Understanding the Impact of Synchronous, Asynchronous, and Hybrid In-Situ Techniques in Computational Fluid Dynamics Applications

eScience Session 7: HPC and eScience

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Motivation

Computational fluid dynamics (CFD)

Characteristics:

- Computationally expensive
- Requiring large storage for the results (tens of GB per simulation step)

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Post-mortem data processing

Workflow:
- Simulation solver write results through IO subsystem to storage
- Data processor read the data through IO subsystem from storage

Disadvantage:
- Bottleneck in IO because of the IO bandwidth
- Limited frequency to preform data processing

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In-situ data processing

Workflow:

- Data processer receive data from simulation solver without via IO subsystem and storage

Challenge:

- Data processing could bring overhead to the simulation
- Data processing could influence the scalability of the simulation

Synchronous, Asynchronous and Hybrid In-Situ Data Processing

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Synchronous in-situ approach

Workflow:

- Simulation waits until data processing finished

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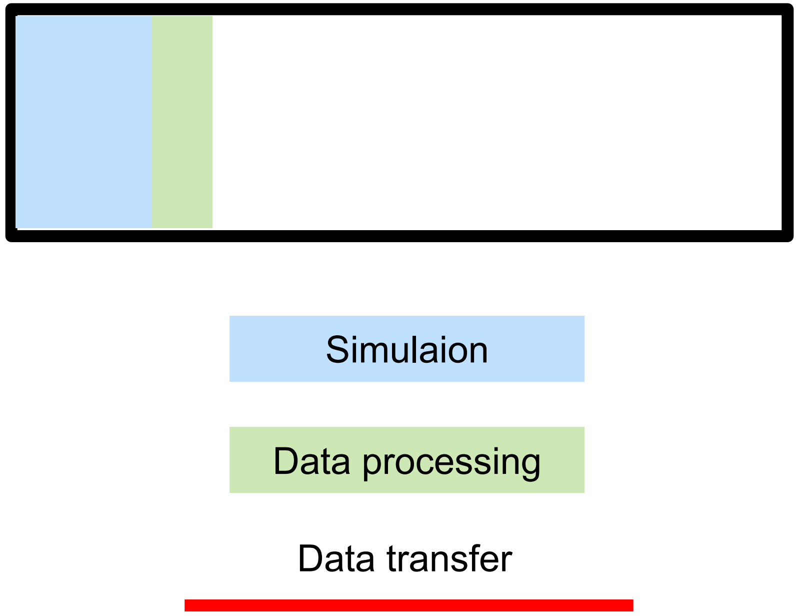

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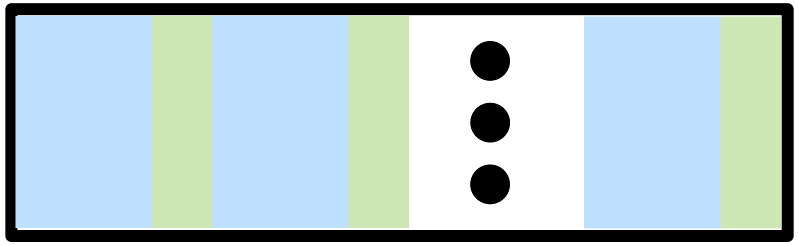

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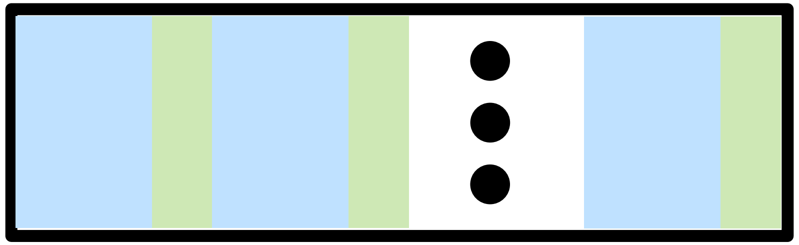

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Workflow:

- Simulation sends data to separate computing resources and continues
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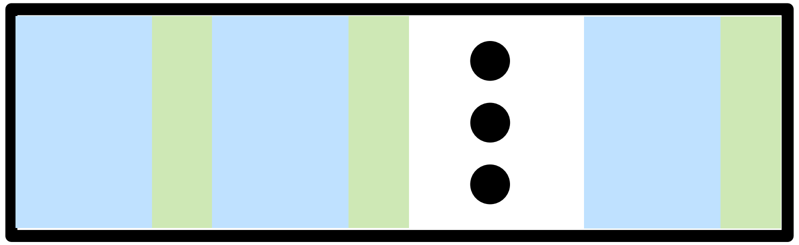

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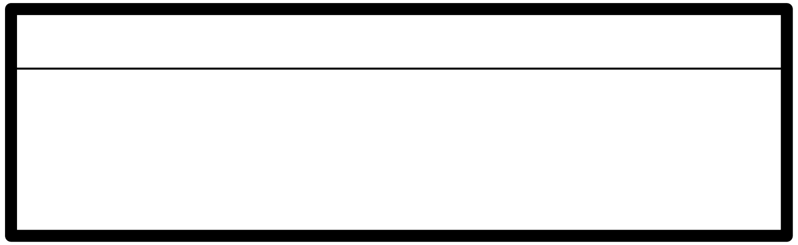

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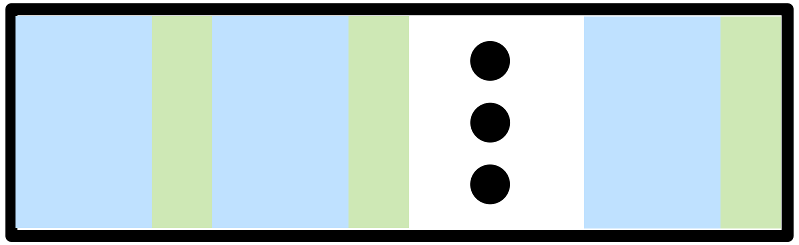

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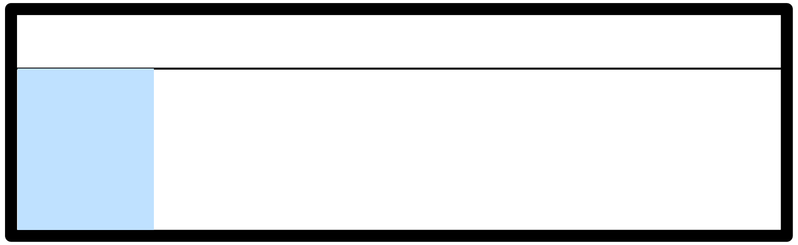

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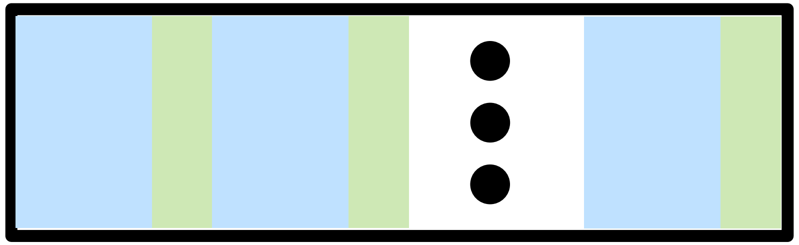

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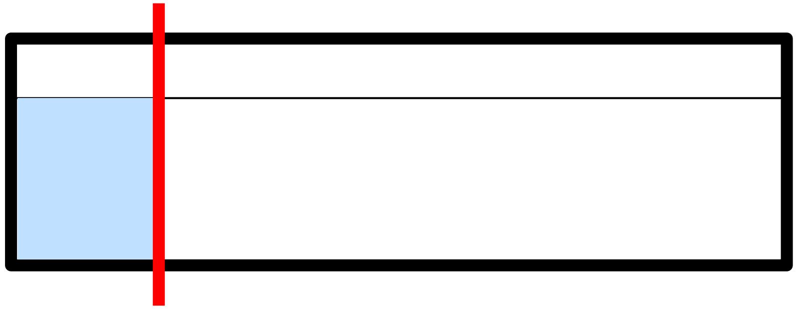

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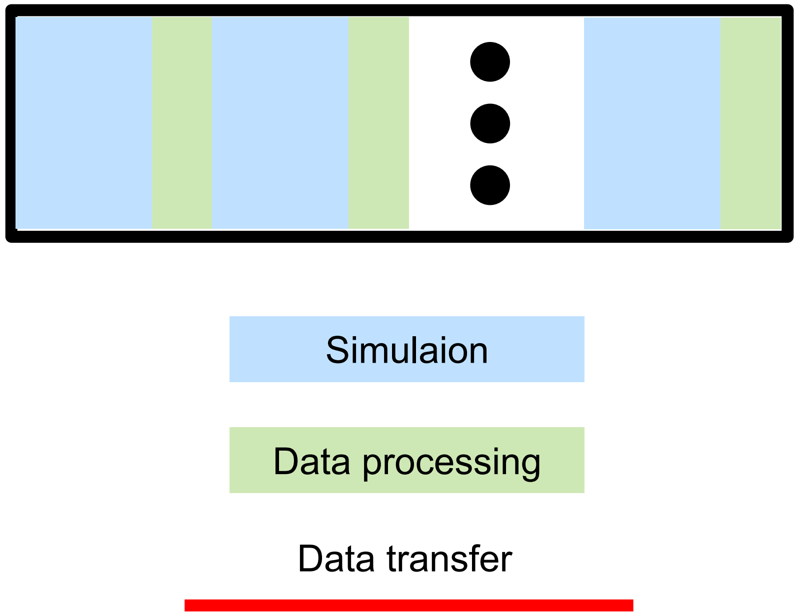

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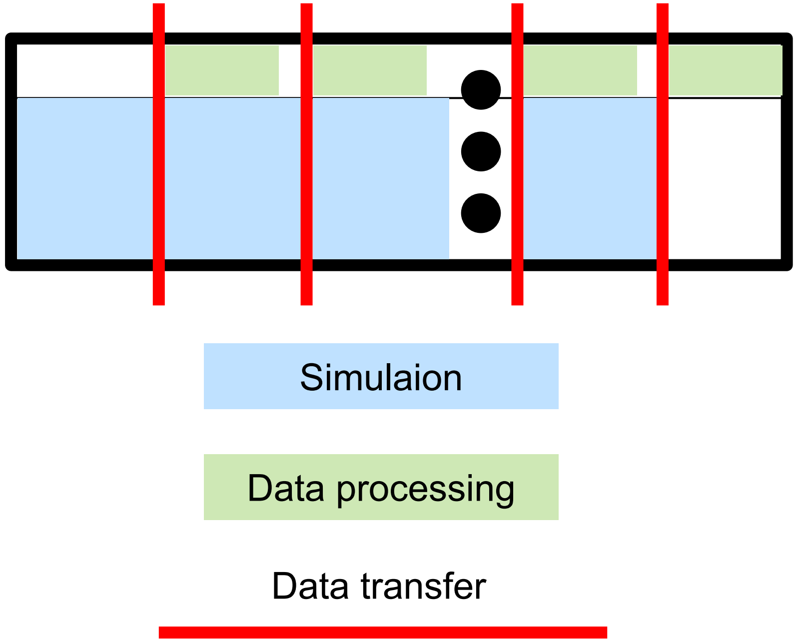

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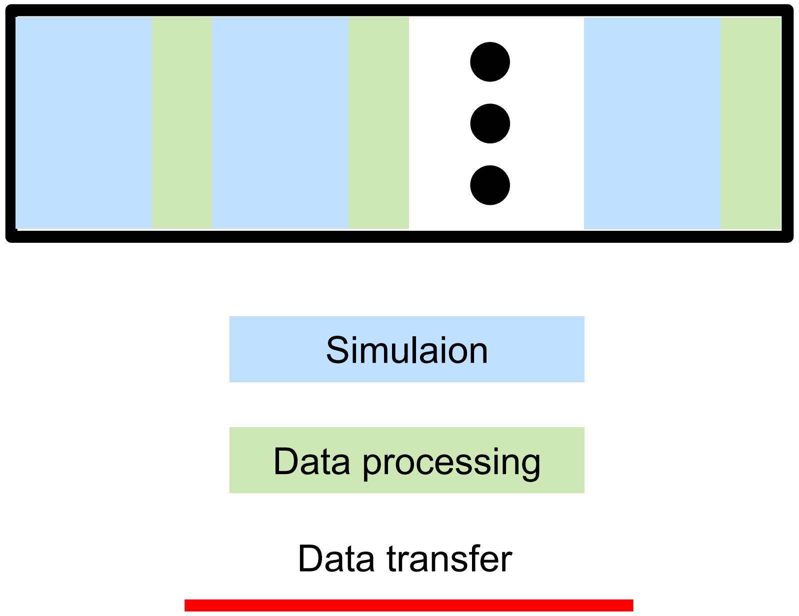

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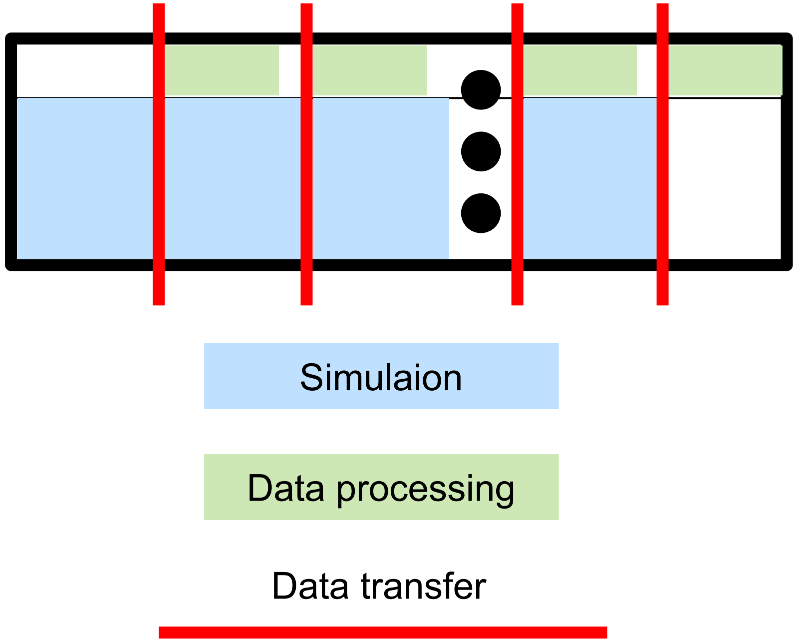

Hybrid in-situ approach

Workflow:

- First part of data processing is synchronous
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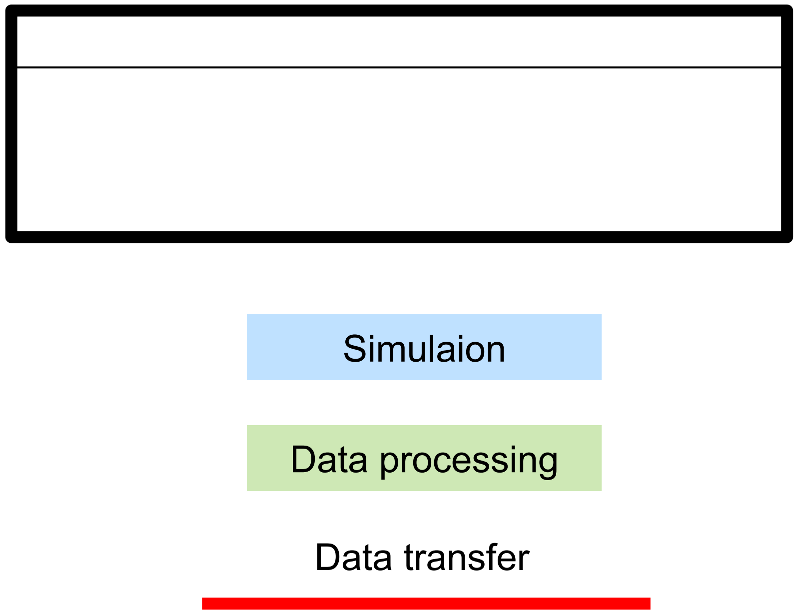

