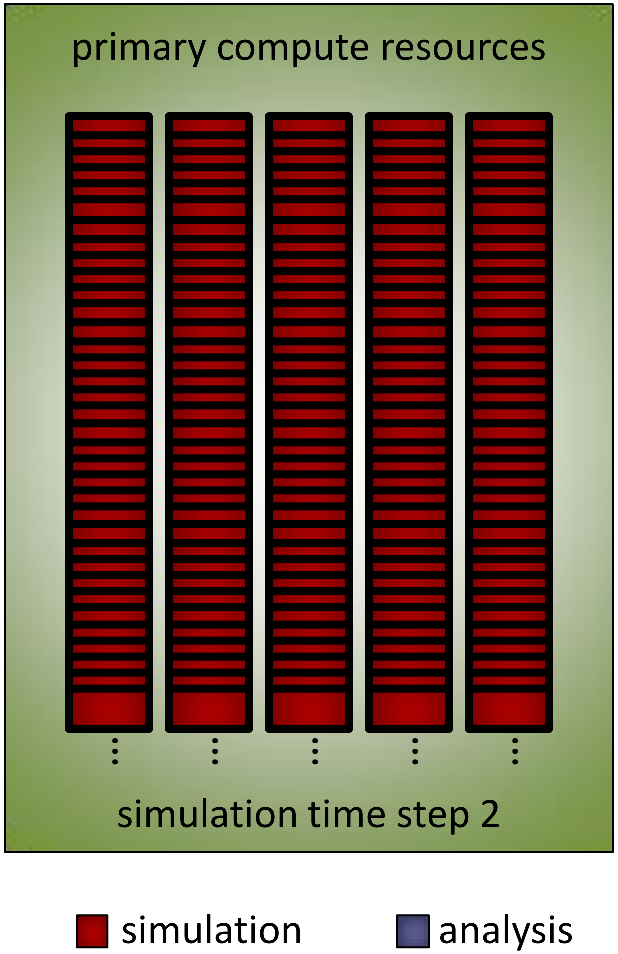

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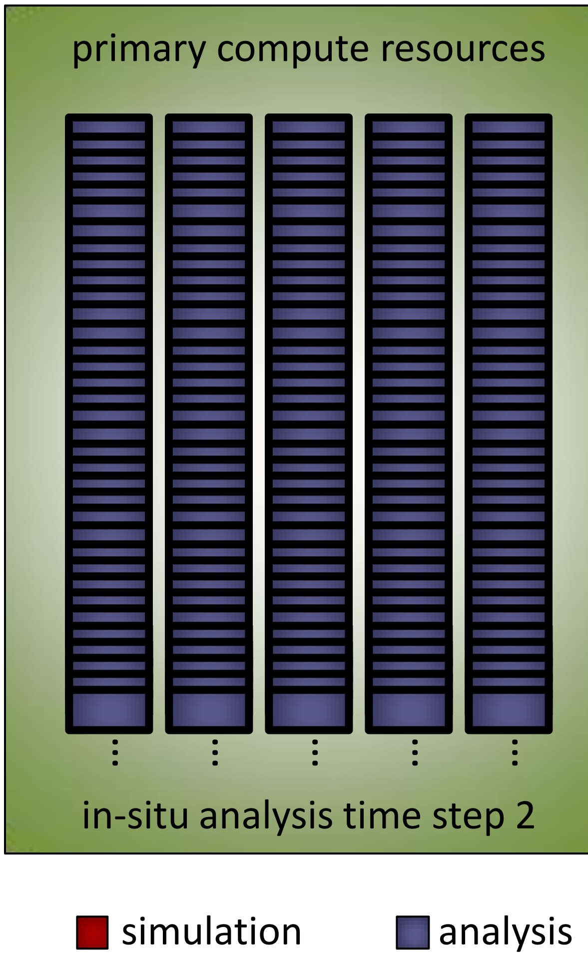

