

Production Ready In Situ and In Transit

Harvest and Process Data Directly from Solver Memory

Presentation for:

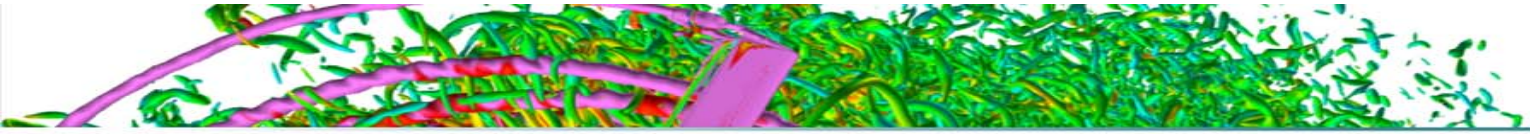
Advanced Modeling and Simulation Seminar Series

NASA Ames Research Center

October 19, 2021

Development supported by Department of Energy SBIR DE-SC0018633

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Intelligent Light: Speeding Workflows, Reducing Risk

- HPC use is coming out of an environment of codes from labs or universities that need to be stitched together
  - Not supported or sustainable (e.g., Catalyst, Libsim, Globus, Galaxy)
- Recognize that some HPC-CAE issues are common and can form the basis for a standardized platform
  - Data location, size, organized metadata
- Simulation and test results and data products have many possible uses beyond original intent
  - Standard formats and metadata needed to enable re-use
- Need to move beyond tightly controlled license management
  - Enterprise open source