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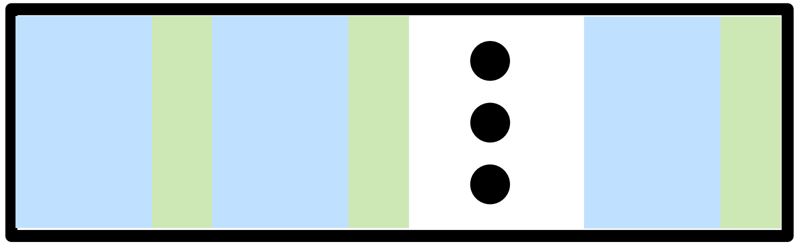

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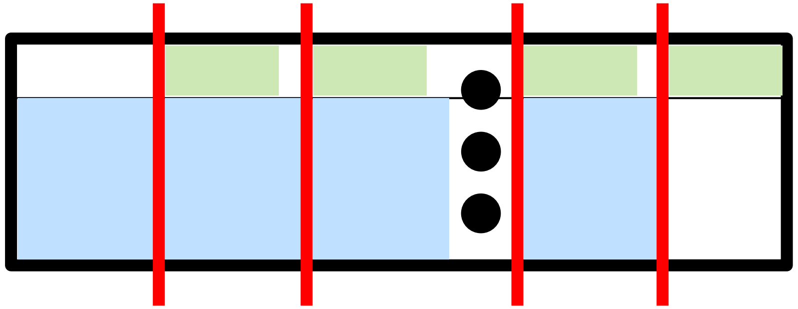

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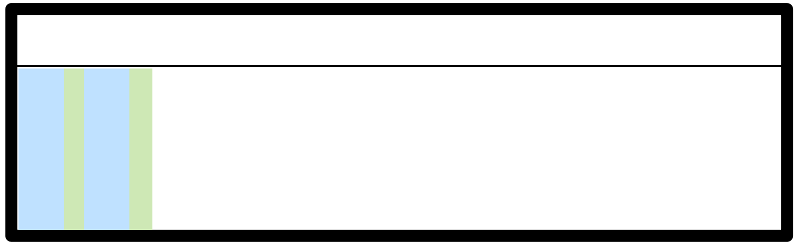

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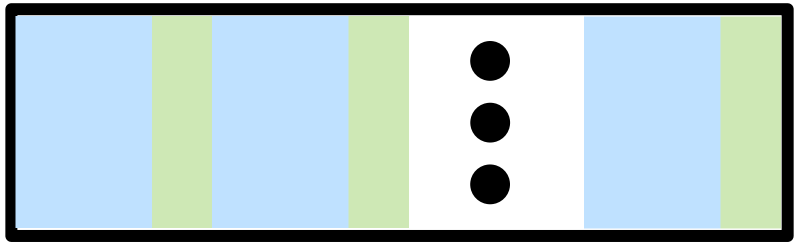

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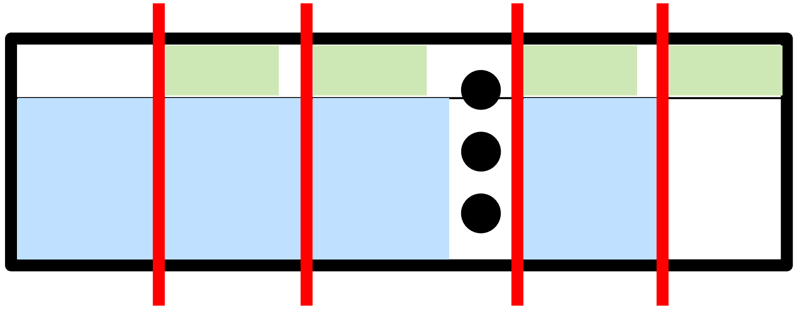

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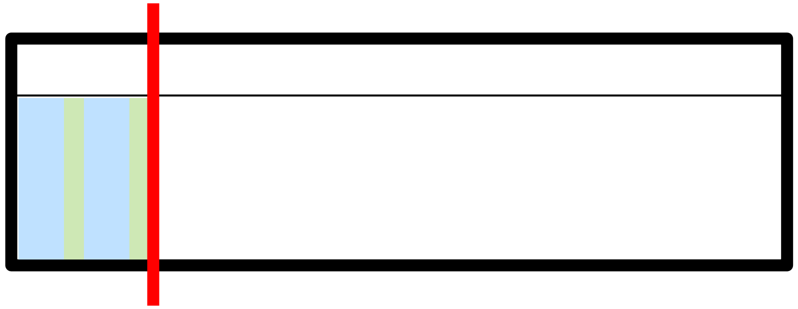

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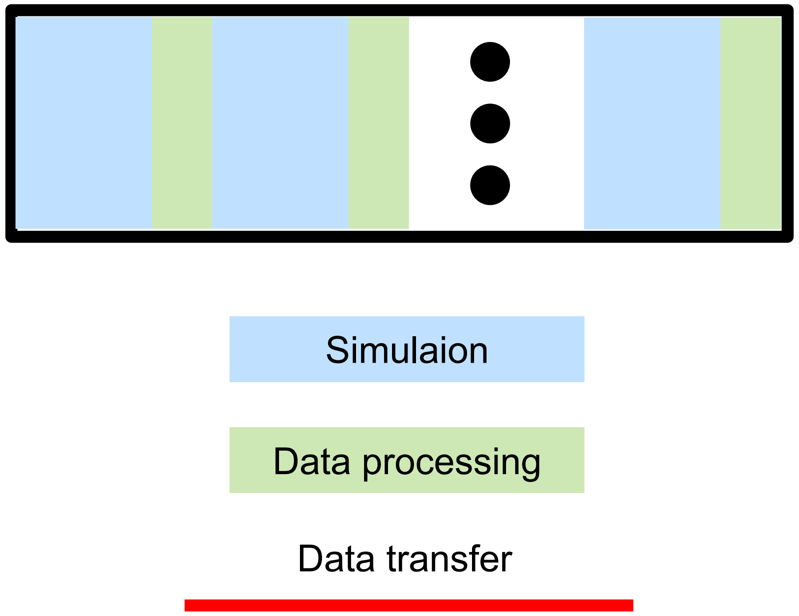

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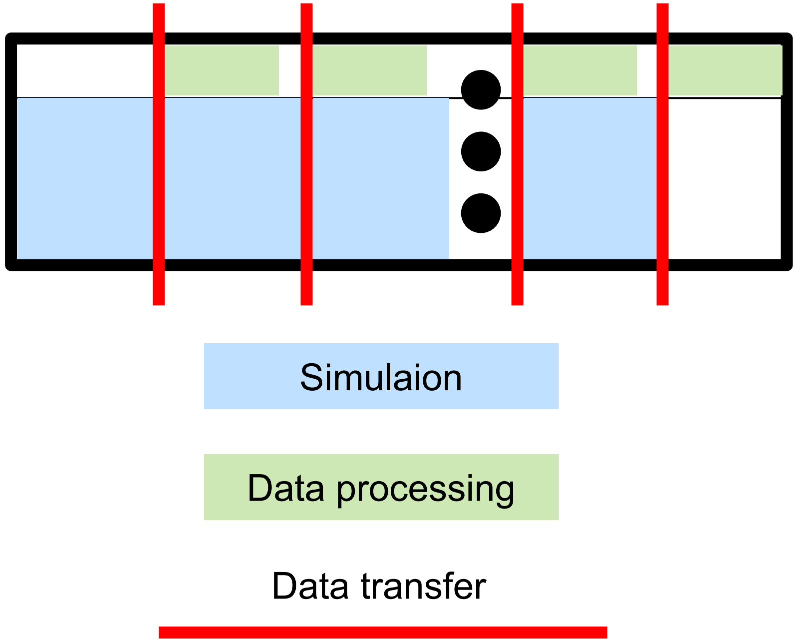

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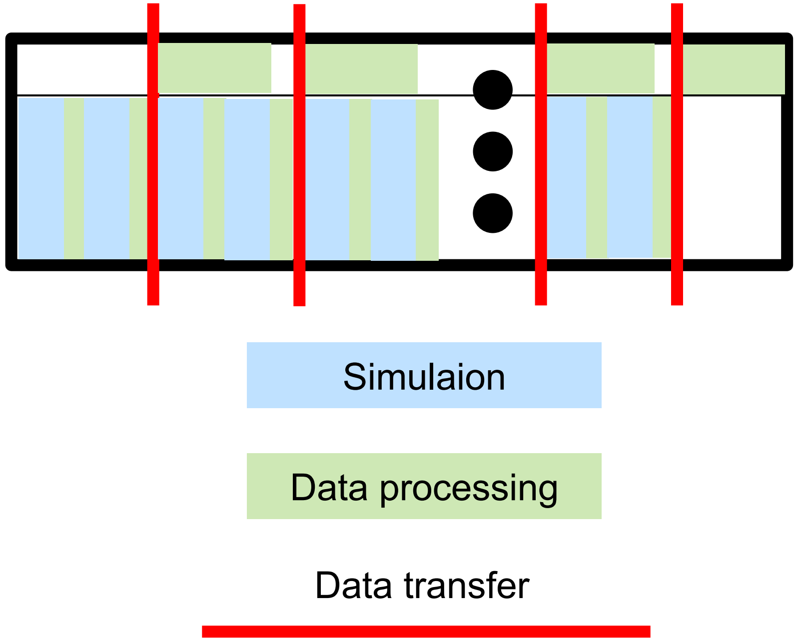
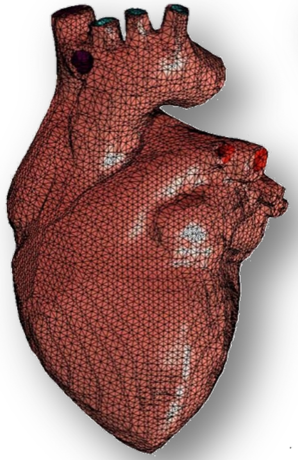


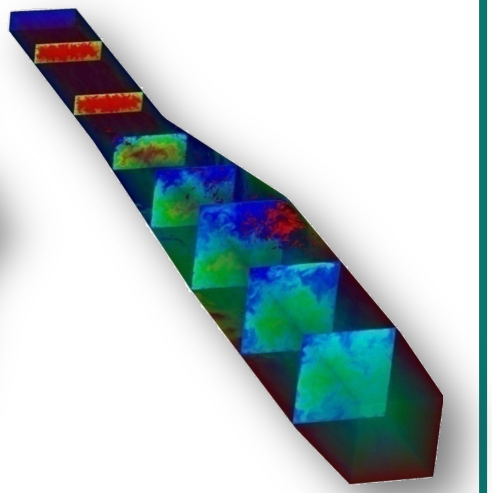
State-of-the-Art

Simulation solver

Nek5000:

- CPU version: Fortran
- GPU version: Fortran with OpenACC





Characteristics:

- Direct Numerical Simulation (DNS) solver
- “Matrix-free”
- Scalability from “local domain”

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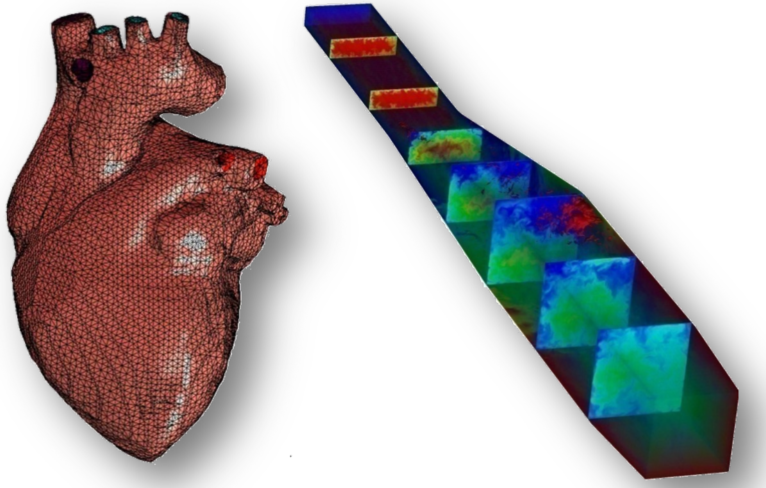

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In-situ systems

- VisIt with Libsim
- ParaView with Catalyst
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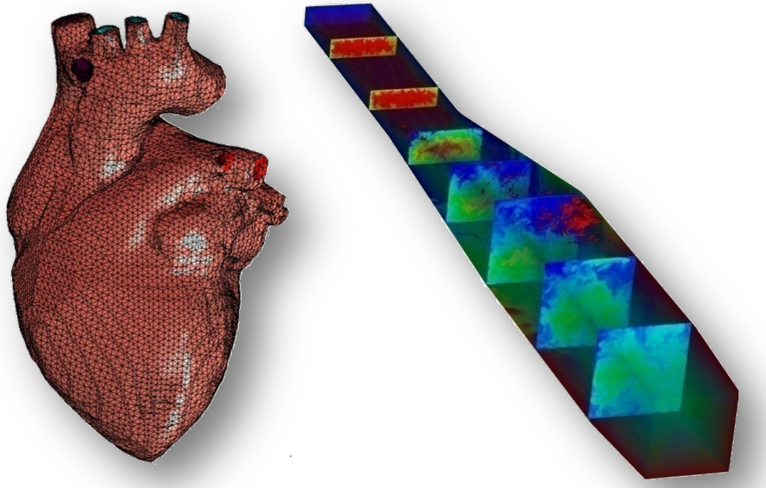

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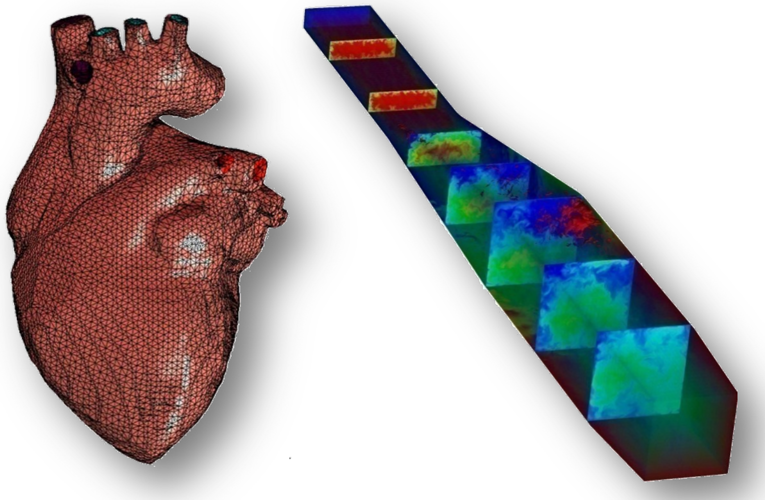

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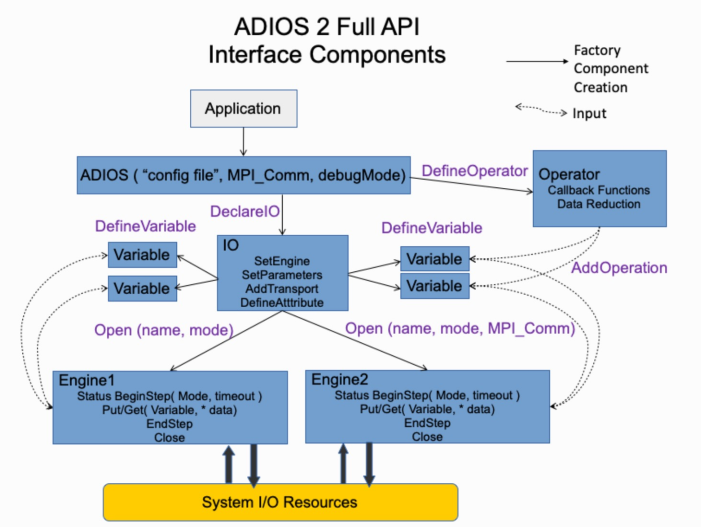
ADIOS

- Arbitrary data structure
- Runtime configuration
- Application programming interfaces (APIs) for multiple programming languages
- Operators such as lossless compression
- MPI-based data communication between arbitrary configuration [1]