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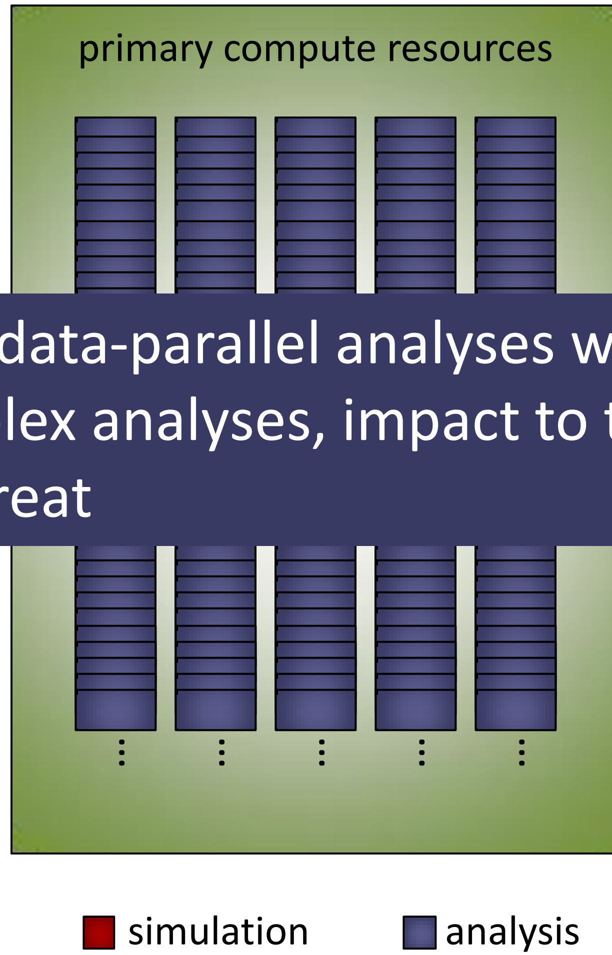
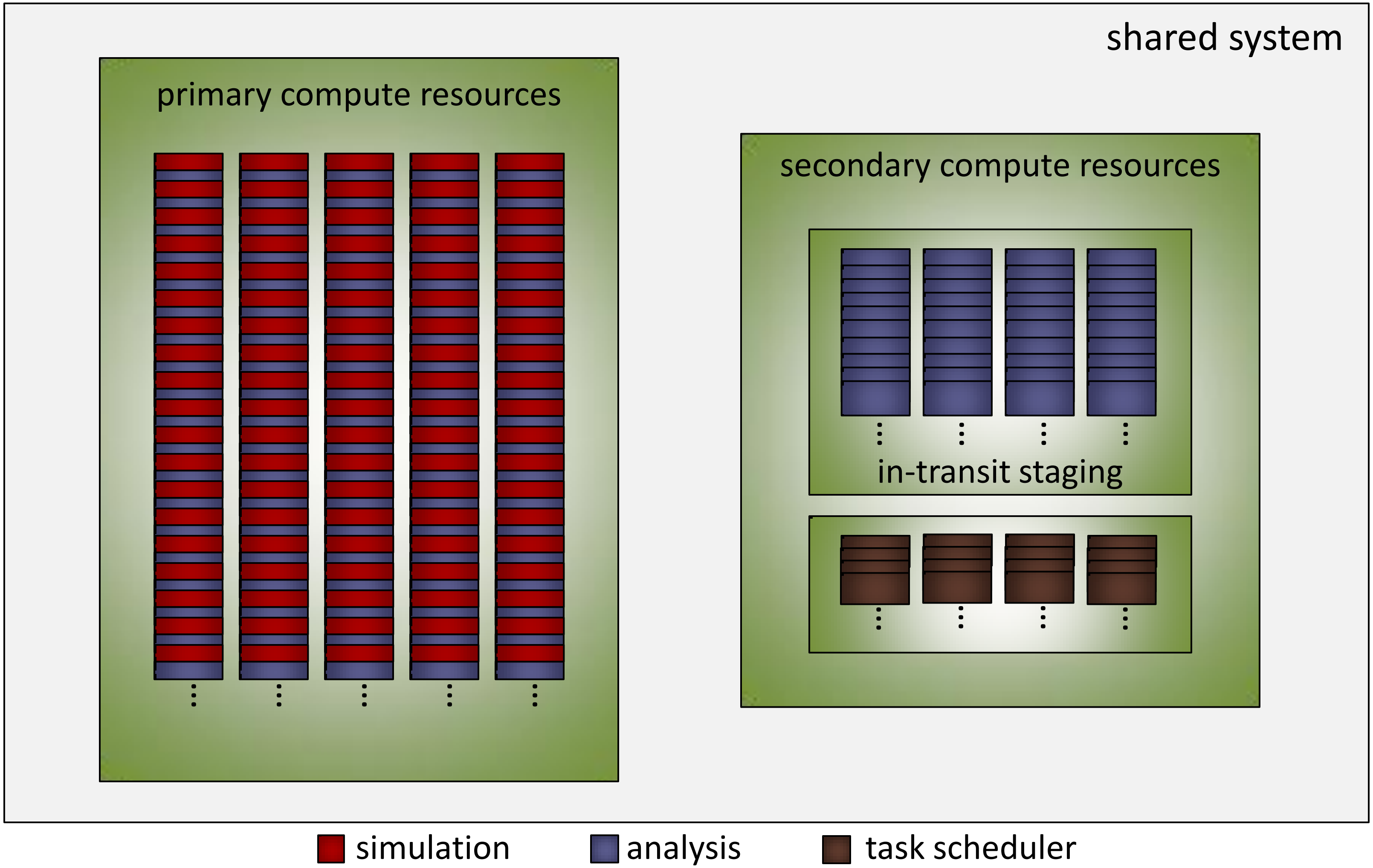


- Works well for data-parallel analyses with short run times
- For more complex analyses, impact to the simulation becomes too great

Exploring the design space of workflows: Temporally multiplexed hybrid in-situ + in-transit workflow



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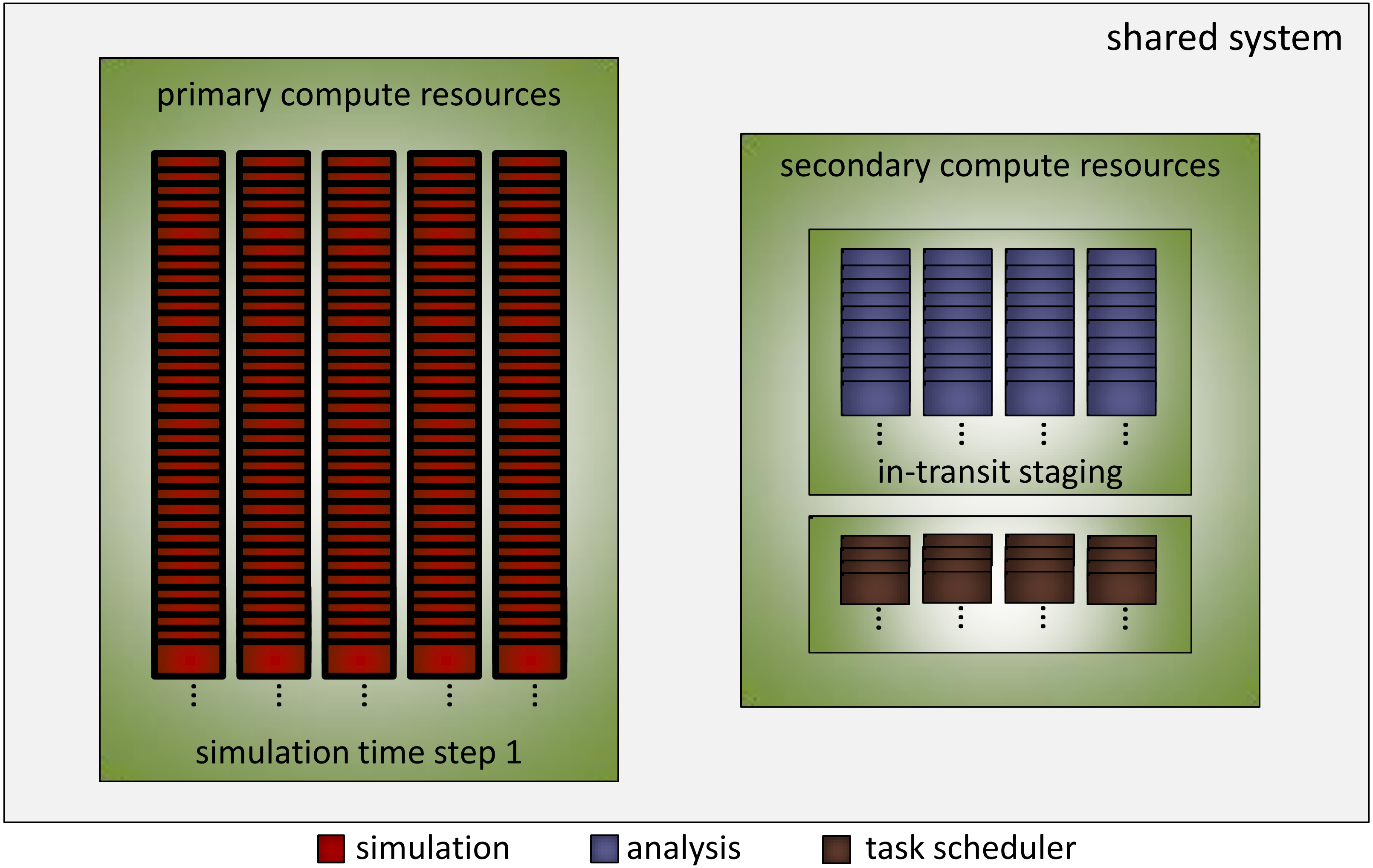