Kombyne

SpectreUQ™

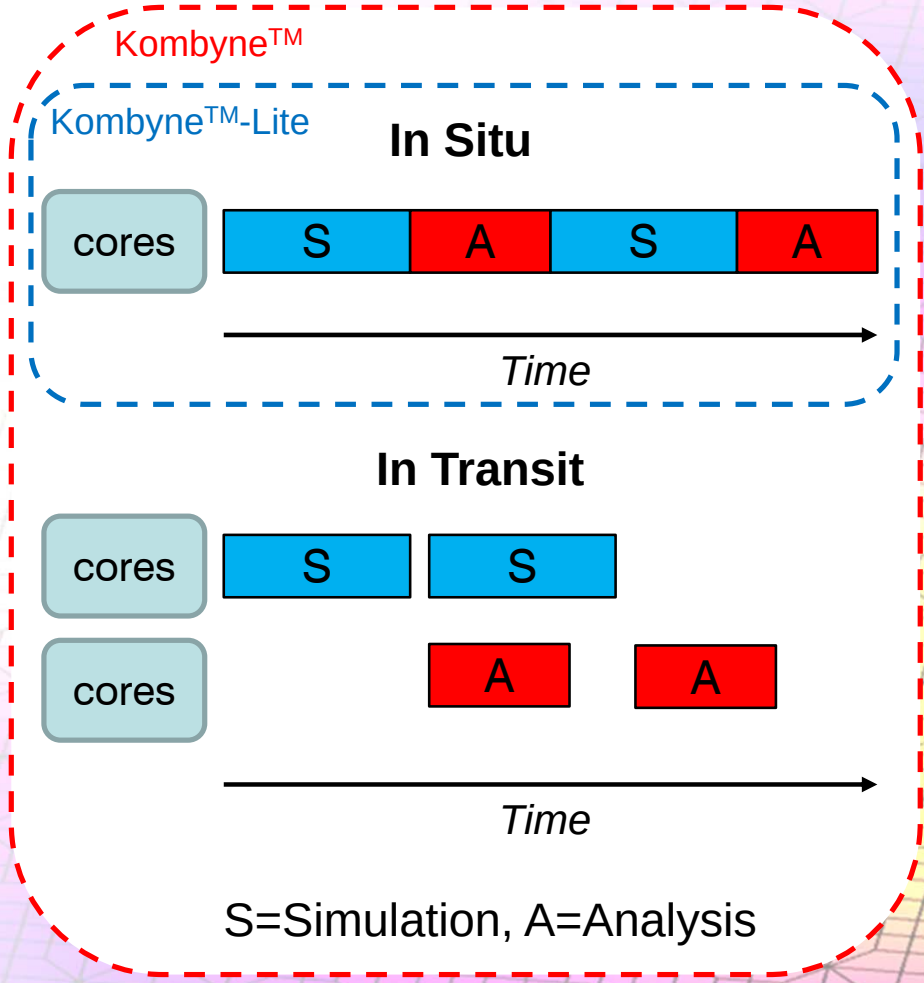
SnapShot™

IntelliTwin™

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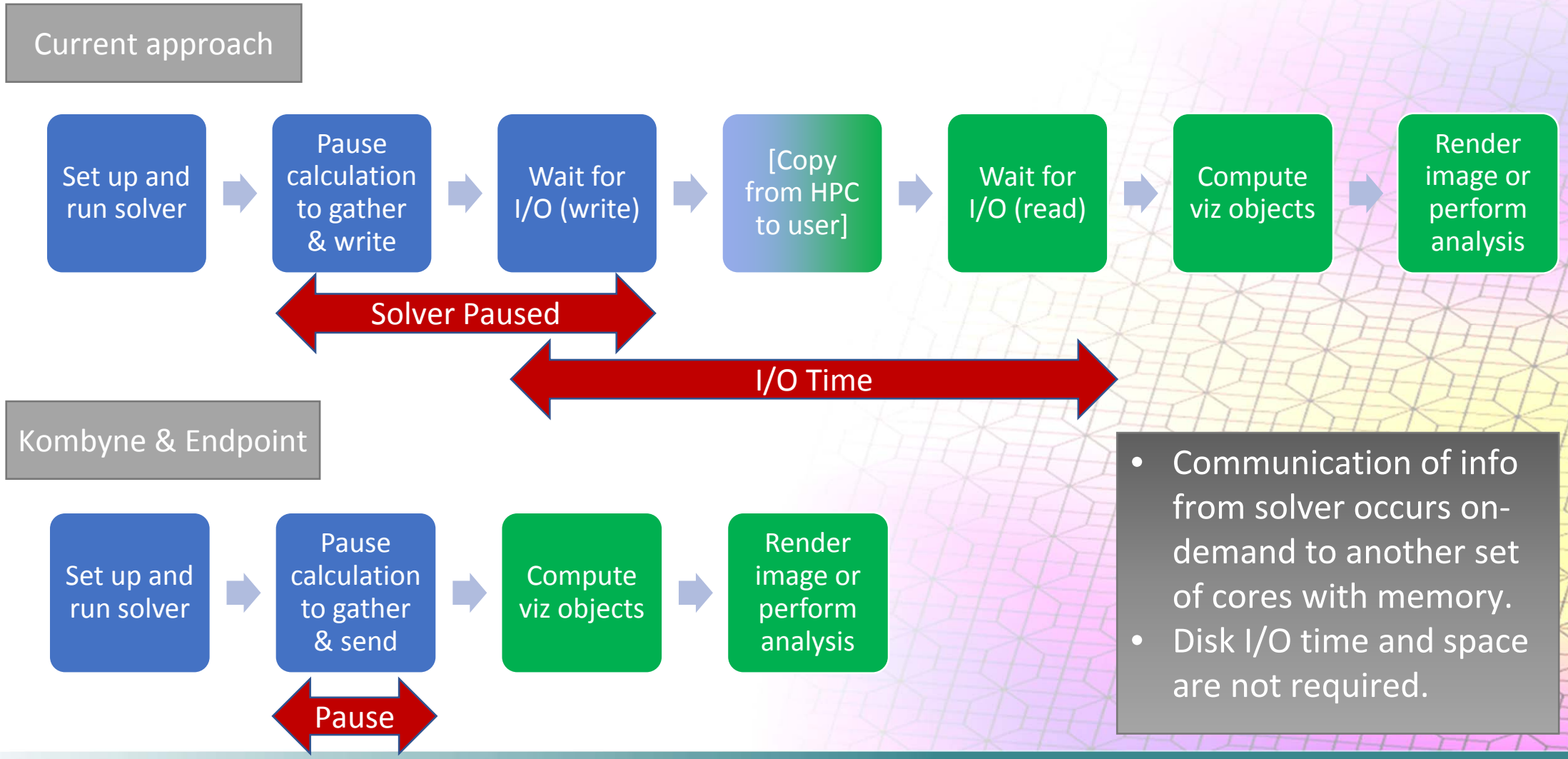
In Situ / In Transit

- Incorporate analysis into running simulation to access data while they are in memory
  - Avoid writing large files
  - Write data products frequently
  - Compute results and return control to simulation
  - Move data to dedicated cores and overlap simulation and analysis (**In Transit – Kombyne™ only**)