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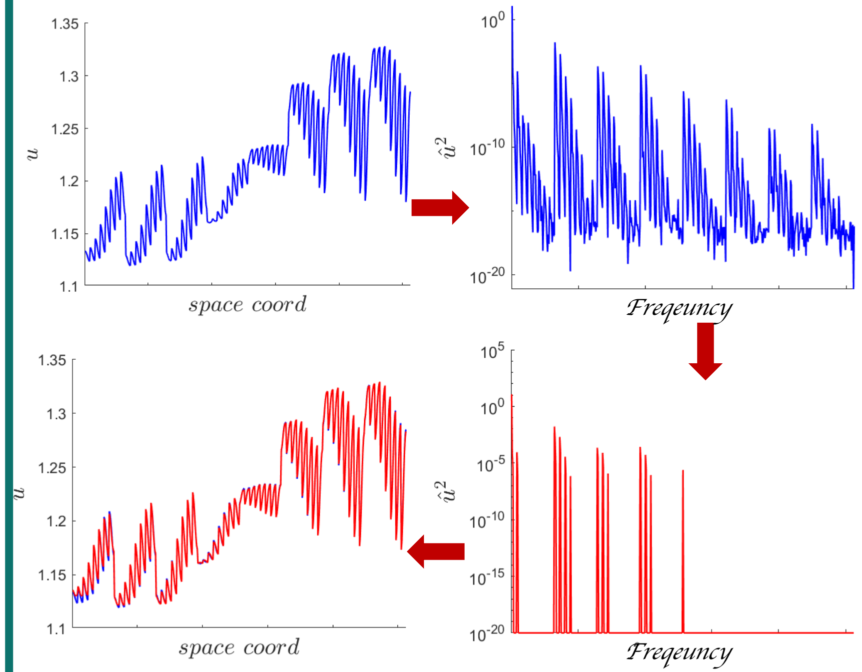
Use Case: Lossy and Lossless Data Compression

Data compression

Lossy compression, physics-based method:
discard the data not associated with the most energetic flow motions [1]



Lossless compression:
ADIOS2 operator with runtime configuration

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malleable data solutions for HPC

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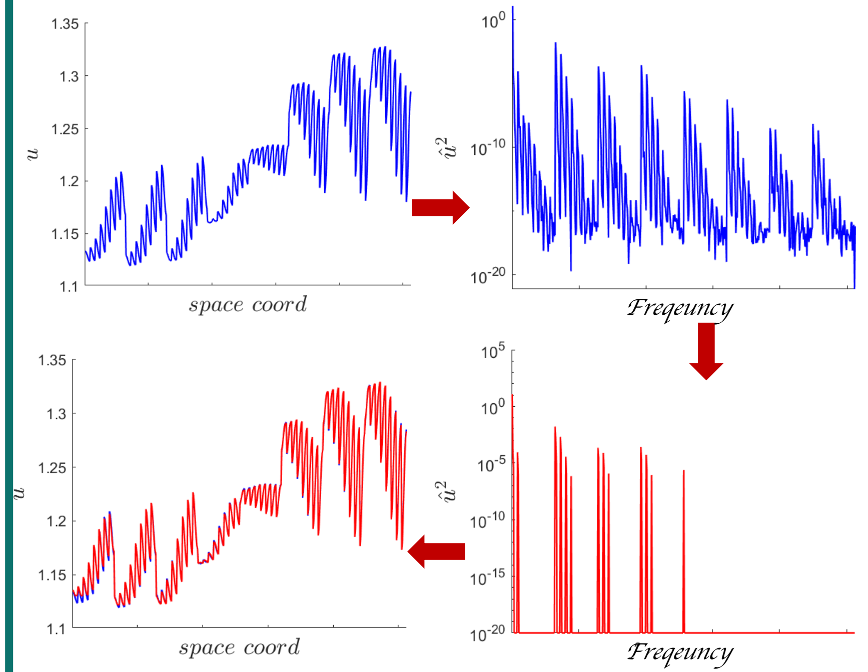

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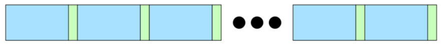
In-situ approach

- Nek5000 with synchronous data compression:



Fortran functions

C/C++ functions called in Fortran

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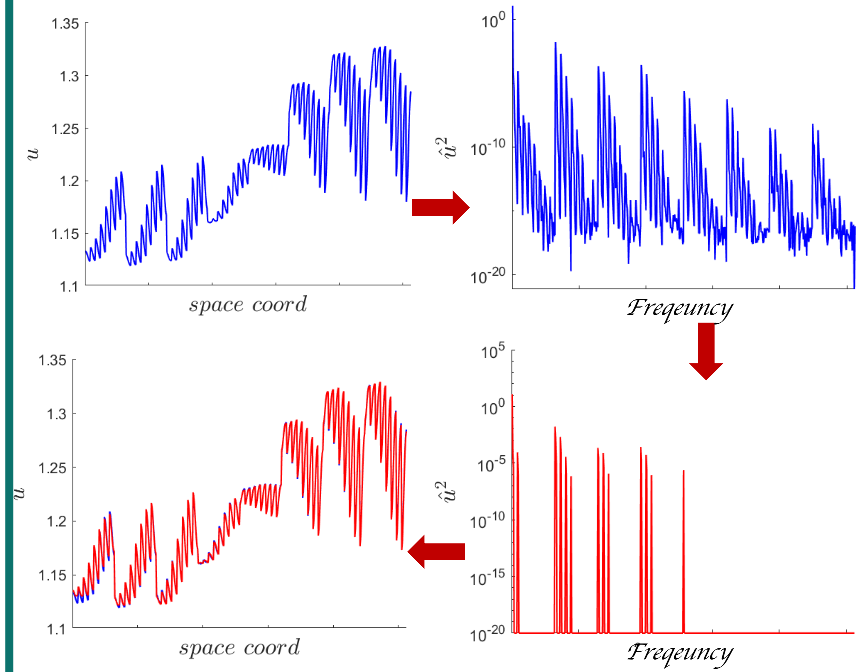

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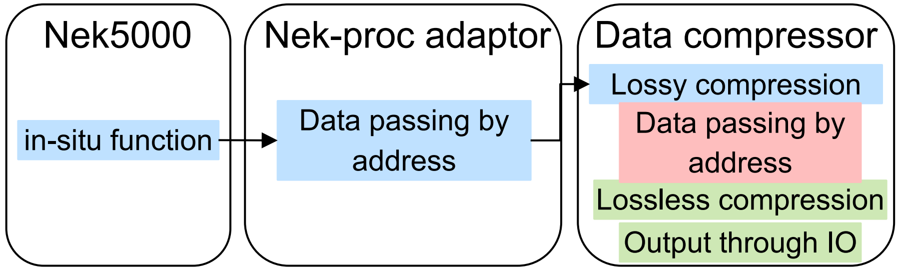

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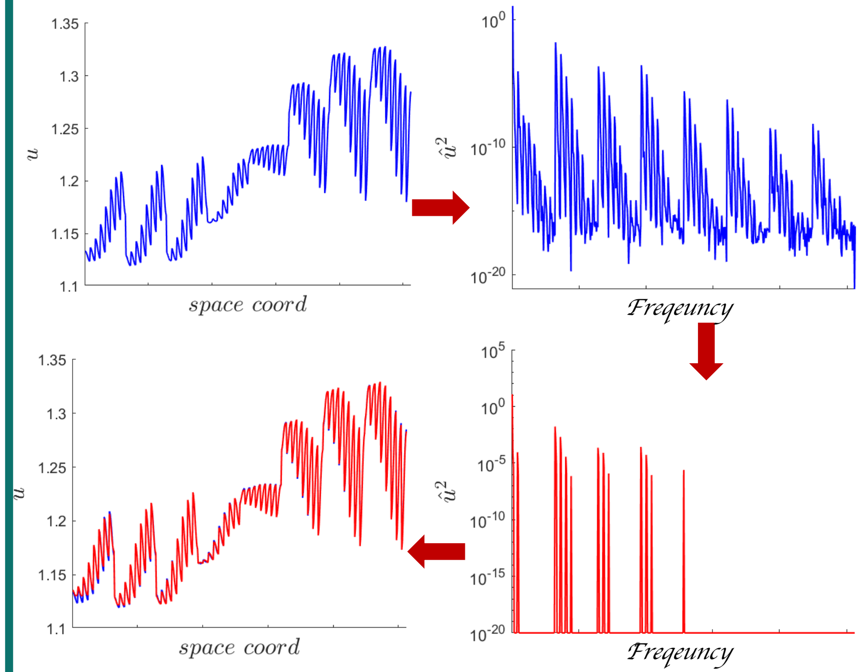

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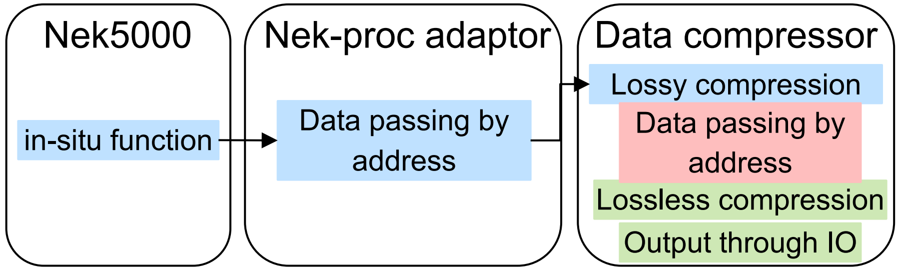

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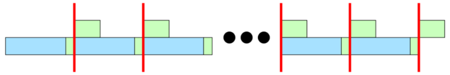

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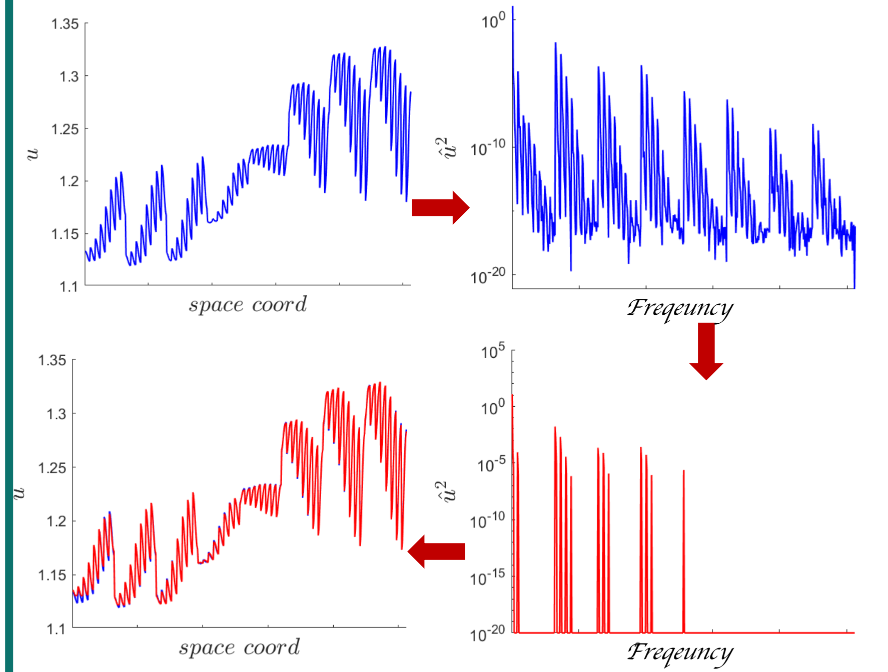

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Nek5000: in-situ function → Nek-proc adaptor: Data passing by address → Data compressor: Lossy compression; Data passing by address; Lossless compression; Output through IO

- Nek5000 with hybrid data compression:

Nek5000: in-situ function → Nek-proc adaptor: Data selection → Data compressor: Lossy compression → Proc-wrtr adaptor: Data passing by address → ADIOS writer: ADIOS *insituMPI* writer

ADIOS reader: ADIOS *insituMPI* reader → Rdr-proc adaptor: Data passing by address → Data compressor: Lossless compression; Output through IO

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CPU-based Nek5000 with Lossy and Lossless Data Compression

(with maximum allowed error $\varepsilon = 10^{-2}$ and compression ratio $c = 98\%$)

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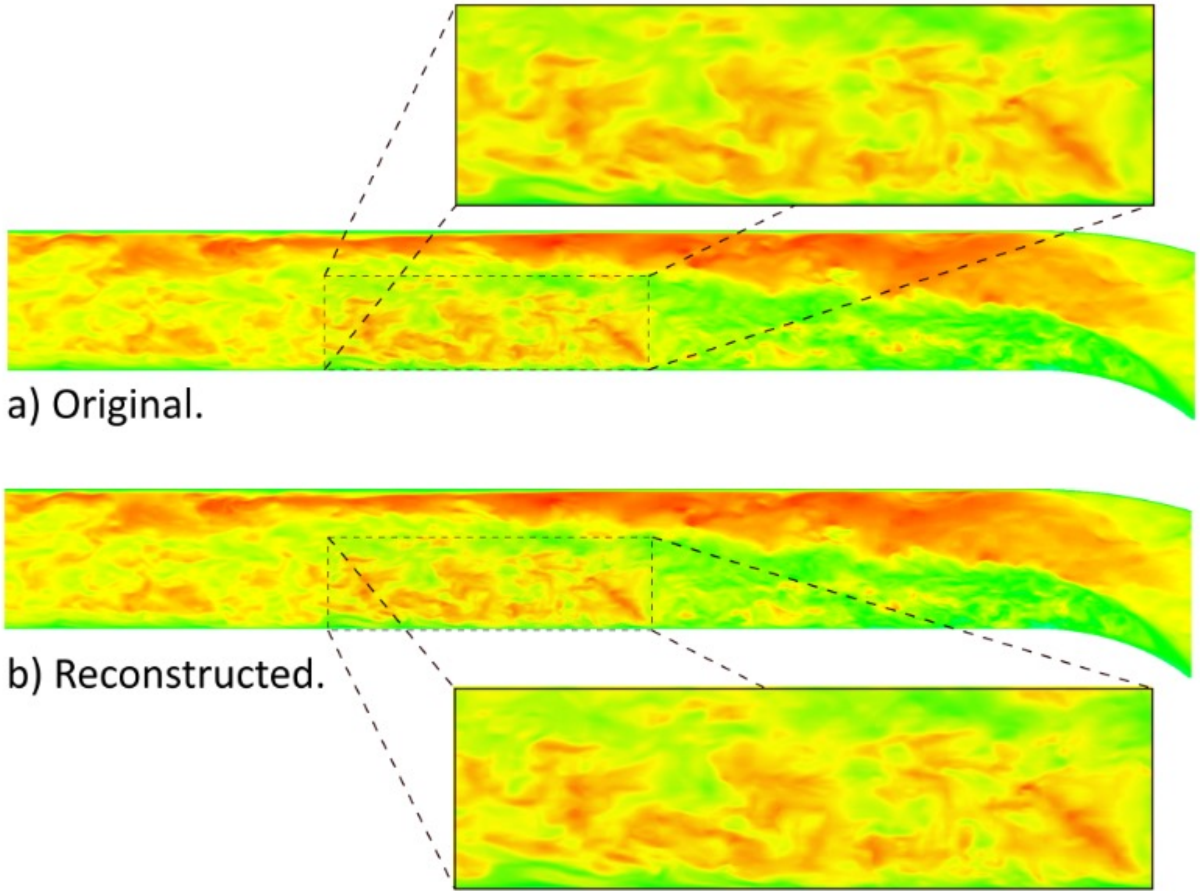

1: Slice of the velocity magnitude downstream from the bent section. a) is the original data set, while b) is the reconstruction of a field compressed with a maximum allowed error of 10^{-2}. 2: RMSE of a slice of the 3D field for a maximum allowed error of 10^{-2}. The error is shown per spectral element.