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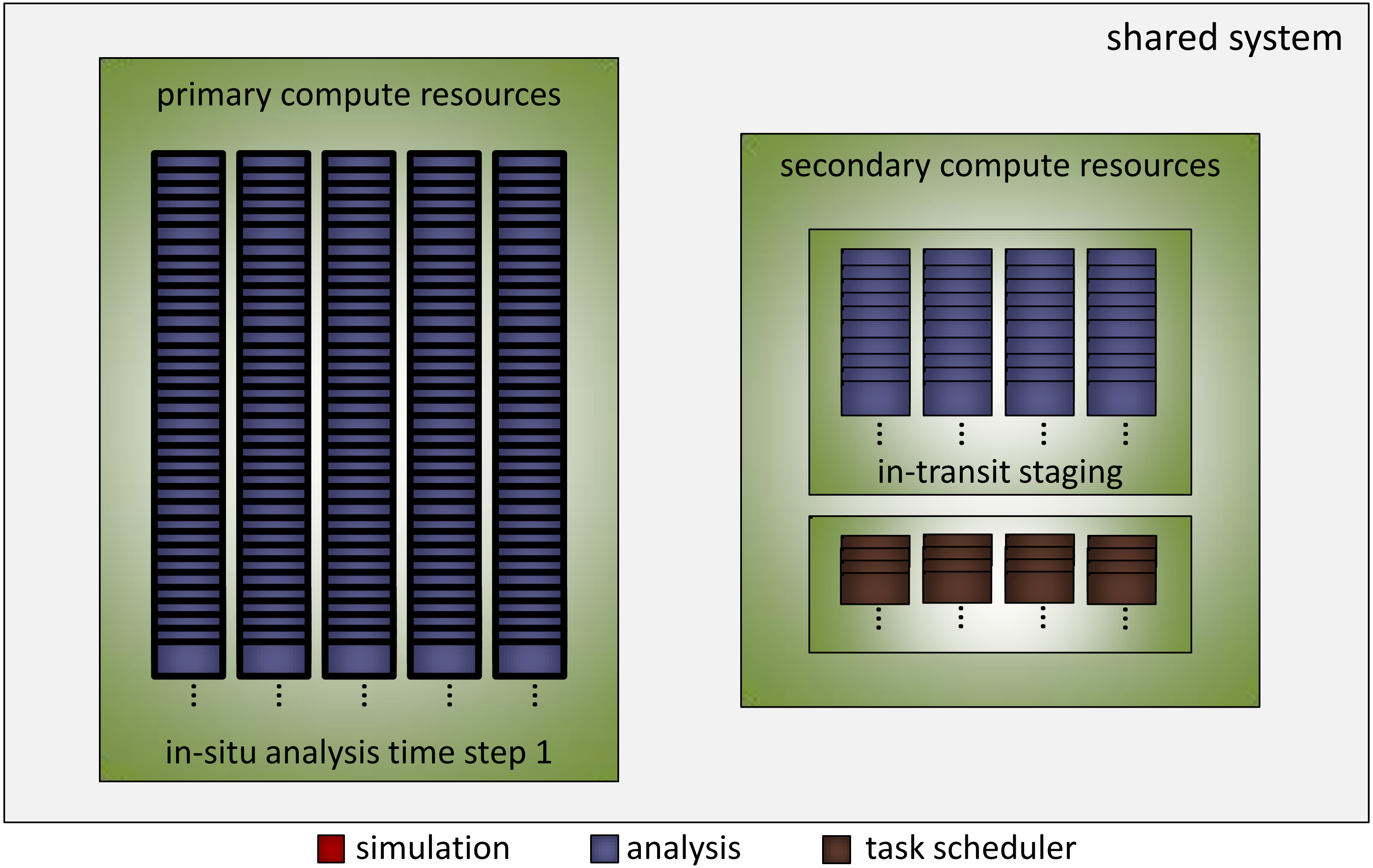