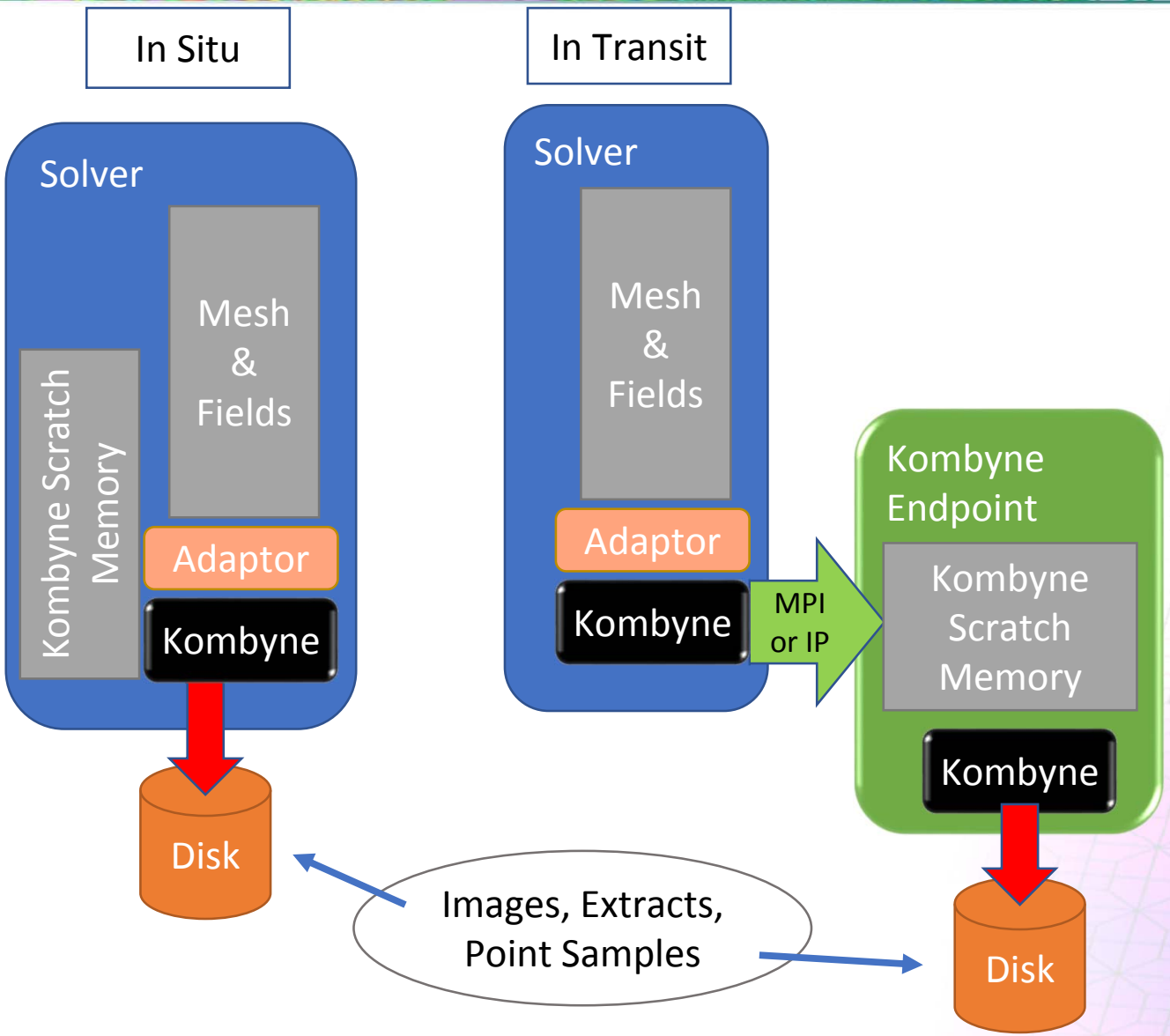
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How does Kombyne change my workflow?



- Communication of info from solver occurs on-demand to another set of cores with memory.
- Disk I/O time and space are not required.

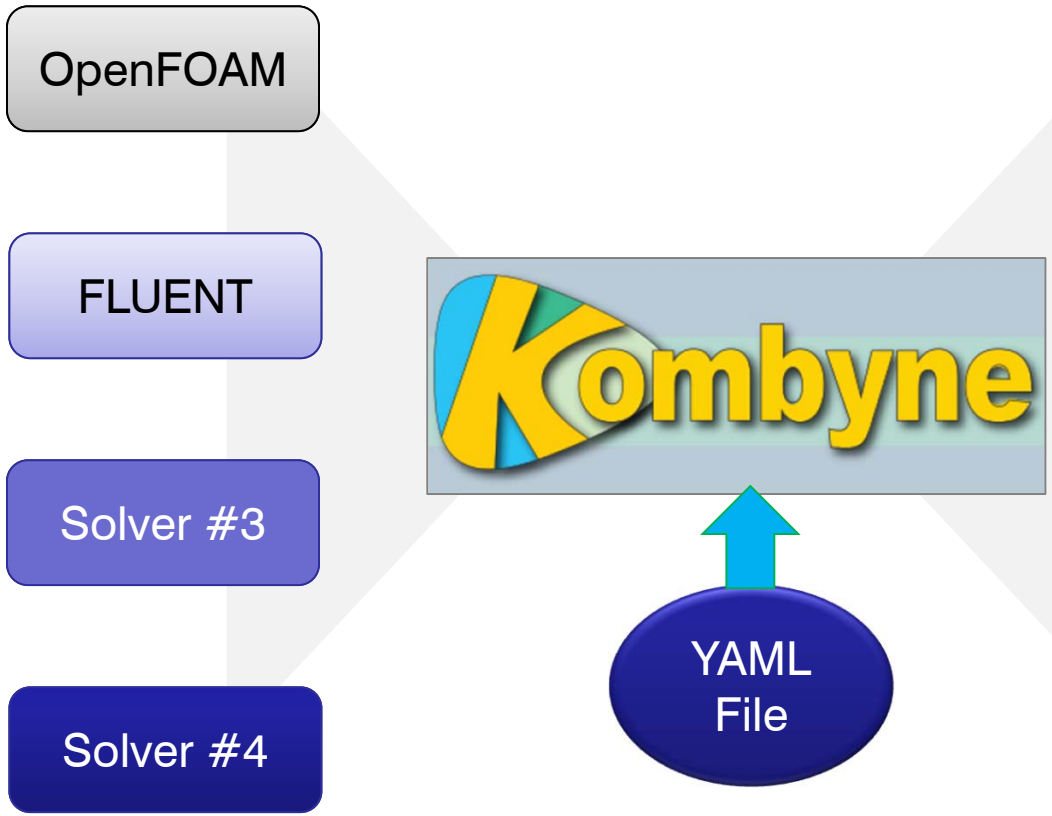
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Feature	Kombyne™	Kombyne-Lite™
In situ, incl. MPI parallel, zero copy	Yes	Yes
In Transit via Endpoint	Yes	No
Interactive connect to VisIt, PV, etc.	Yes	No
Steering and monitoring	Yes	No
Source code available	Yes	Limited
Licensing, support	Pricing based on enterprise size (annual)	No-cost to use, support via Forum or Maint. contract