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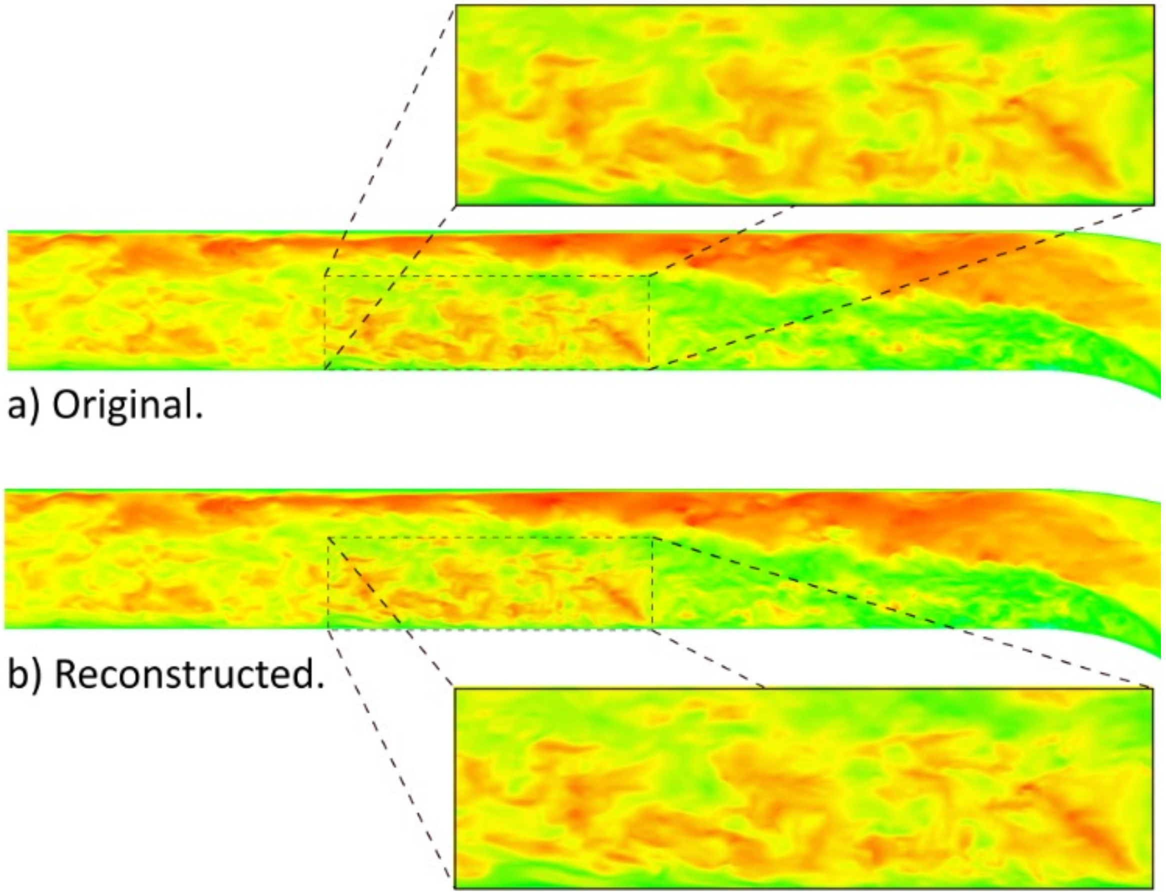

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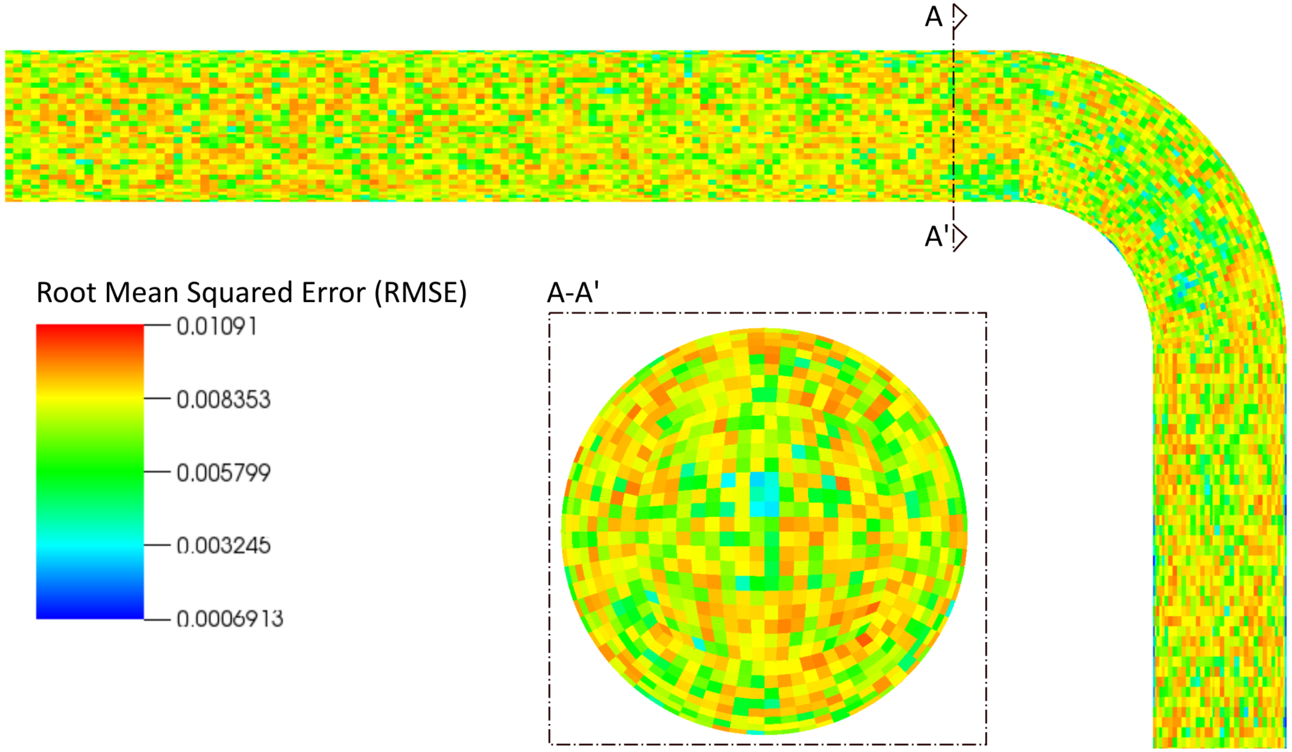

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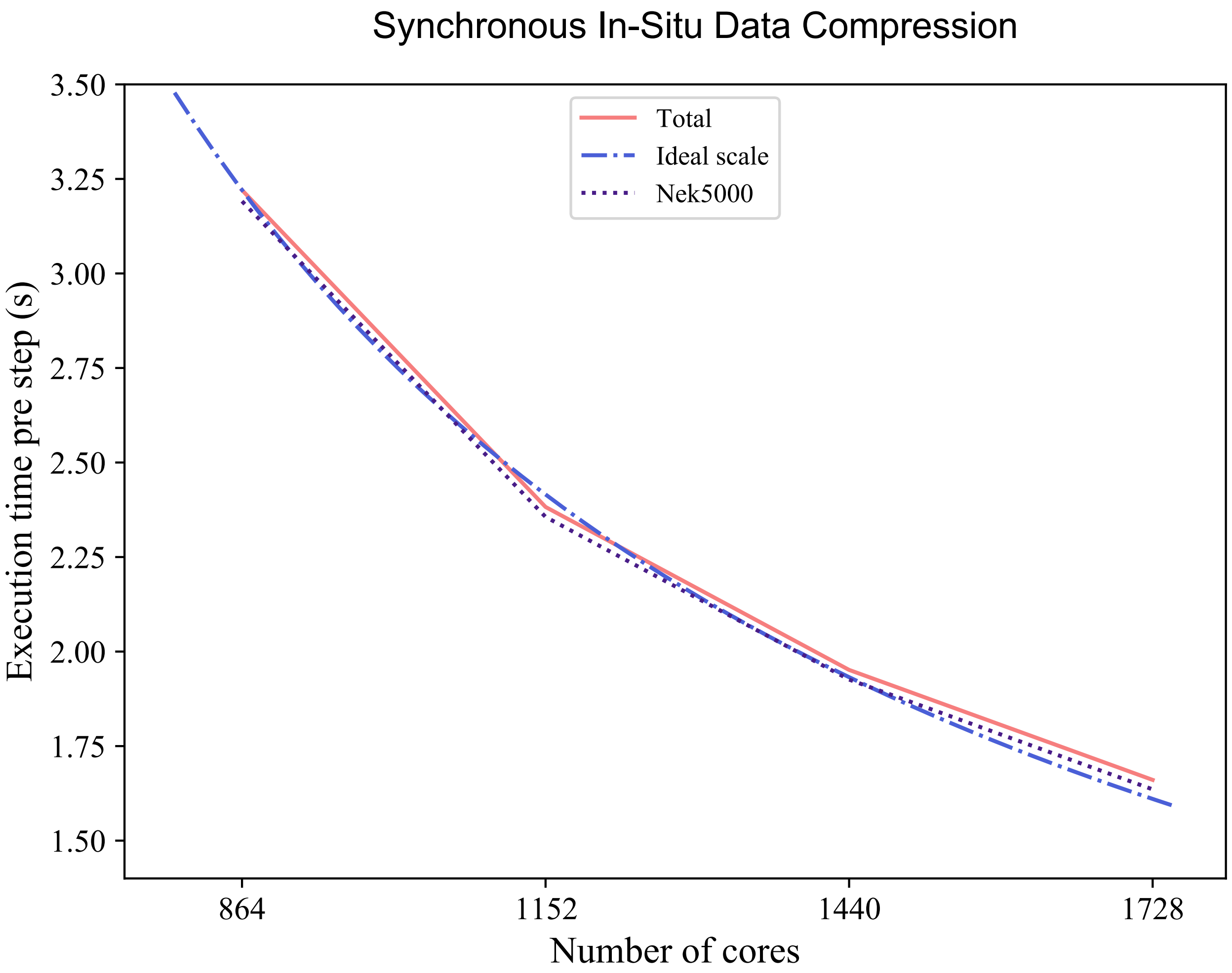
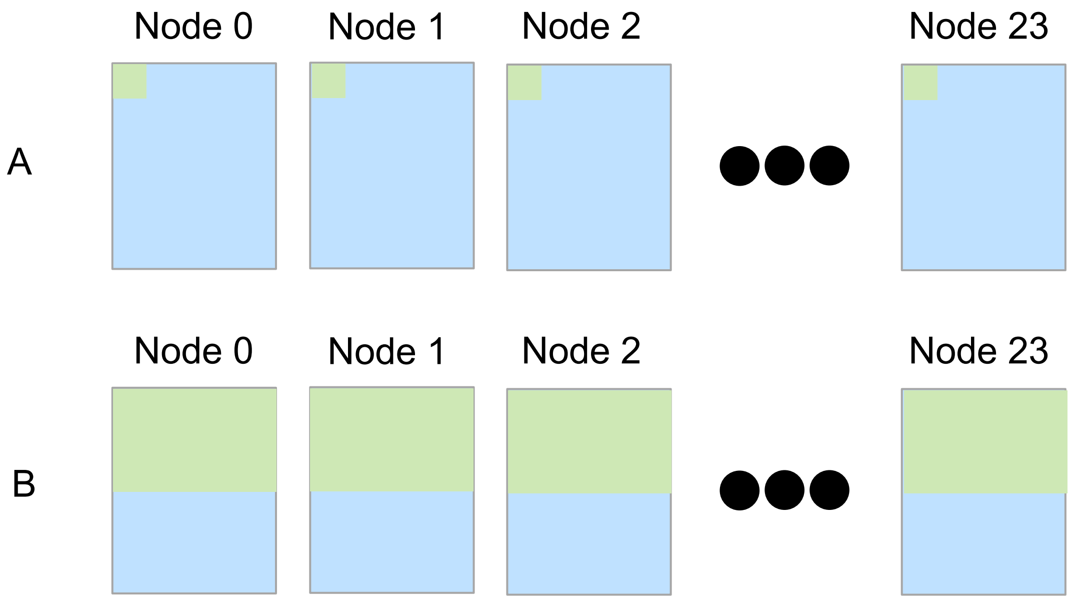


1: execution time of Nek5000 with synchronous in-situ compression with lossy compression maximum allowed error ε = 10^{-2} on Raven supercomputer (left) and hybrid in-situ compression with lossy compression maximum allowed error ε = 10^{-2} on 24 Raven nodes (right).

CPU-based Nek5000 with Synchronous and Hybrid In-Situ Data Compression

(with maximum allowed error $\varepsilon = 10^{-2}$ and compression ratio $c = 98\%$)



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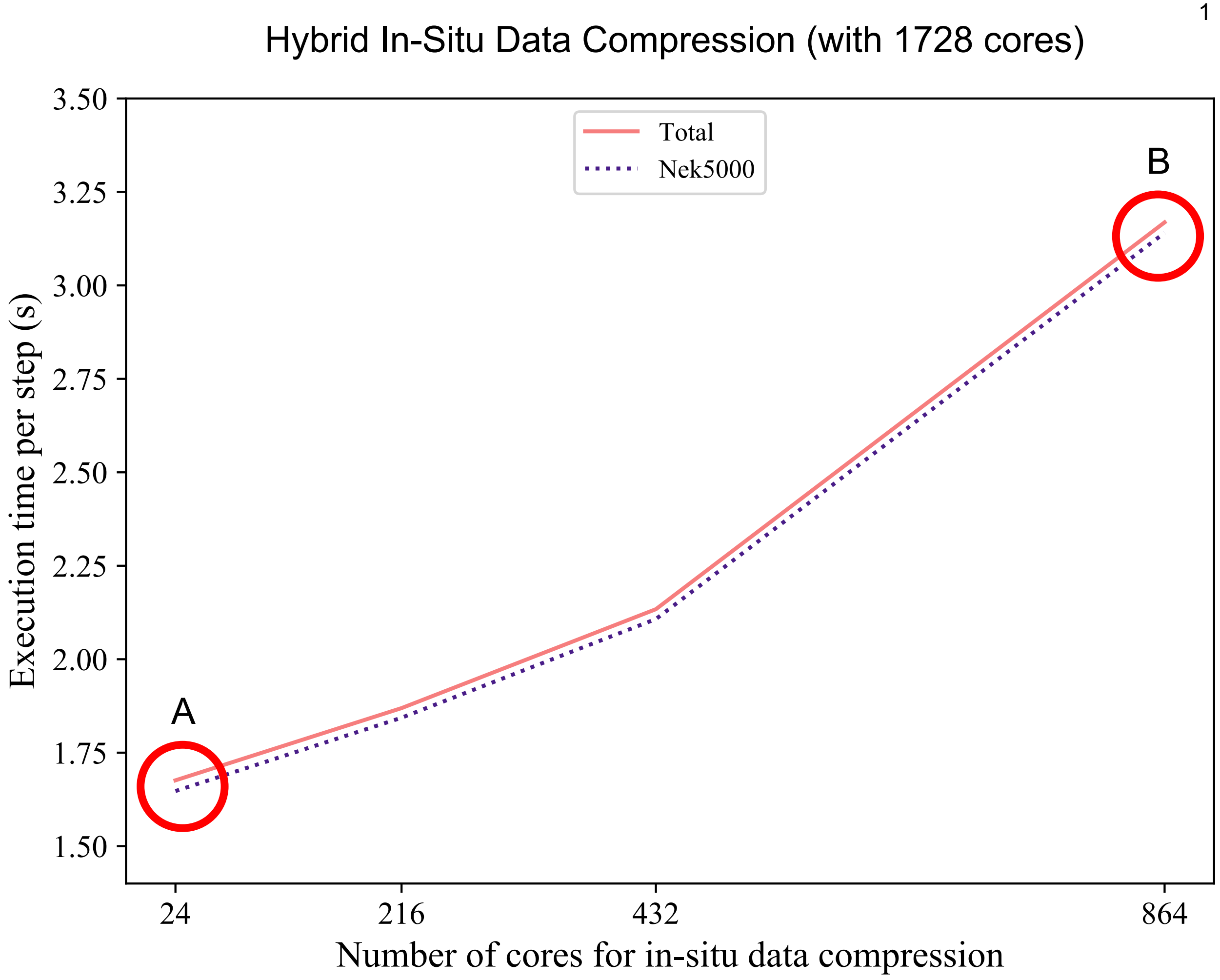