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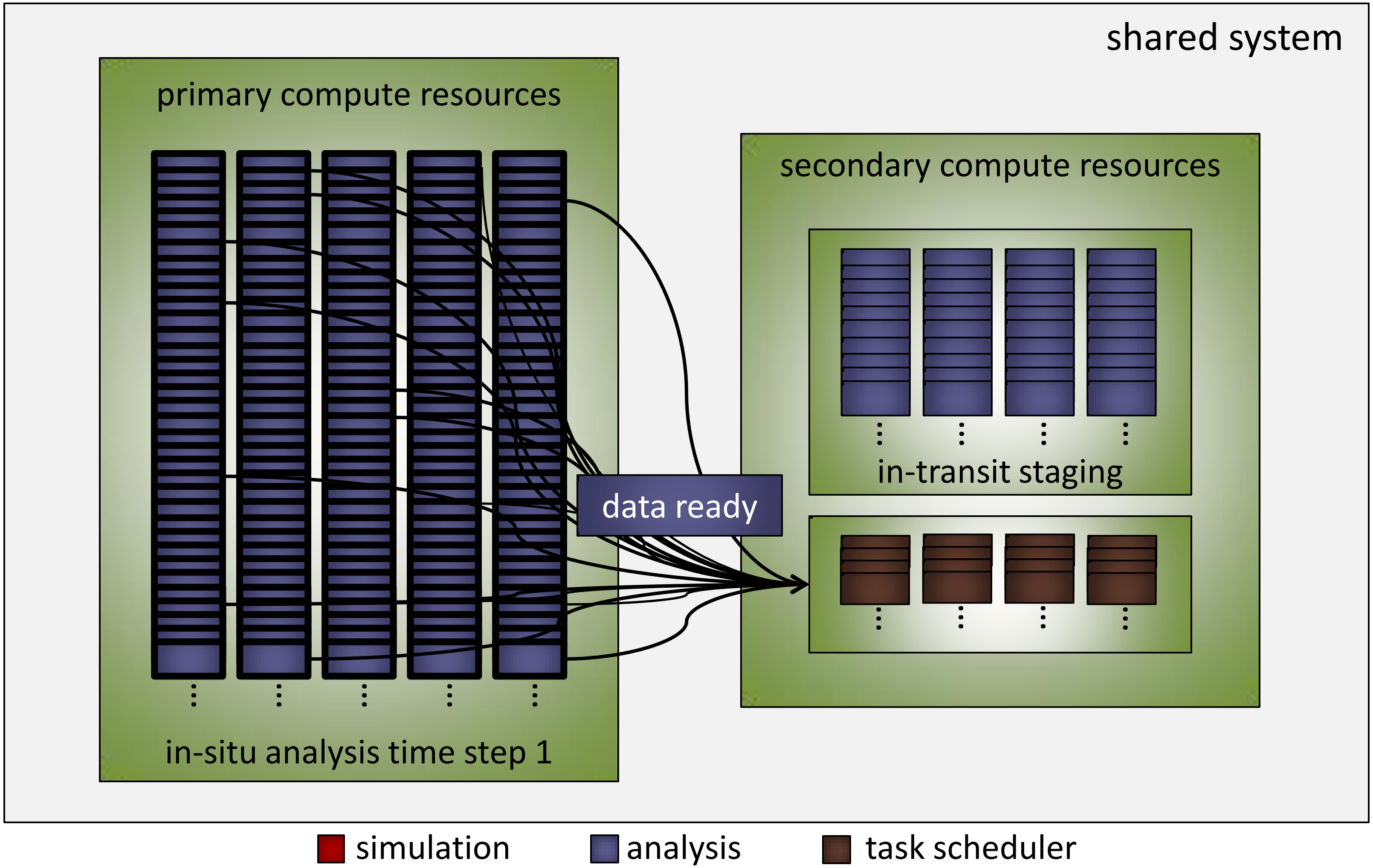

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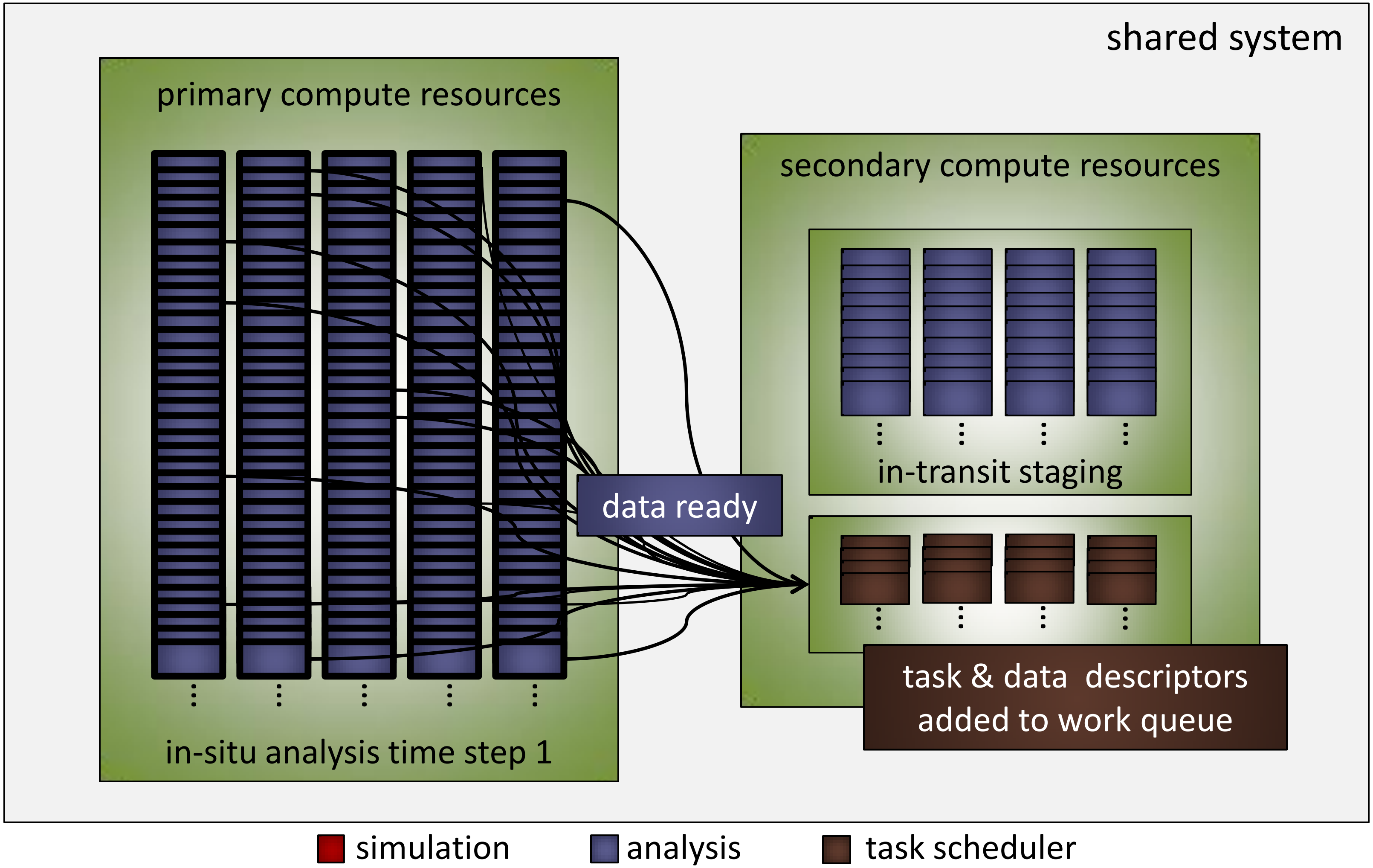