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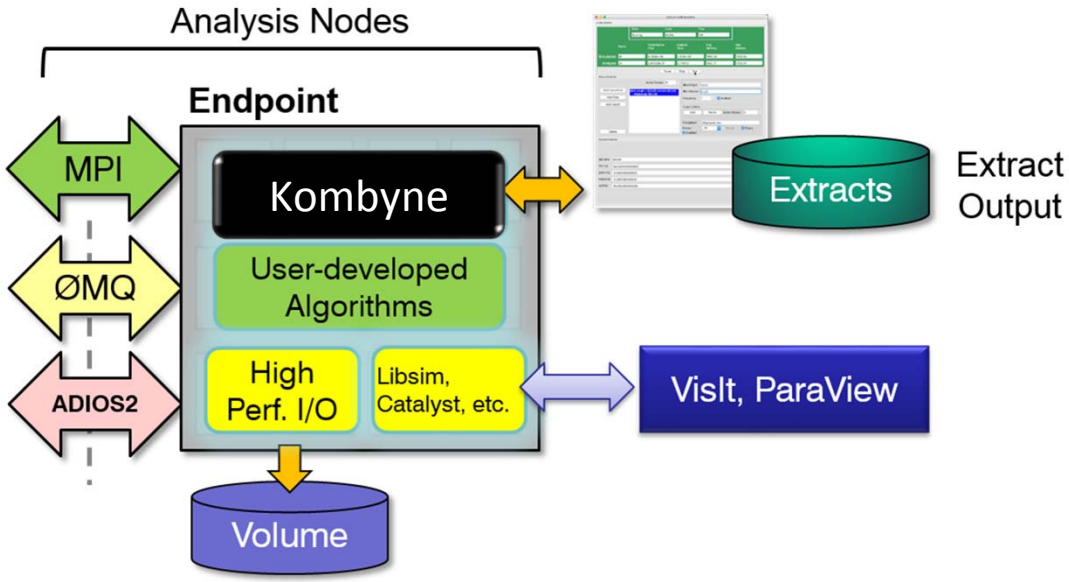
Choice of many data products



- Extracts in various formats
  - XDB, vtk
- Structured point samples
  - CSV, Matlab
- Samples mapped to mesh
  - Plot3D
- Rendered images
  - PNG, CINEMA

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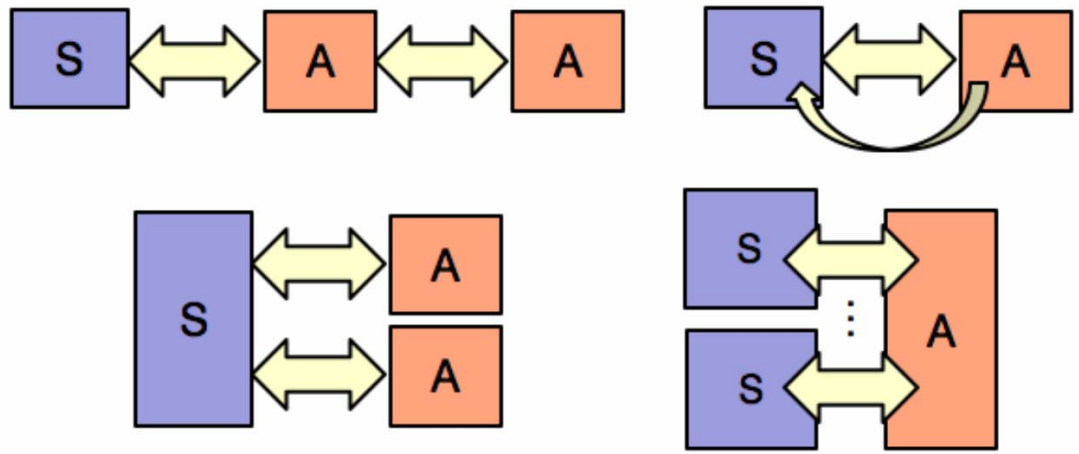
Endpoint Operation: In Transit