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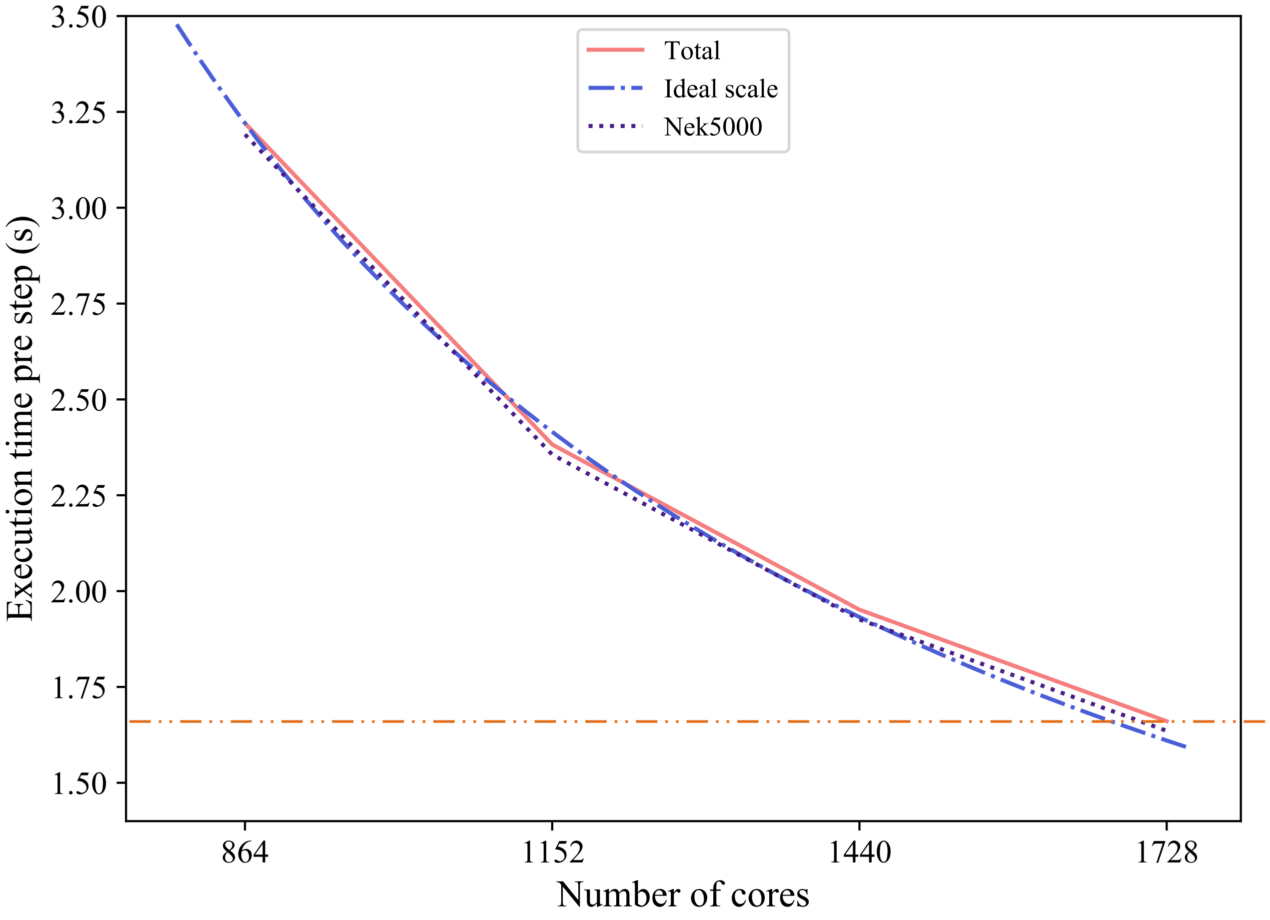
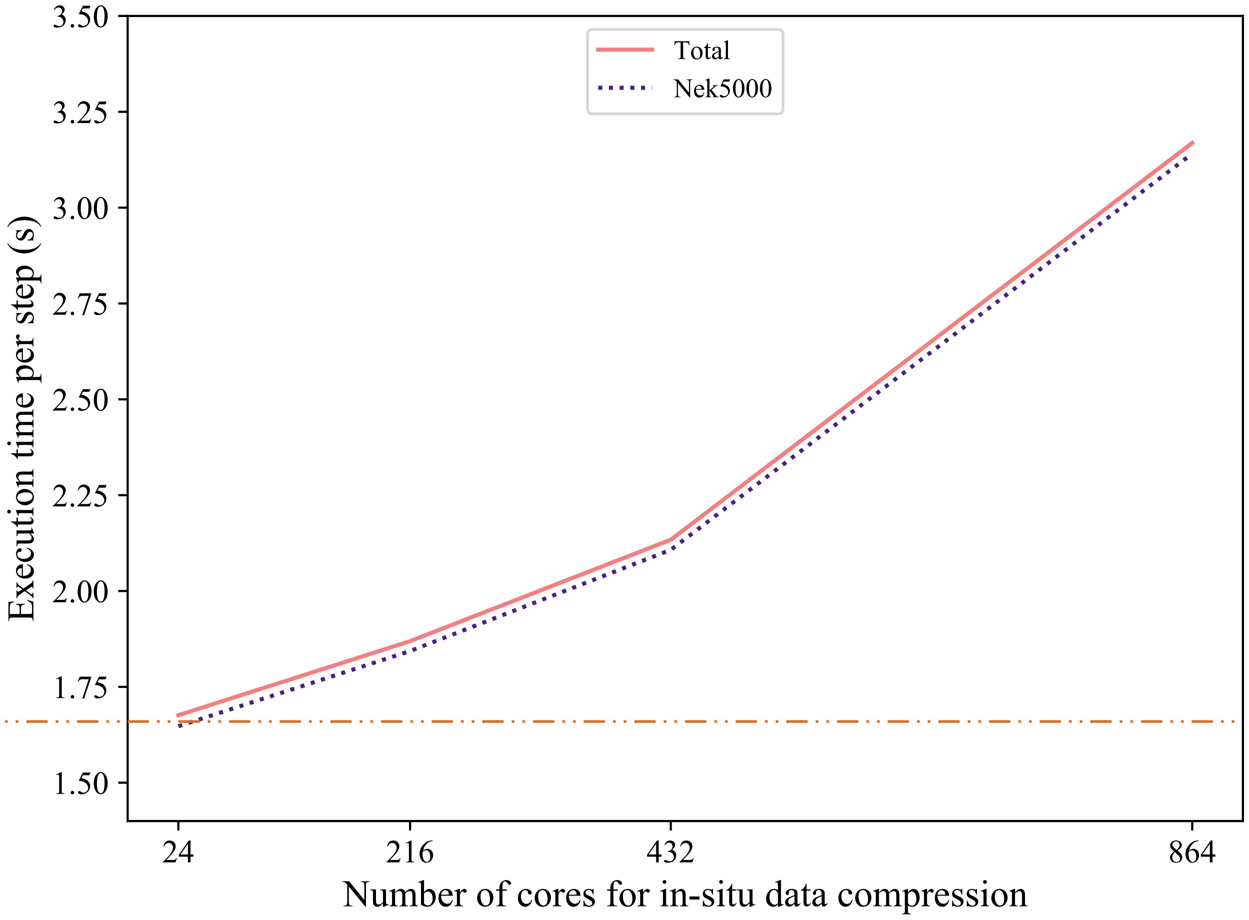
[1]

Synchronous In-Situ Data Compression

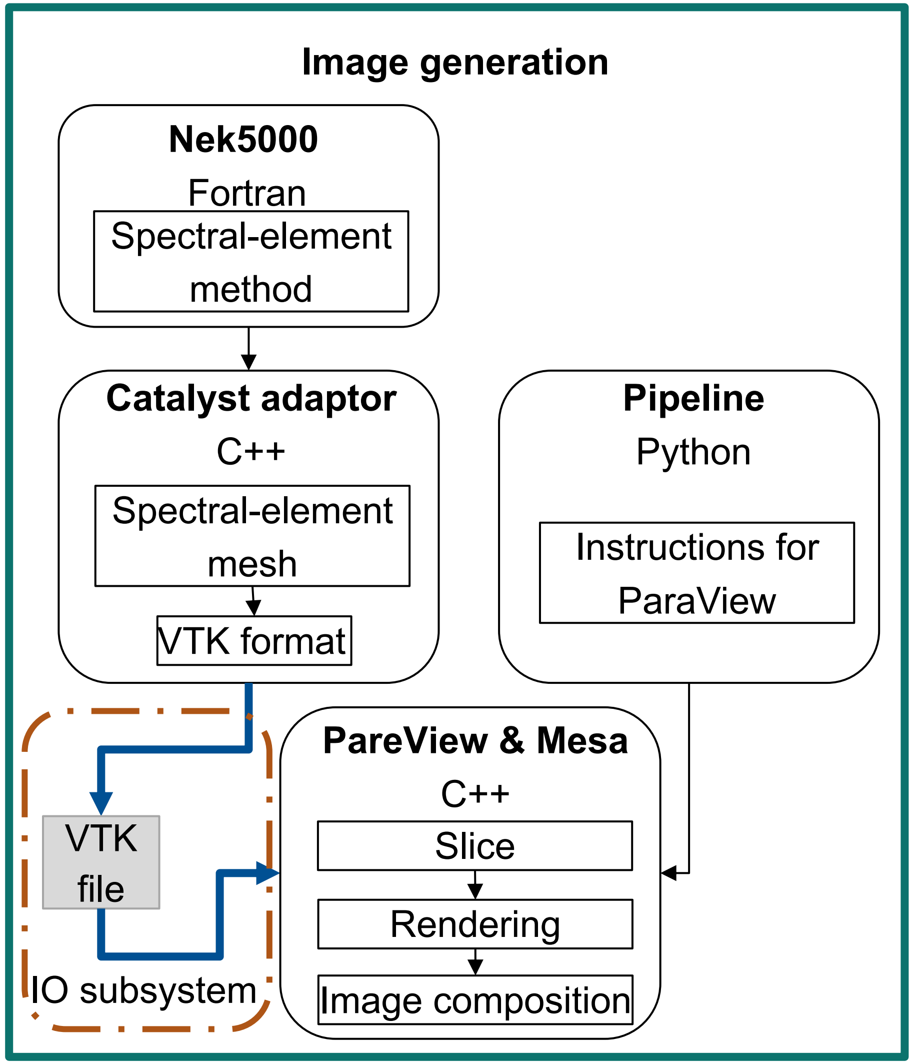


Hybrid In-Situ Data Compression (with 1728 cores)



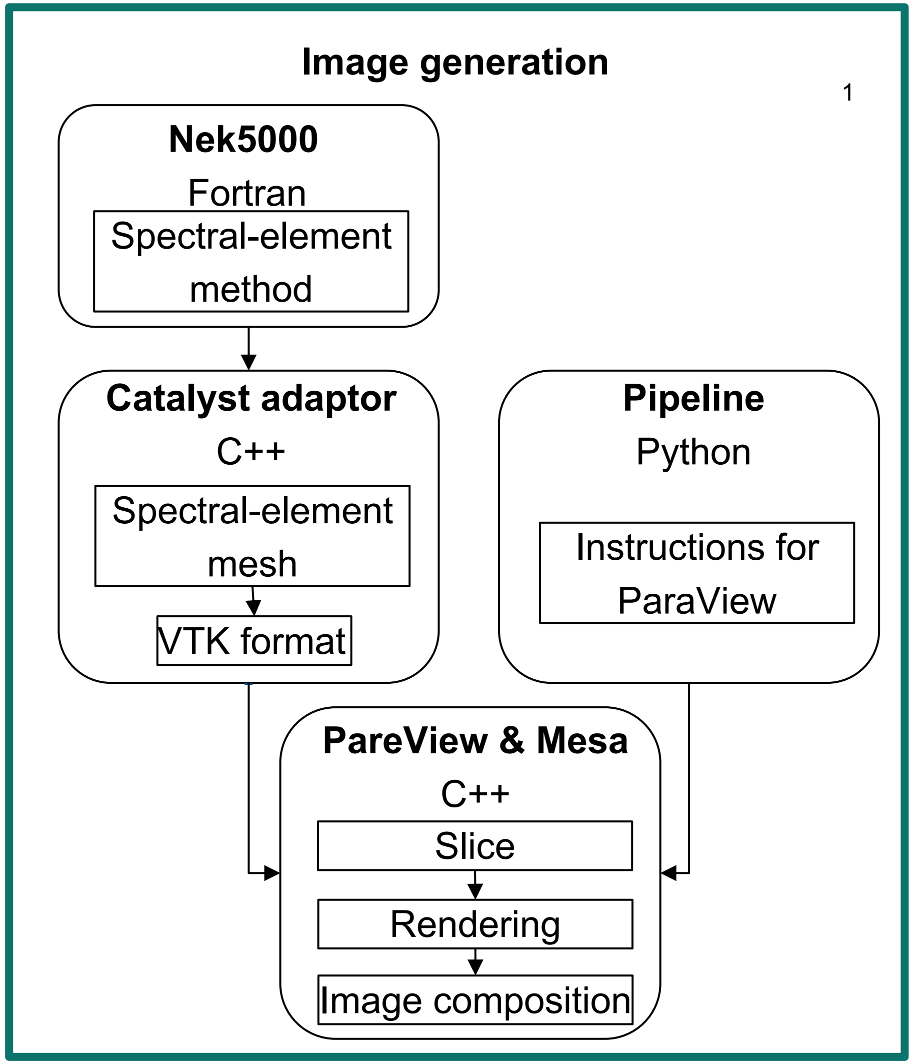
1: execution time of Nek5000 with synchronous in-situ compression with lossy compression maximum allowed error ε = 10^{-2} on Raven supercomputer (left) and hybrid in-situ compression with lossy compression maximum allowed error ε = 10^{-2} on 24 Raven nodes (right).

Use Case: Image Generation with ParaView/Catalyst



1: Original from "M. Atzori, W. Ko¨pp, S. W. Chien, D. Massaro, F. Mallor, A. Peplinski, M. Rezaei, N. Jansson, S. Markidis, R. Vinuesa et al., "In situ visualization of large-scale turbulence simulations in nek5000 with paraview catalyst," The Journal of Supercomputing, vol. 78, no. 3, pp. 3605–3620, 2022."