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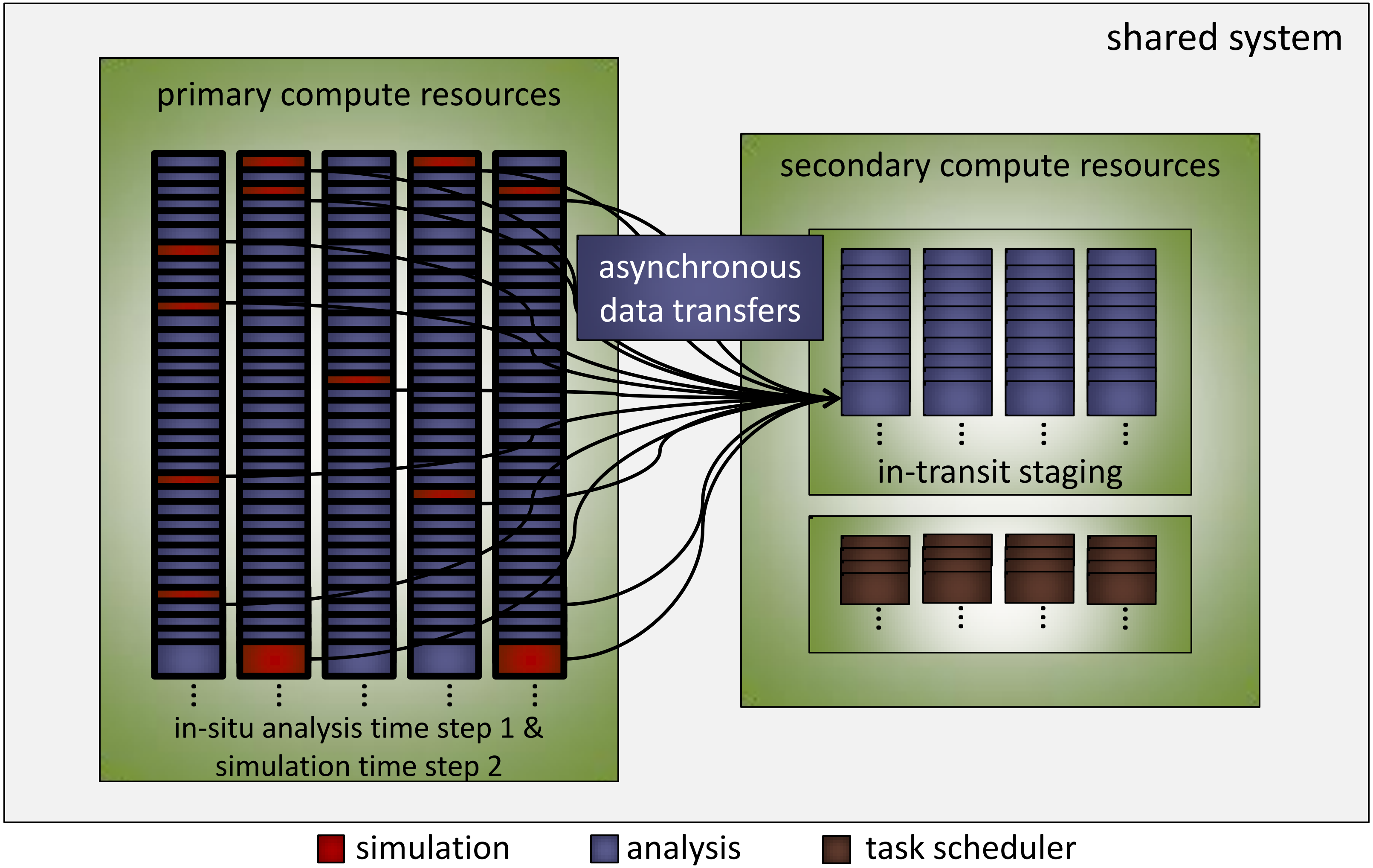