- The simulation and analysis cores truly overlap operation
- Flexible M:N rank assignment, fully parallel
- **Customers/OEMs can integrate their advanced physics & vtk visualization pipelines**

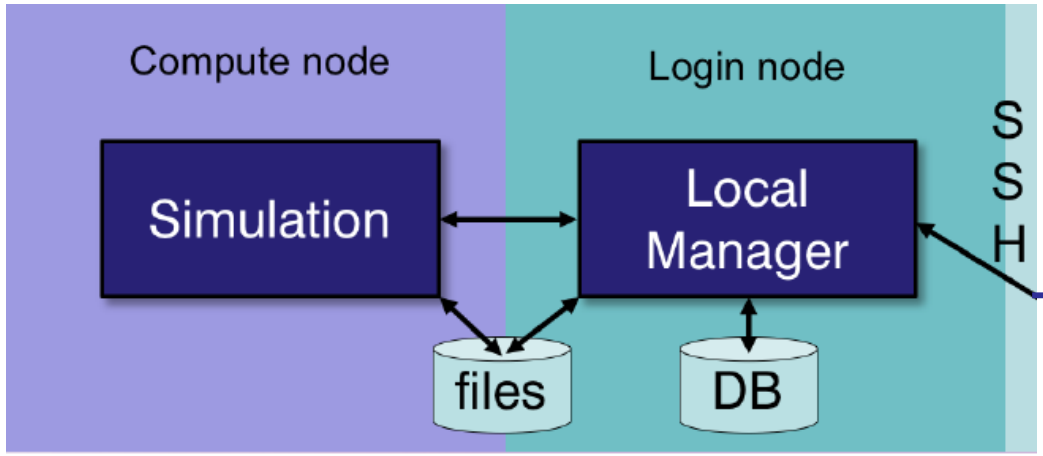
Endpoints have been designed to support flexible topologies that coupled solvers and data science require

S = simulation; A = analysis endpoint



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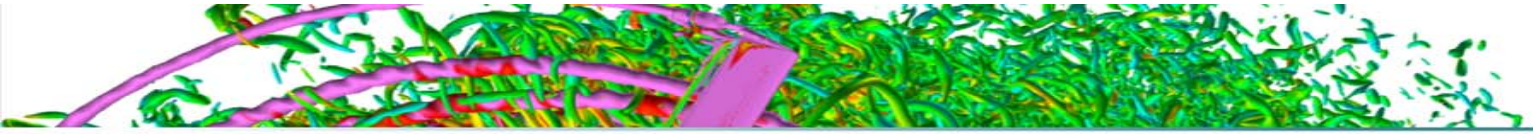
Monitoring and Steering





- Monitor and archive all Kombyne™ jobs
- Display strip charts, performance statistics
- Keep track and review extract and image production
- **Interactive control of visualization and solver parameters**

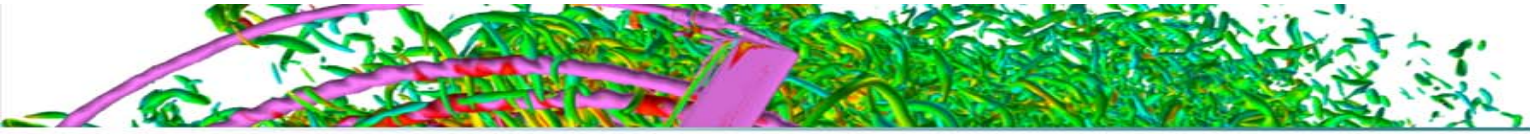
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Benefits

- ✓ In transit operation minimizes interference with solver resources (memory and CPU)
- ✓ Simplify integration into solver codes, reducing library dependencies – *no* vtk, *no* mesa, …
- ✓ Permits data science type of post-processing which prefer to retain blocks of timesteps in memory – sampling can be at solver timestep rate
- ✓ Simplify extract creation workflow
- ✓ Monitor and control multiple local or remote solver jobs

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Features

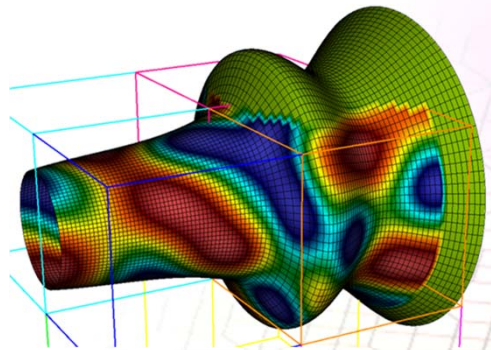
- In situ and In transit
- Parallel (MPI + OpenMP, CUDA)
- Languages: FORTRAN, C/C++, Python, Julia
- Meshes: Rectilinear, Structured, Unstructured, Polyhedral
- Pass data zero-copy
  - Flexible memory layouts
  - Cell data, point data