Use Case: Image Generation with ParaView/Catalyst



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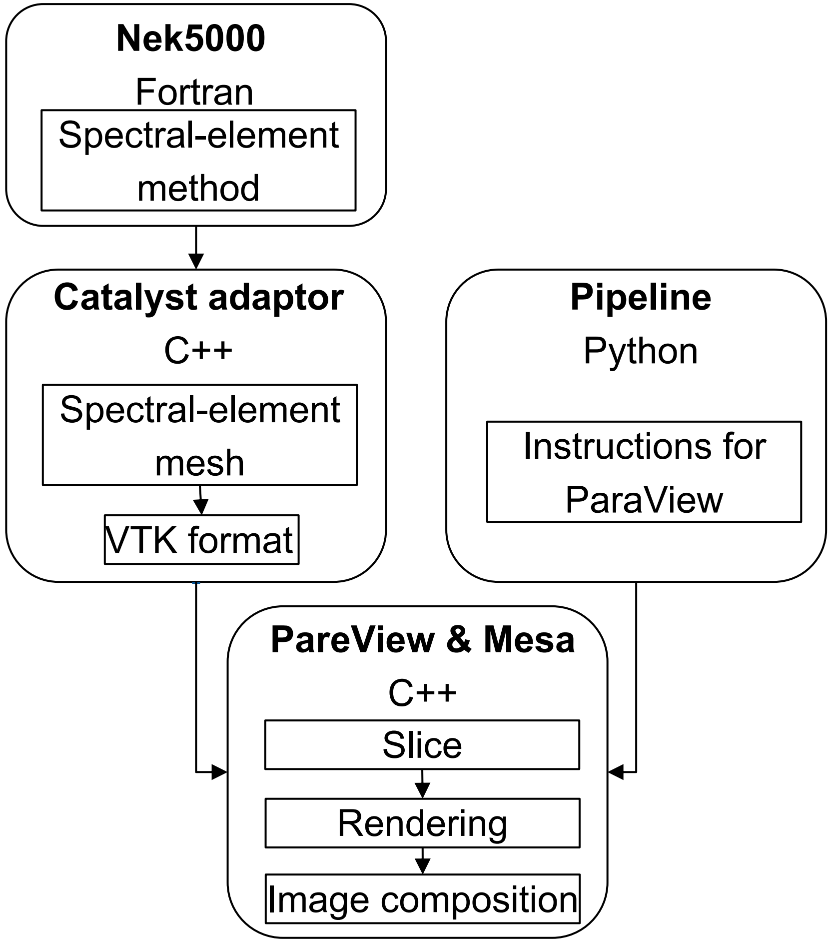
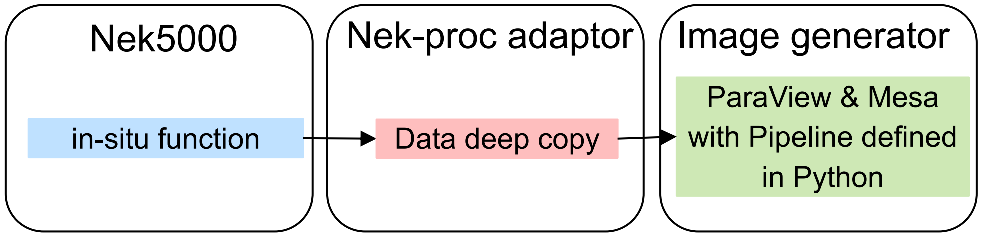
Use Case: Image Generation with ParaView/Catalyst

Image generation [1]



In-situ approach

- Nek5000 with synchronous image generation:



Fortran functions

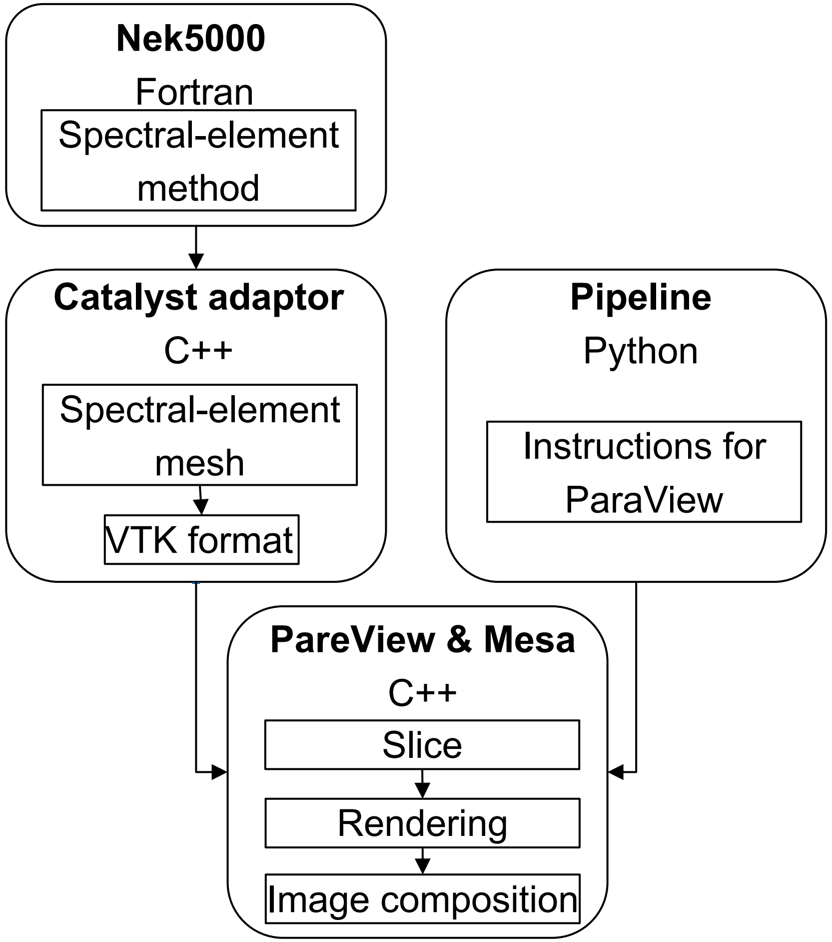
C/C++ functions called in Fortran

C++ functions

1: Original from "M. Atzori, W. Ko¨pp, S. W. Chien, D. Massaro, F. Mallor, A. Peplinski, M. Rezaei, N. Jansson, S. Markidis, R. Vinuesa et al., "In situ visualization of large-scale turbulence simulations in nek5000 with paraview catalyst," The Journal of Supercomputing, vol. 78, no. 3, pp. 3605–3620, 2022."

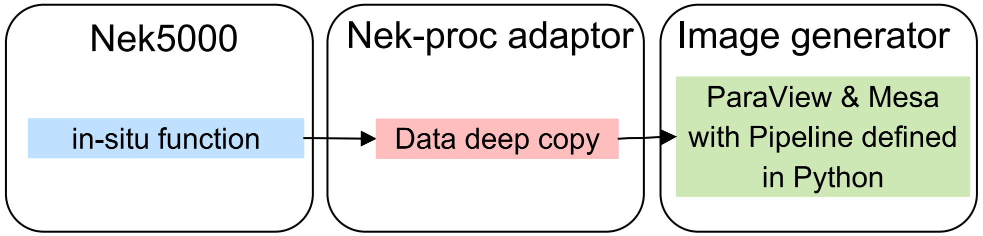
Use Case: Image Generation with ParaView/Catalyst

Image generation [1]

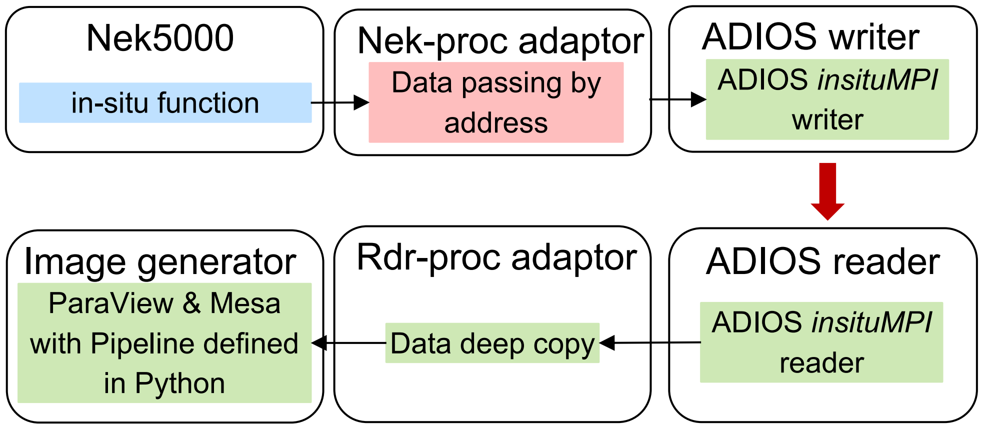


In-situ approach

- Nek5000 with synchronous image generation:



- Nek5000 with asynchronous image generation:



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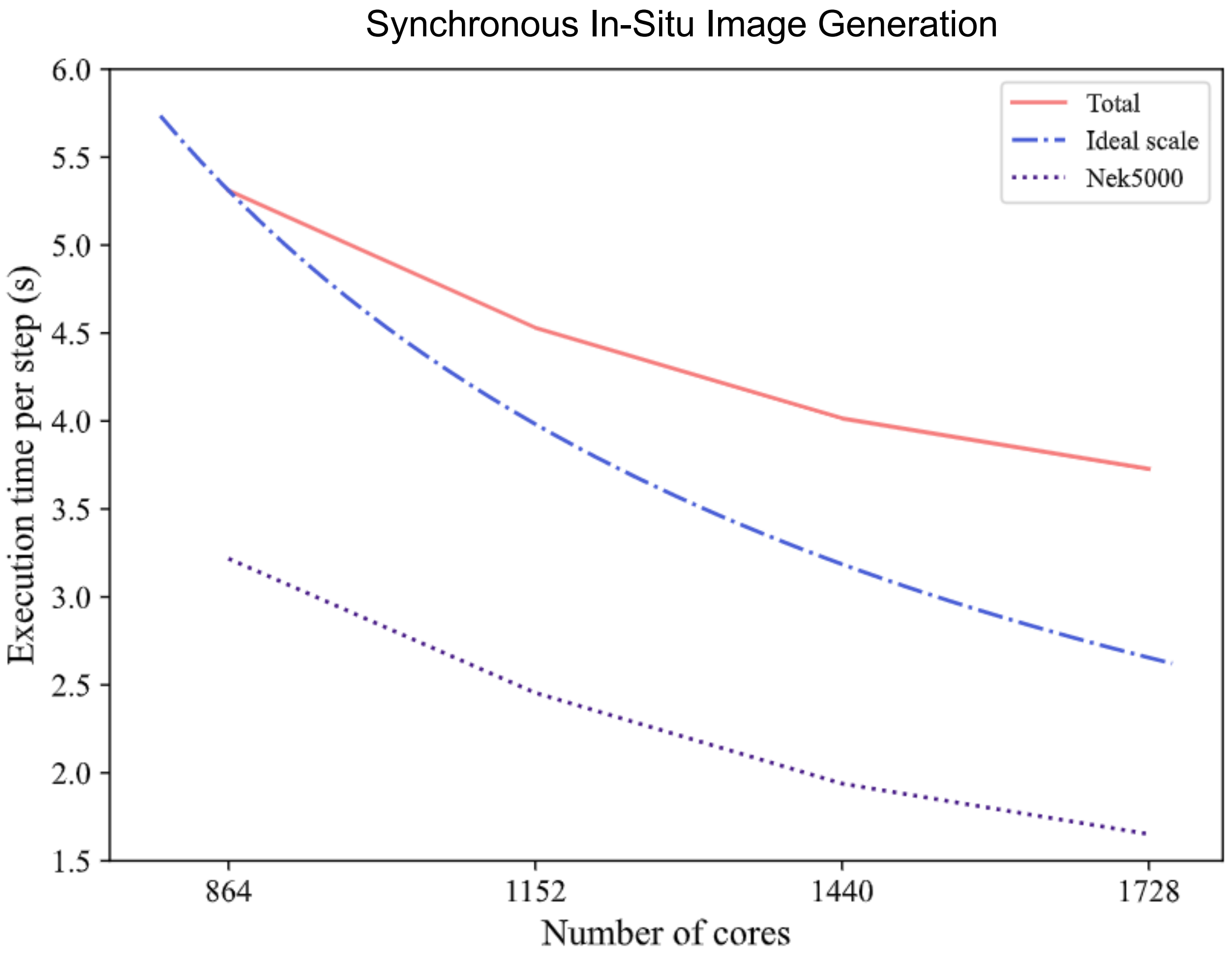
CPU-based Nek5000 with Synchronous and Asynchronous Image Generation

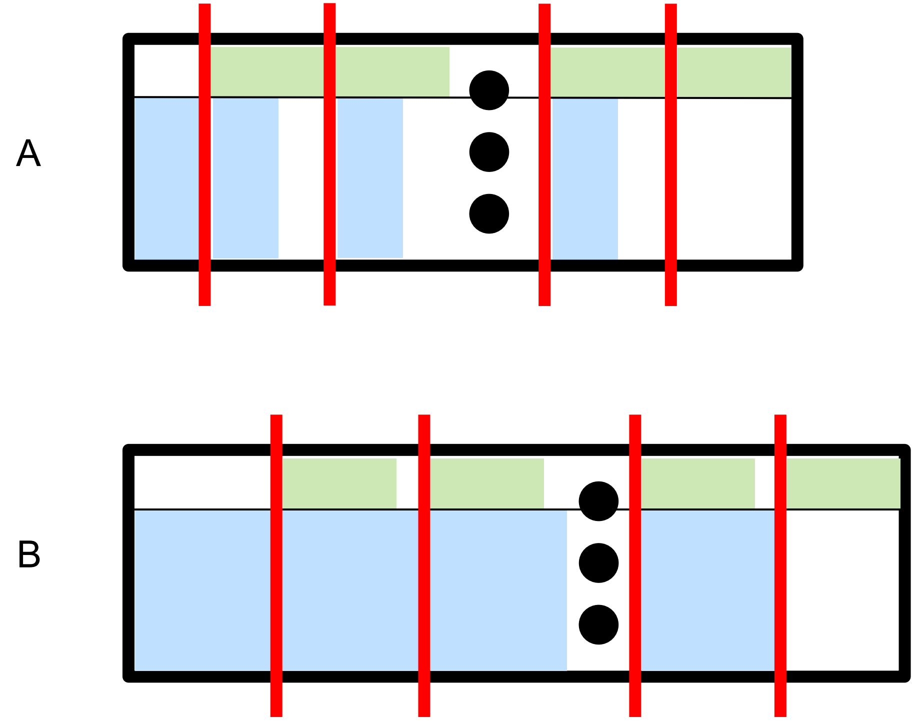
(45G VTK file for one image avoided) 1



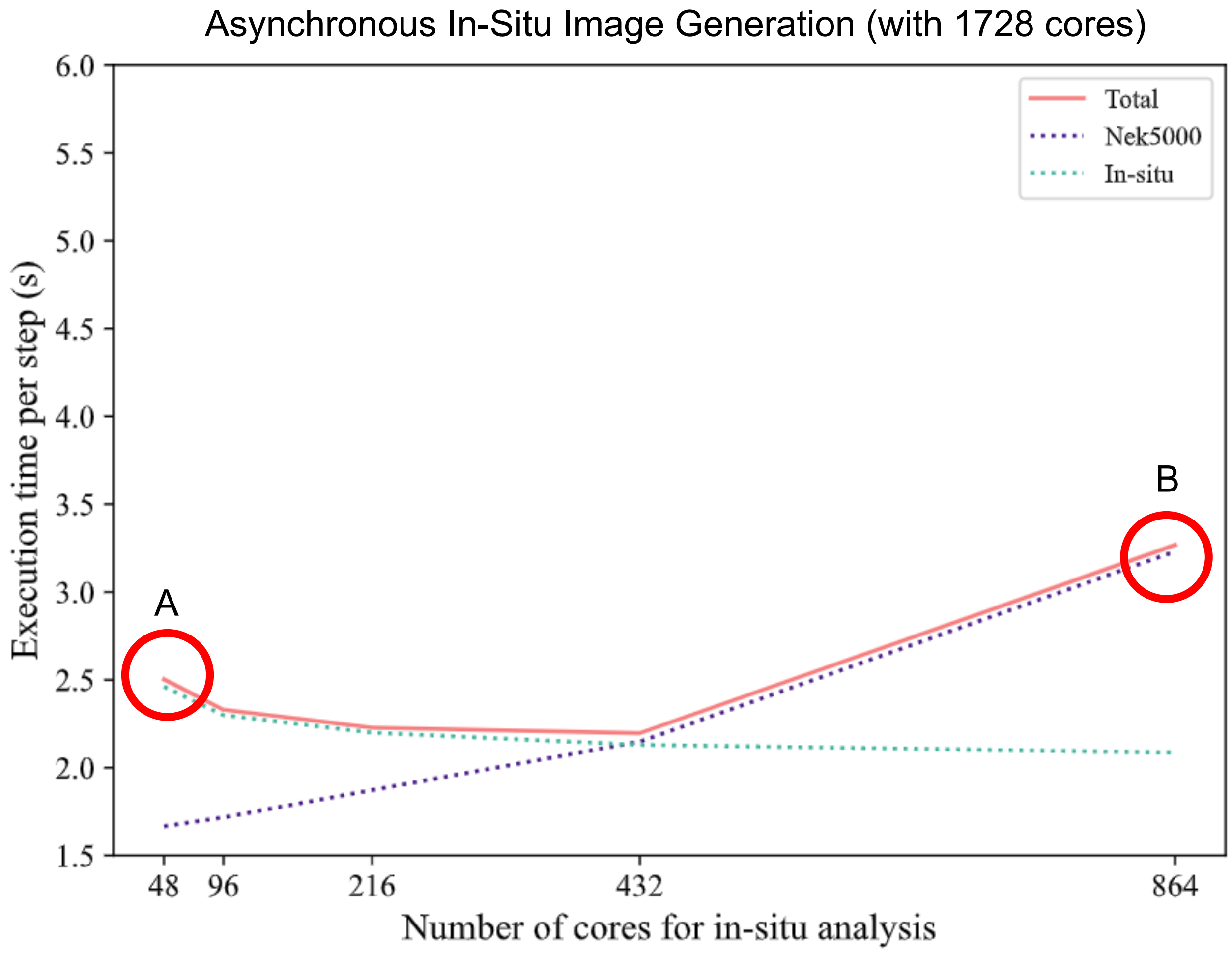
1: Execution time of Nek5000 with synchronous in-situ image generation every two steps on Raven supercomputer (left) and asynchronous in-situ image generation every two steps on 24 Raven nodes (right).