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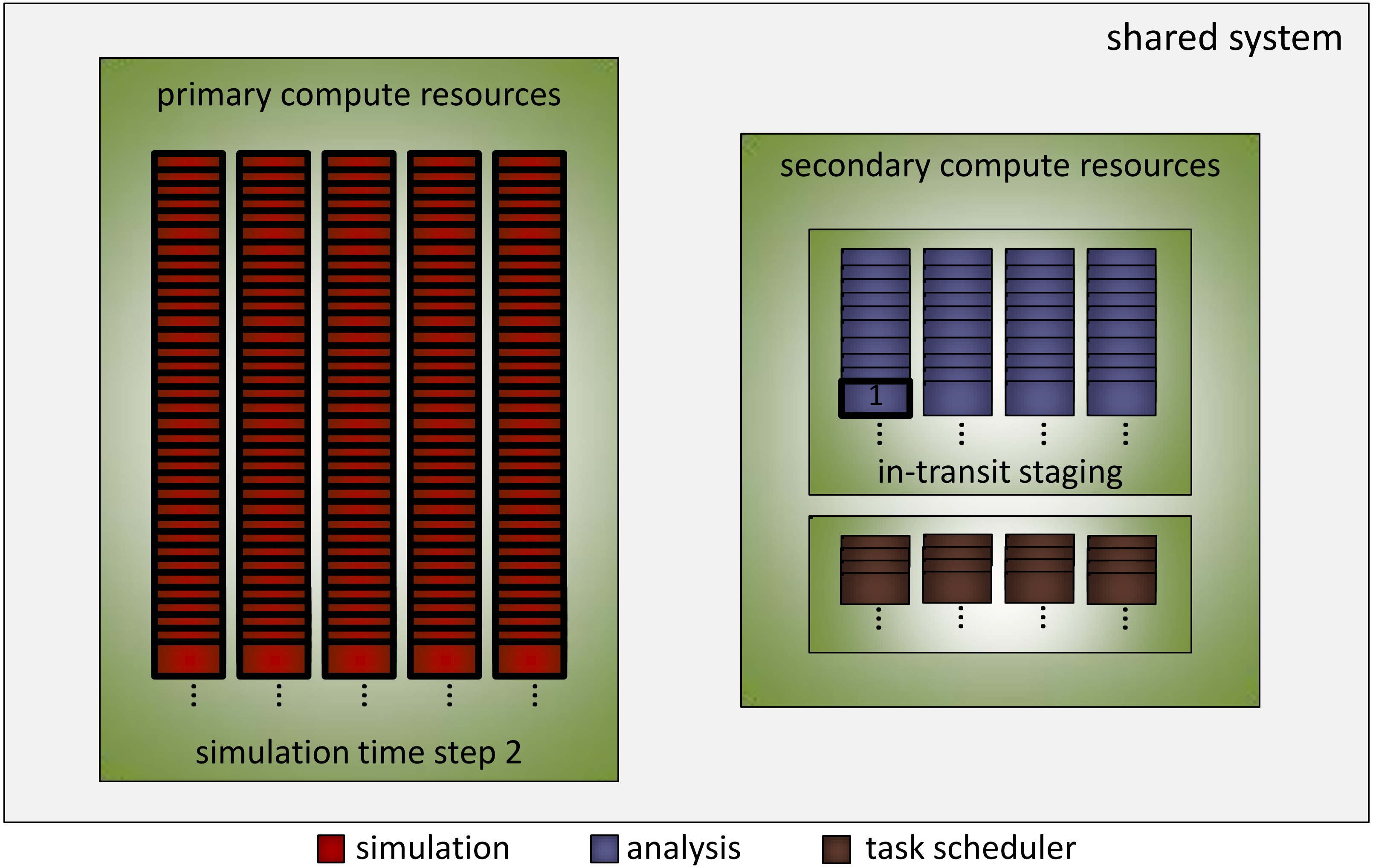


Hybrid workflow design impacts the manner in which analysis is performed

Hybrid analysis requires decomposition of algorithms into 2 stages

In-situ	In-transit
Data-parallel	More forgiving of complex communication needs
Short run time with respect to simulation	Can have longer run times while minimizing impact to simulation
Limited amount of memory; minimize cache impacts	Limited to memory and processing constraints of secondary resources
Should minimize the amount of data sent in-transit	Can only require data sent by in-situ stage

In situ techniques and methods

Data Reduction

The transform by itself should be reversible

Subsample, **Single precision or double precision,**

Quantization ***Direct scalar quantization***,, ***Adaptive scalar quantization***,, ***Vector quantization (VQ)*** or block quantization groups (LBG, k means, Codebook training) (*VQ is computationally expensive as an in-situ processing method*)

Transform-based compression (FT, wavelet, …)

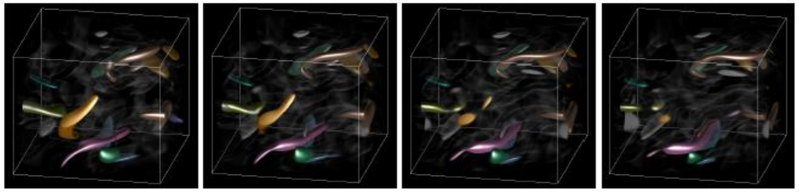


Figure 3. Feature tracking on a turbulent vortex data set [14]. Four selected time steps are shown. Each tracked feature is rendered with a distinct color.

Feature Extraction

Large-scale scientific simulations generate massive amounts of data that must be validated and analyzed for understanding and possibly new discovery.

Basic visualization algorithms exist for feature identification, extraction, and tracking, which incorporate principles from **image processing, computer vision, and machine learning (especially new deep learning).**

Quality Assessment

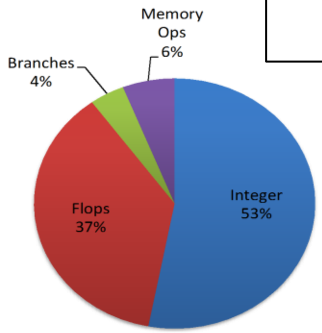
If data has to be reduced, the corresponding information loss must be conveyed to the user of the reduced data set. Quality assessment thus plays a crucial role in large-scale data analysis and visualization since in many cases the reduced versions of data rather than the original version are used for evaluating the simulation and modeled phenomena.

Issues In Situ Visualization

Compared with a traditional visualization task that is performed in a postprocessing fashion, in-situ visualization brings some unique challenges.

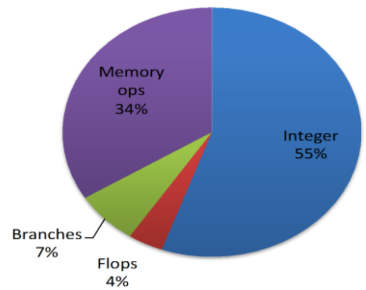
Efficient In situ Data Processing: Coupling 3 Algorithms with different characteristics

In Situ Uncertainty Quantification Guided by Analytics



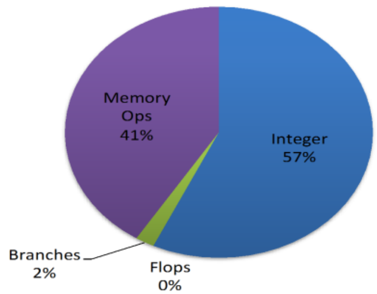
- Complexity: not data dependent
- Communication: small, fixed