- I/O: VTK, CSV, MatLab, Plot3D, FieldView XDB
- Raytrace rendering: PNG, Cinema
- Data extraction (via input file)
  - Null (for export)
  - Slice
  - Iso
  - Boundary Surfaces
  - Point Sample
- Derived fields and Triggers
- Monitoring / steering

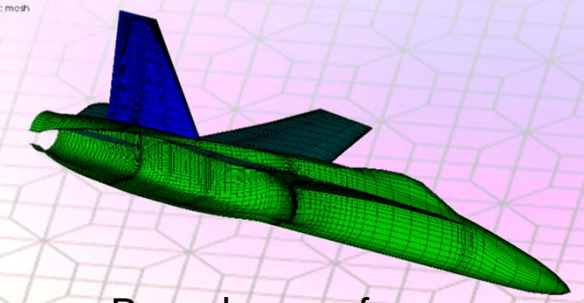
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Types of Pipelines

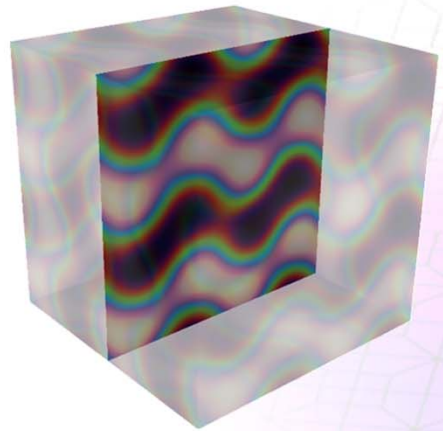
- Pipelines transform data and can export geometry
- Pipelines are specified via a YAML or JSON input file
- Types
  - Null (operate on volume)
  - Slice
  - Isosurface
  - Boundary surface
  - Sample (point clouds)



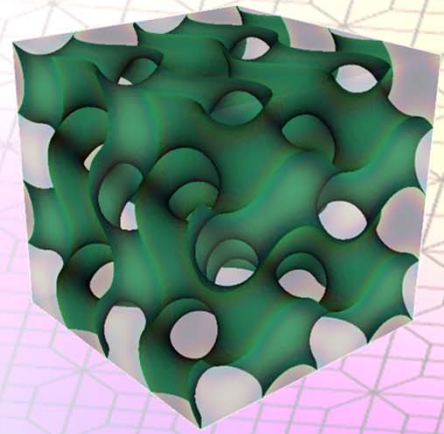
Point Sample



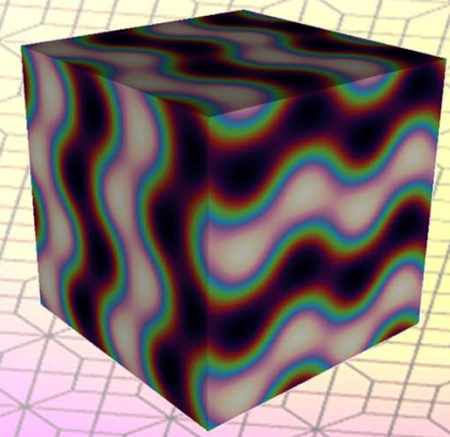
Boundary surface



Slice



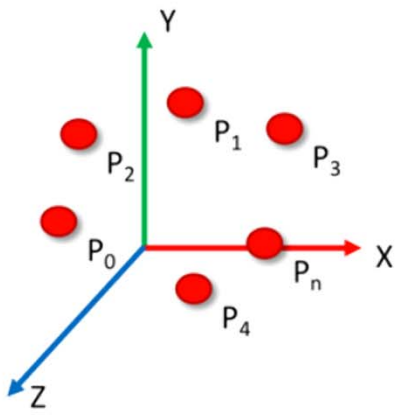
Isosurface



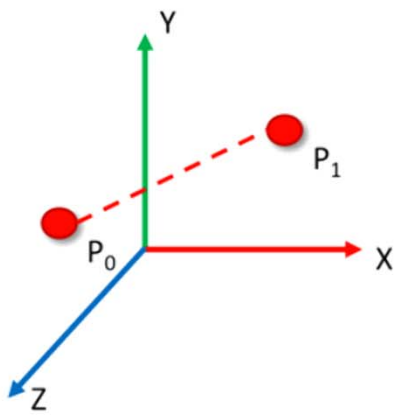
Null (export)

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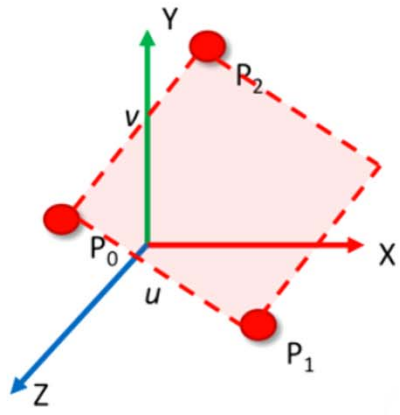
Parametric, Repeatable Sampling