CPU-based Nek5000 with Synchronous and Asynchronous Image Generation

(45G VTK file for one image avoided)



[1]



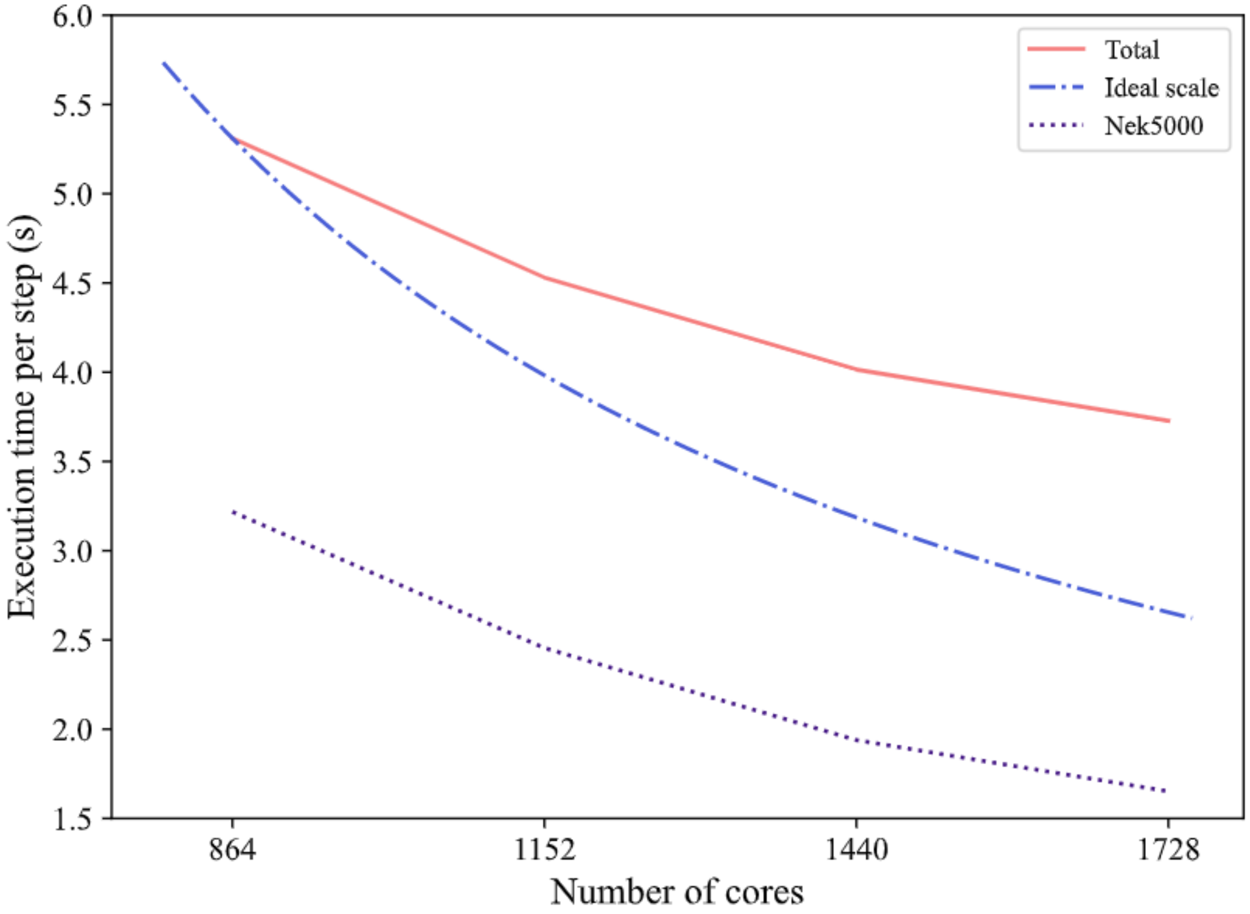
1: Execution time of Nek5000 with synchronous in-situ image generation every two steps on Raven supercomputer (left) and asynchronous in-situ image generation every two steps on 24 Raven nodes (right).

CPU-based Nek5000 with Synchronous and Asynchronous Image Generation

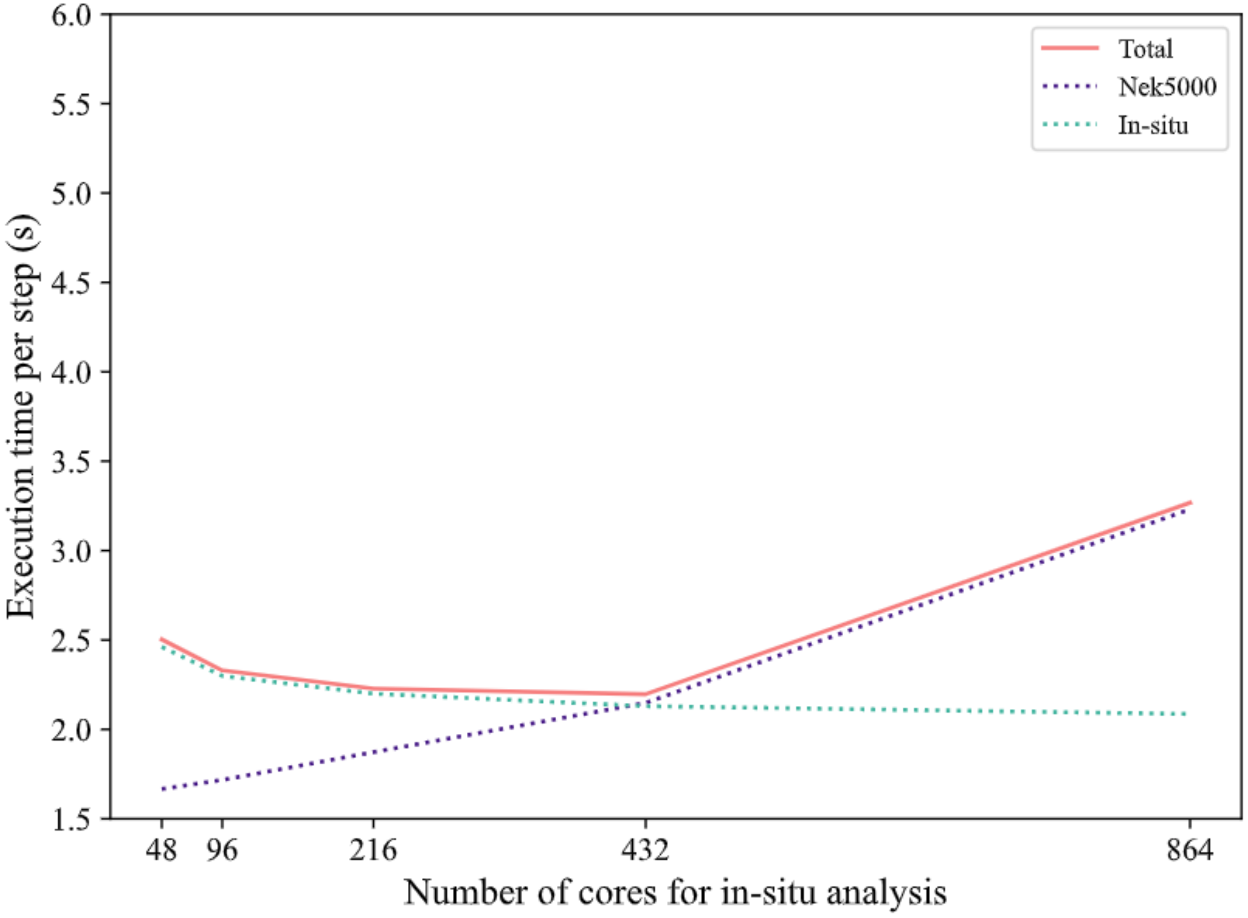
(45G VTK file for one image avoided)

1

Synchronous In-Situ Image Generation



Asynchronous In-Situ Image Generation (with 1728 cores)



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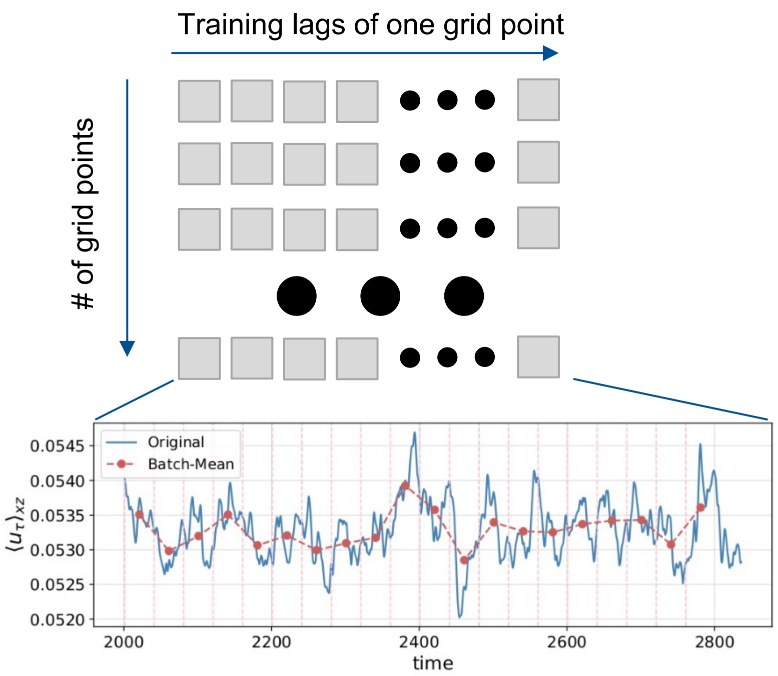
Use Case: Uncertainty Quantification

Uncertainty Quantification



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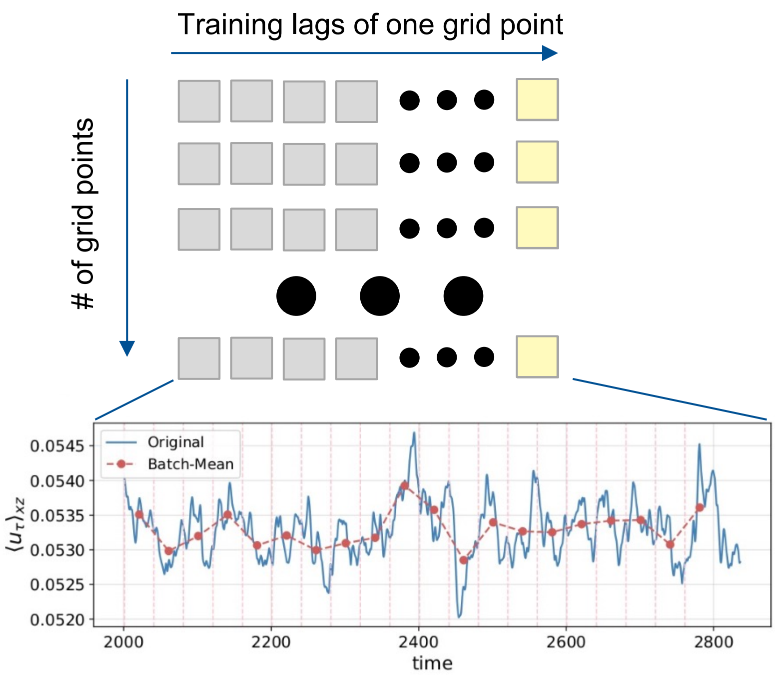
Use Case: Uncertainty Quantification