Statistics



- Complexity: data dependent
- Communication: data dependent

Volume Rendering



- Complexity: very data dependent
- Communication: very data dependent

Topology

Statistics

- Debugging and Analysis, Filtering and averaging (spatial and temporal)
- Statistical moments (conditional)
  - In-situ local moments & aggregation
  - In-situ local moments + in-transit aggregation
- Statistical dimensionality reduction
- Spectra (scalar, velocity, coherency)

Volume Rendering

- Qualitative visual depiction of data
- Local data: partial images via image compositing
- In-situ down-sampling + in-transit rendering & compositing

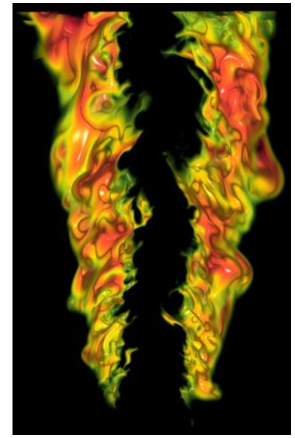
Topological Segmentation and Tracking

- Distance field (level set)
- Compute local merge trees
- Integrate to resolve features spanning multiple cores
- Adjust local merge trees

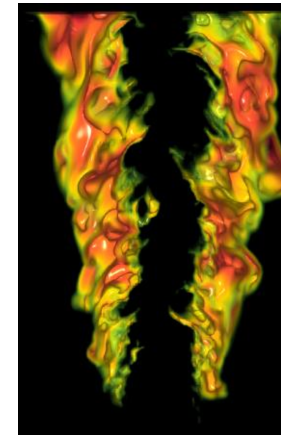
In-situ Visualization

Parallel volume rendering

- Design grid adaptor mechanism
- Visualization directly takes data regions from grid adaptor
- Highly scalable parallel volume rendering, particle rendering and image compositing
- Down sampling



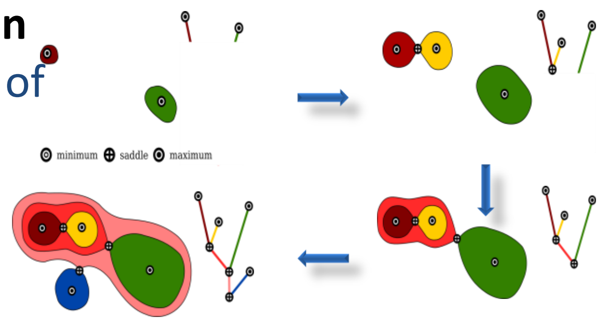
full resolution



down sampled

Reduced topology computation

- Complete characterization of level-set behavior of simulation variables
- Used to define features of interest
- Compute local merge trees
- Integrate to resolve features spanning multiple cores
- Adjust local merge trees



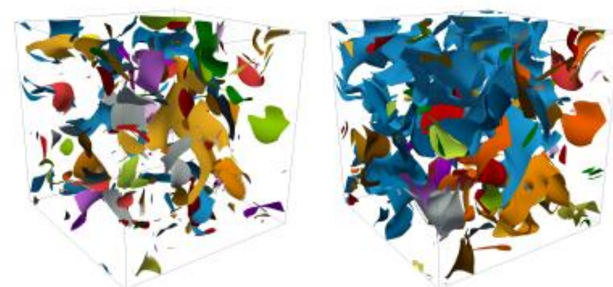
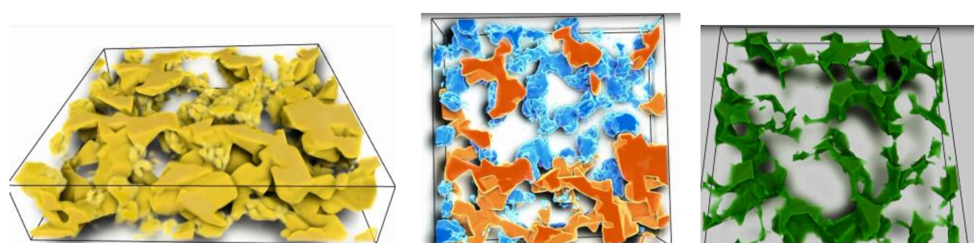


Fig. 13. Features extracted from the HCCI simulation for a diff-OH threshold of 0.12 (left) and 0.09 (right).



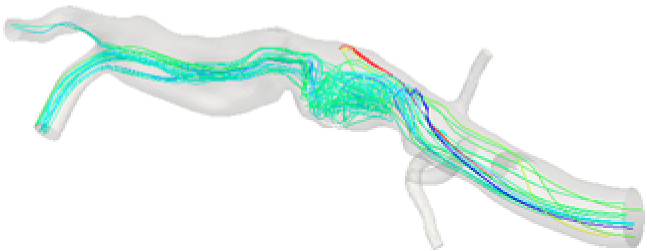
Digital Rocks Properties

On the fly Visualization

In-situ Visualization

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \mu \nabla^2 \vec{v}$$

Simulation Code+ ParaView CoProcessing



User

- LEVEL 1
  - User wants to see !
  - Is the simulation converging?
  - Monitoring

In-Situ Visualization : Collaboration between simulation and visualization

On the fly Visualization : Accessing to In-situ Visualization at "simulation time"

On the fly Visualization

In-situ Visualization

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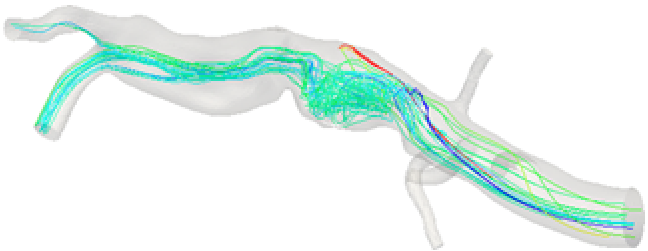


User

- LEVEL 2
  - User wants to change the visualization
  - Change an initial choice?
  - Modify the pipeline at "simulation time"

In-Situ Visualization : Collaboration between simulation and visualization

On the fly Visualization : Accessing to In-situ Visualization at "simulation time"