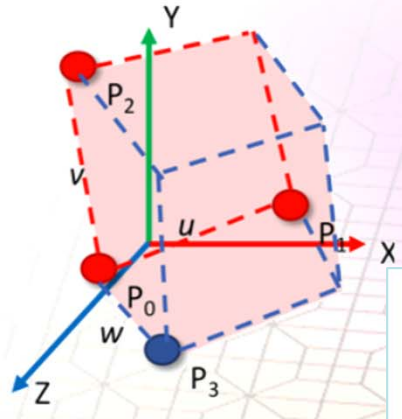
Points



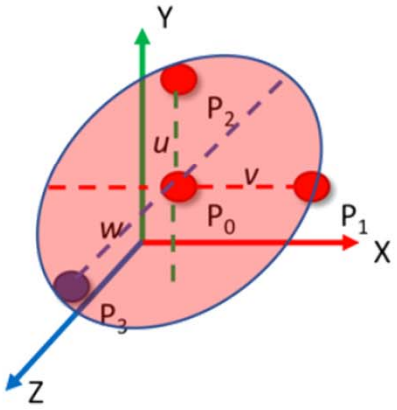
Line



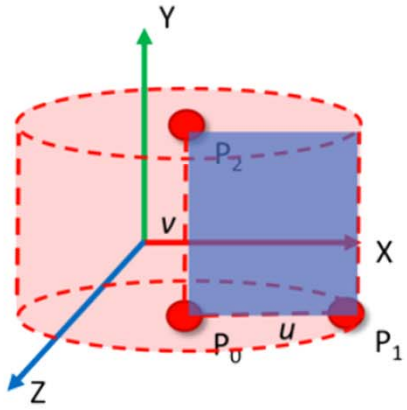
Plane



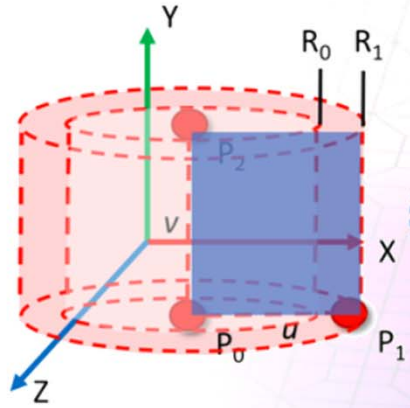
Box



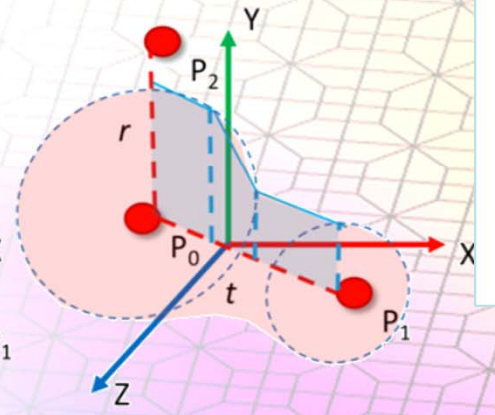
Ellipsoid



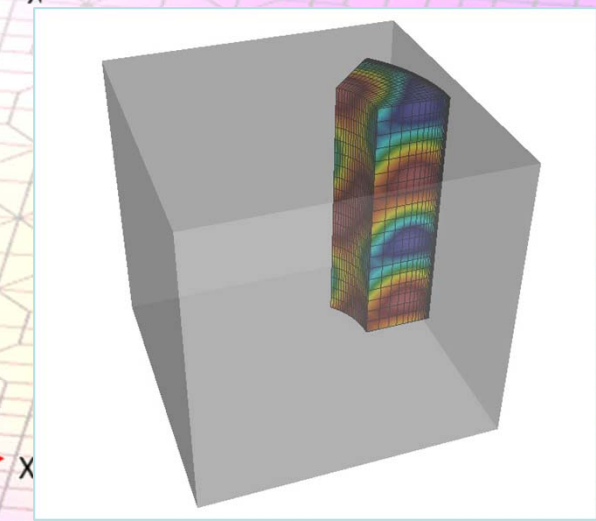
Cylinder



Annular Cylinder



Revolved curve



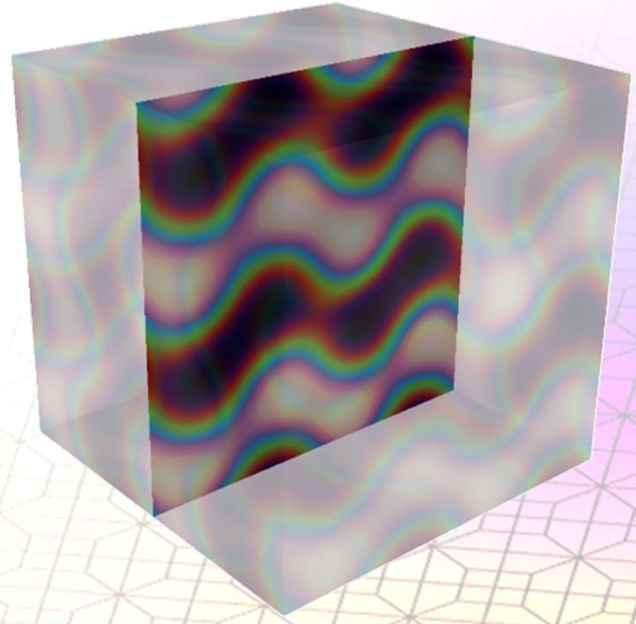
Timestep driven

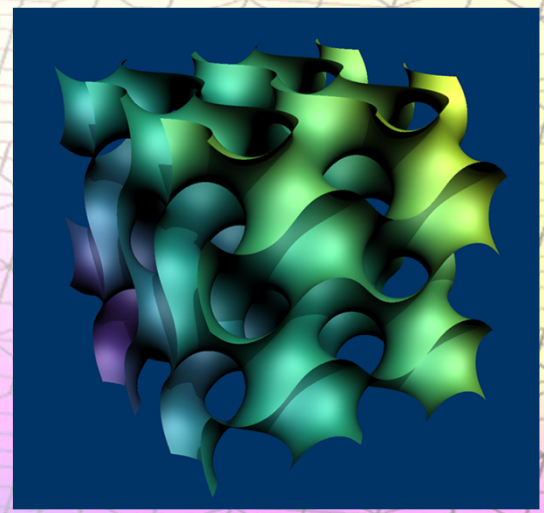
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Pipelines

- Expressed via YAML files
- Pipelines are applied to simulation data to make extract data
- Extract data is sent to one or more outputs to make files
- Pipelines can operate at different frequencies or use triggers to be invoked in response to conditions

```
pipelines:
  -
    type: "slice"
    enabled: "true"
    frequency: 1
    attributes:
      origin: [0.0, 0.0, 6.28]
      normal: [0.0, 0.0, 1.0]
   outputs:
     -