On the fly Visualization

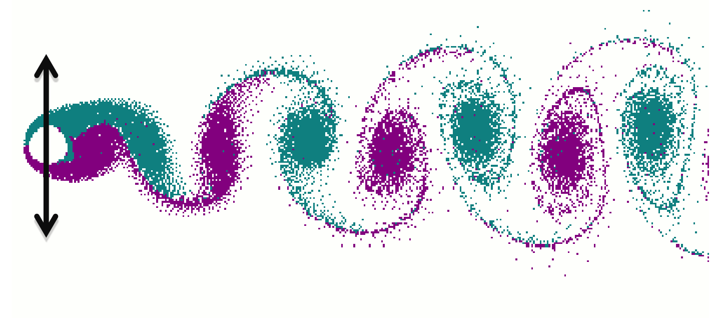
In-situ Visualization

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + \mu \nabla^2 \vec{v}$$

Simulation
Code+
Paraview
CoProcessing

User

Karman Vortex Street

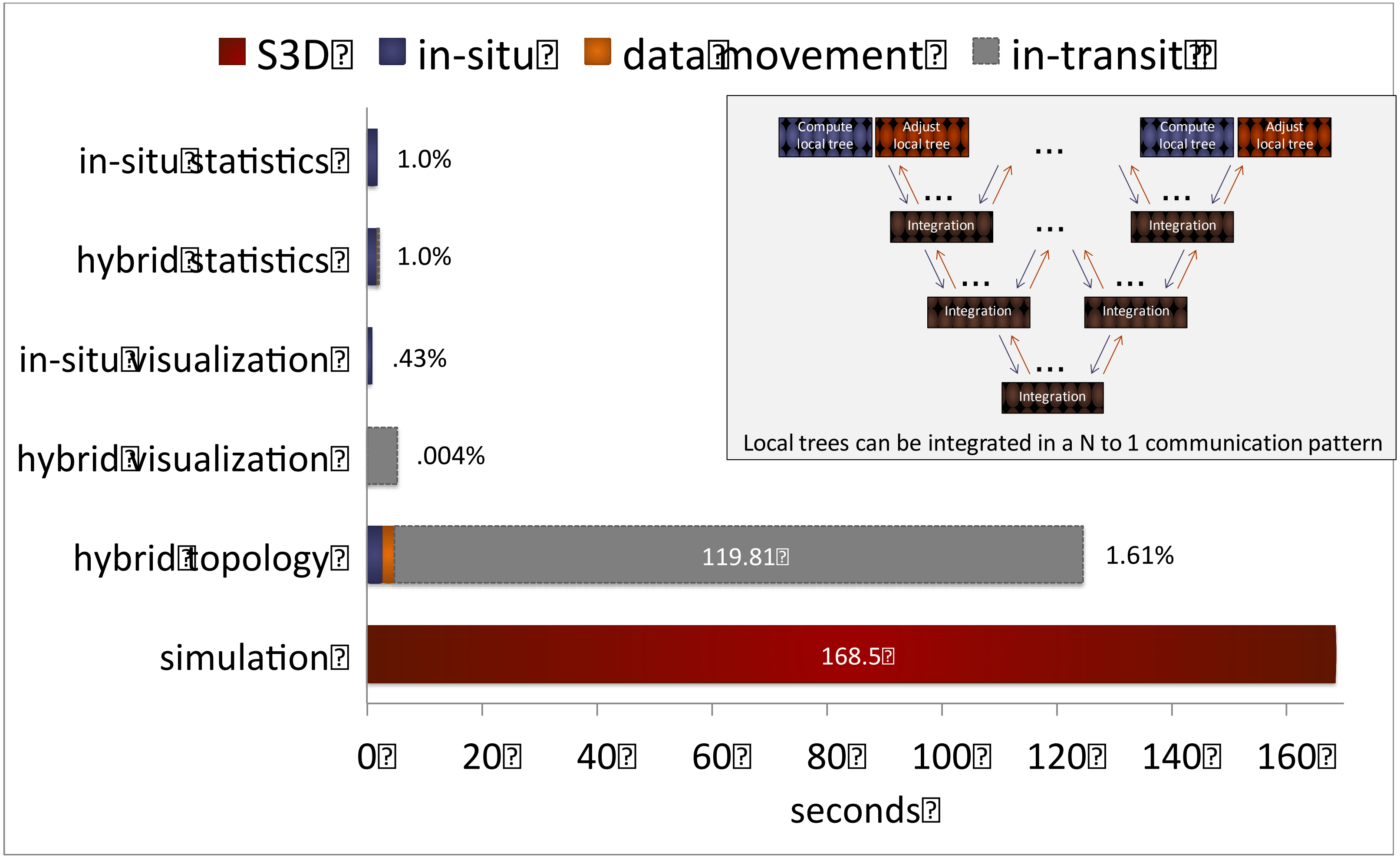


- LEVEL 3
  - User wants to DRIVE!
  - Computational steering
  - Real time response

In-Situ Visualization : Collaboration between simulation and visualization

On the fly Visualization : Accessing to In-situ Visualization at "simulation time"

Simulation case study with S3D (CT): Timing results for 4896 cores and analysis every 10th simulation time step



Courtesy of Jackie Chen, EXaCT, Sandia

new

Data Centric Approaches

Proposal : Fund R&D programs in order to explore

- The design space of future workflows: Real Time (In situ) data-related energy/performance trade-offs for end-to-end simulation workflows running at scale on current high-end computing systems
- Take into account future multi tiered storage architectures and asynchronous data transfers
- Design and implement new analysis techniques typically performed on large-scale scientific simulations: topological analysis, descriptive statistics, surrogate data model, filtering, compression, active learning, pattern/feature discovery, error analysis …
  - Identify metrics required to characterize classes of analyses
  - Identify which classes of algorithms perform best under which workflow designs
  - Algorithmic shifts – subsampling with quantification of error
- Explore disruptive approaches like sub-linear algorithms addressing the fundamental mathematical problem of understanding global features of a data set using limited resources.
- The use of in situ data analysis for tracking and checking fault or error propagation into the simulation, associating a resilience aspect with the execution of workflows on parallel systems.

Some Biblio on In situ Data Processing & Extreme Computing

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THANK YOU FOR ATTENTION