       type: "export"
       file_pattern: "slice%domain.%ts"
       file_format: "vtk"
       attributes:
         binary: "true“
   type: ”iso"
      enabled: "true"
      frequency: 10
      attributes:
        variable: "gyroid"
        value: 0.0
     outputs:
       -
         type: "export"
         file_pattern: ”iso%domain.%ts"
         file_format: "vtk"
         attributes:
           binary: "true"
```

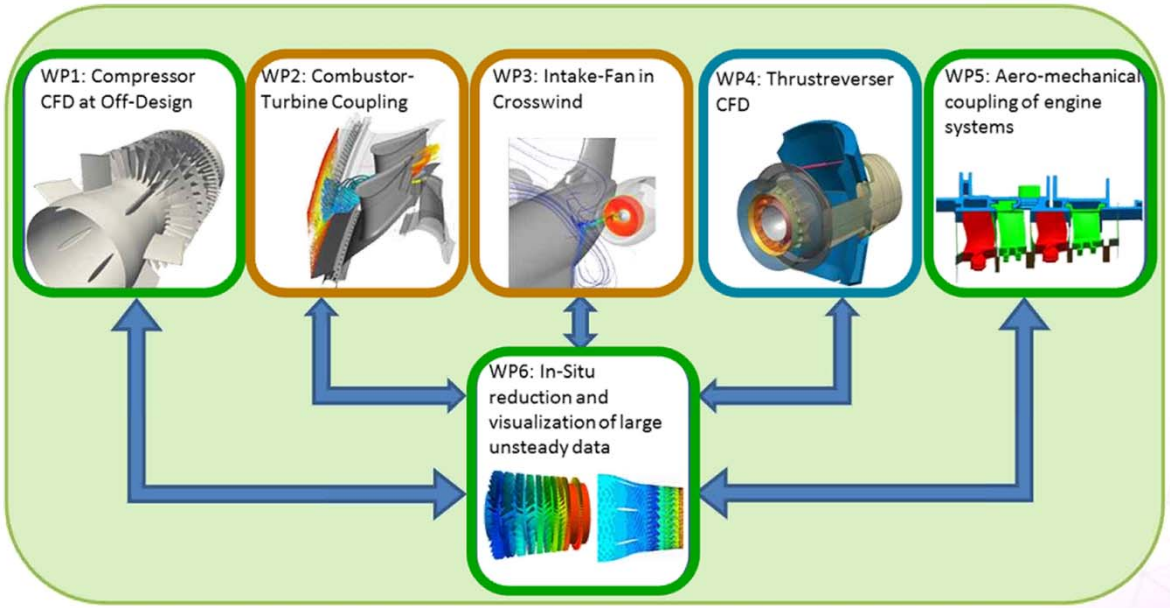




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Progress to date…

PRESTIGE



Start: 1.5.2018; Duration: 3.25 years
Budget: 5 mio €

Rolls-Royce

"successfully demonstrated on a high pressure compressor model with more than 5 Billion mesh nodes on the high-performance compute cluster of the TU Dresden."

Adapters built or in progress:

- OVERFLOW2
- RR Hydra
- OpenFOAM
- FLUENT

Planned:

- FUN3D
- SU2

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