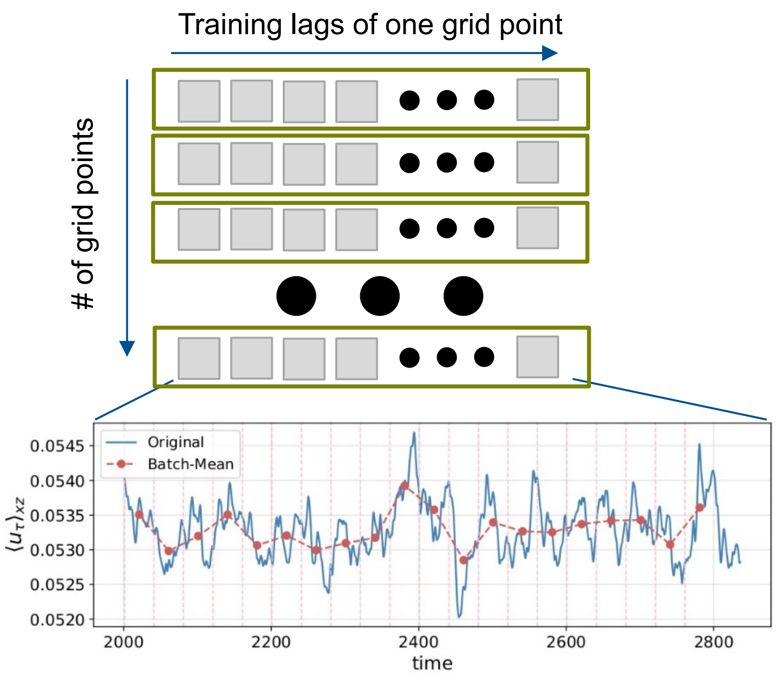
Uncertainty Quantification



Frequent training lag update

Use Case: Uncertainty Quantification

Uncertainty Quantification

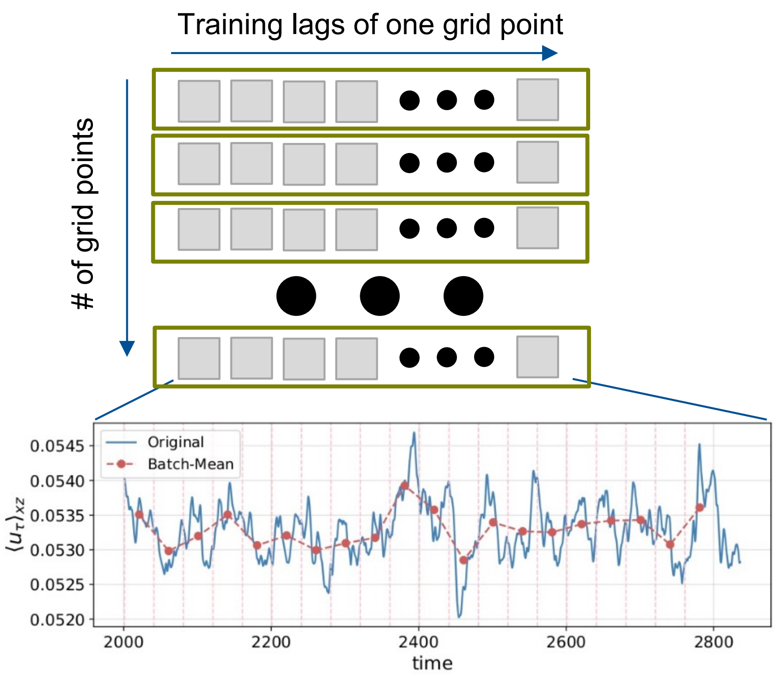


Frequent training lag update

Expensive model and uncertainty update

Use Case: Uncertainty Quantification

Uncertainty Quantification

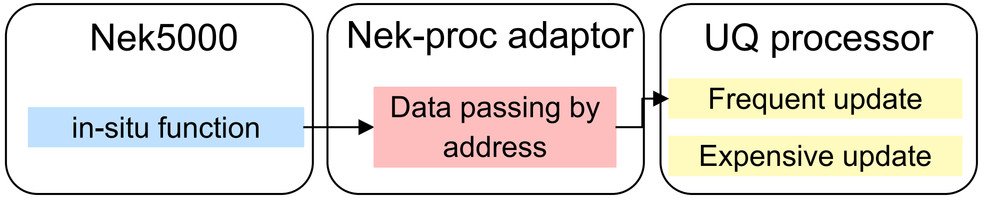


Frequent training lag update

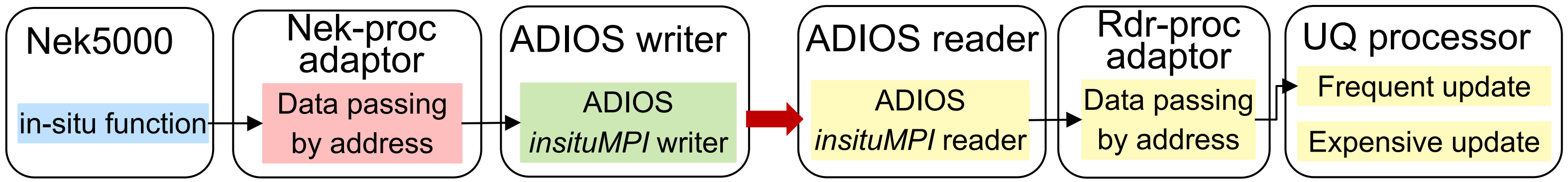
Expensive model and uncertainty update

In-situ approach

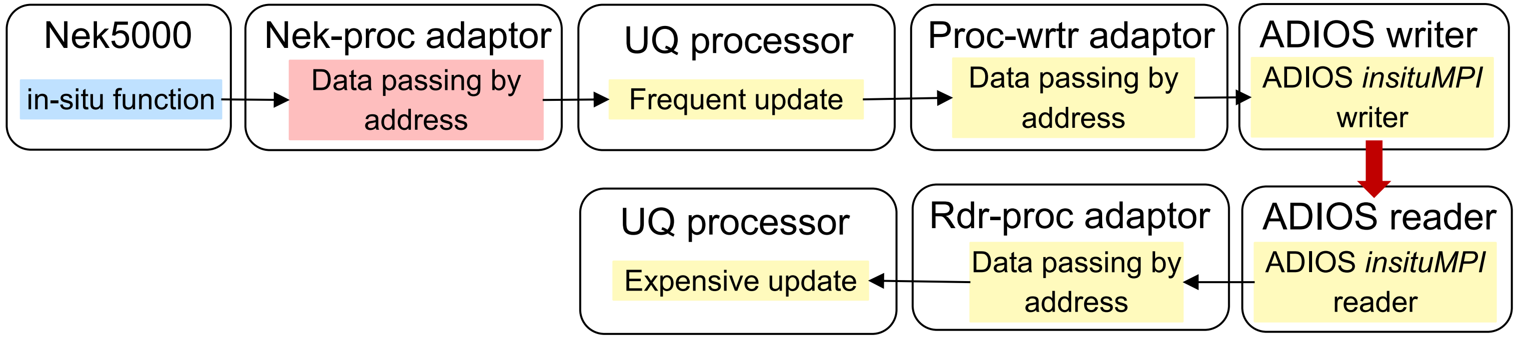
- Nek5000 with synchronous uncertainty quantification:



- Nek5000 with asynchronous uncertainty quantification:



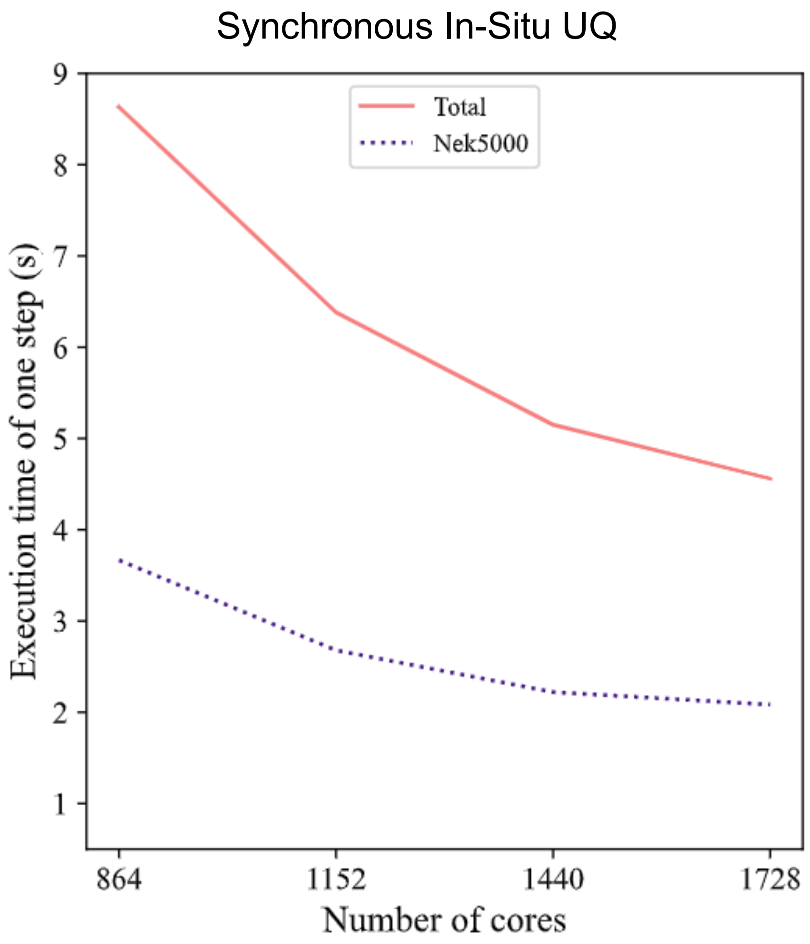
- Nek5000 with hybrid uncertainty quantification:



Fortran functions | C/C++ functions called in Fortran | Python functions | C++ functions

CPU-based Nek5000 with In-Situ Uncertainty Quantification (UQ)

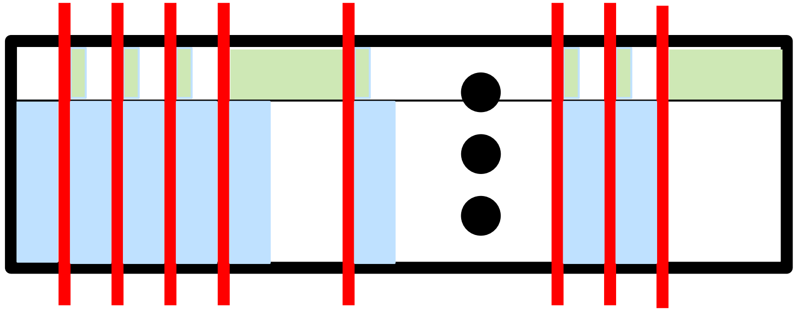
1



1: Execution time of Nek5000 with synchronous in-situ uncertainty quantification (left), asynchronous in-situ uncertainty quantification on 24 Raven nodes (middle) and hybrid in-situ uncertainty quantification on 24 Raven nodes (right).

CPU-based Nek5000 with In-Situ Uncertainty Quantification (UQ)

Asynchronous



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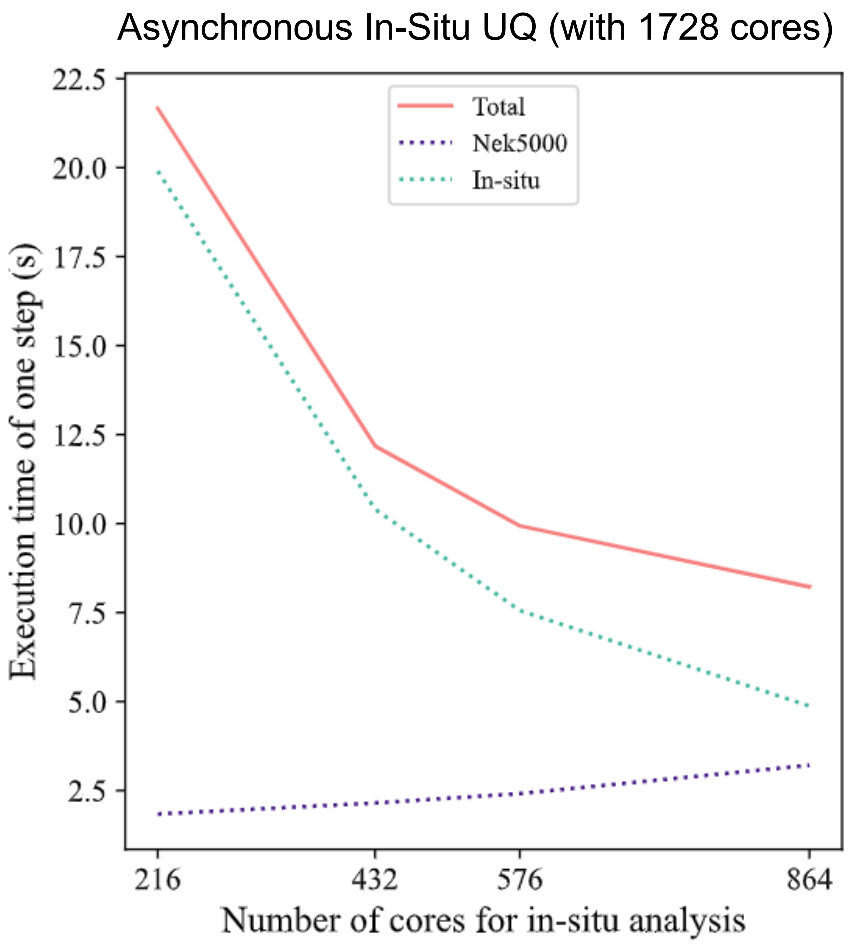

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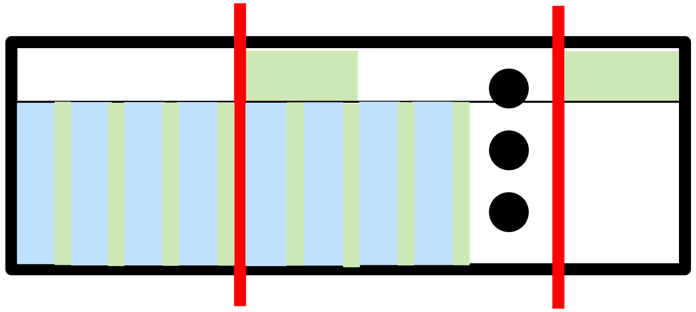
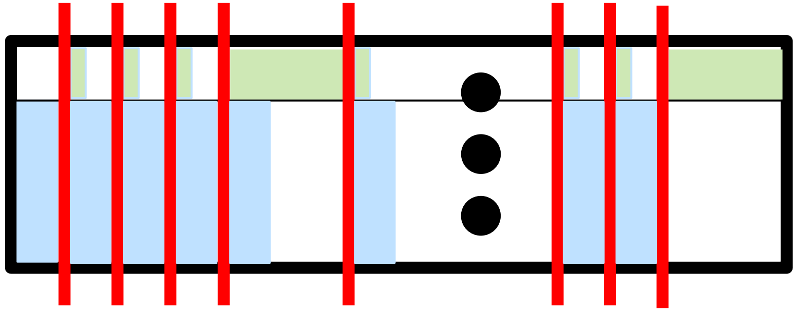
CPU-based Nek5000 with In-Situ Uncertainty Quantification (UQ)

[1]

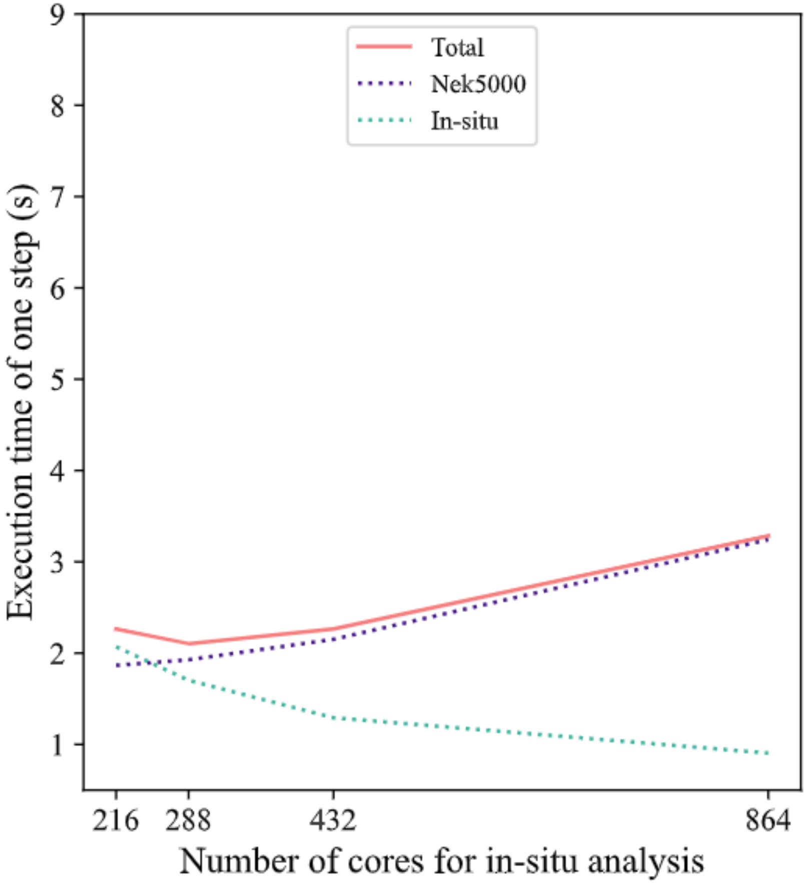
Hybrid



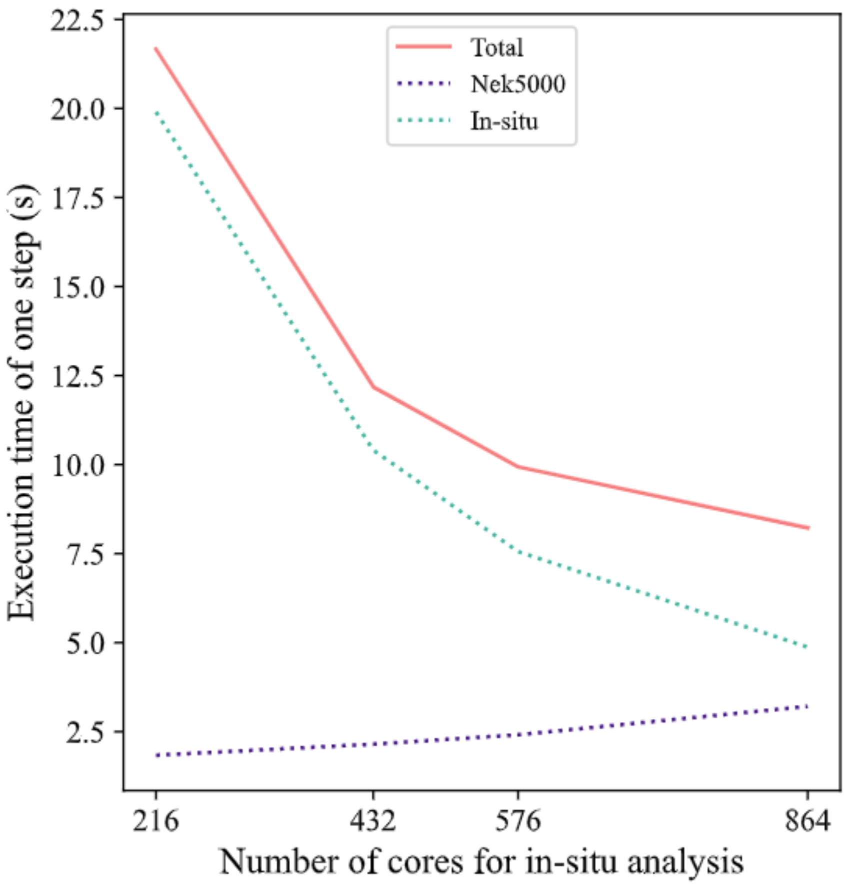
Asynchronous



Hybrid In-Situ UQ (with 1728 cores)



Asynchronous In-Situ UQ (with 1728 cores)



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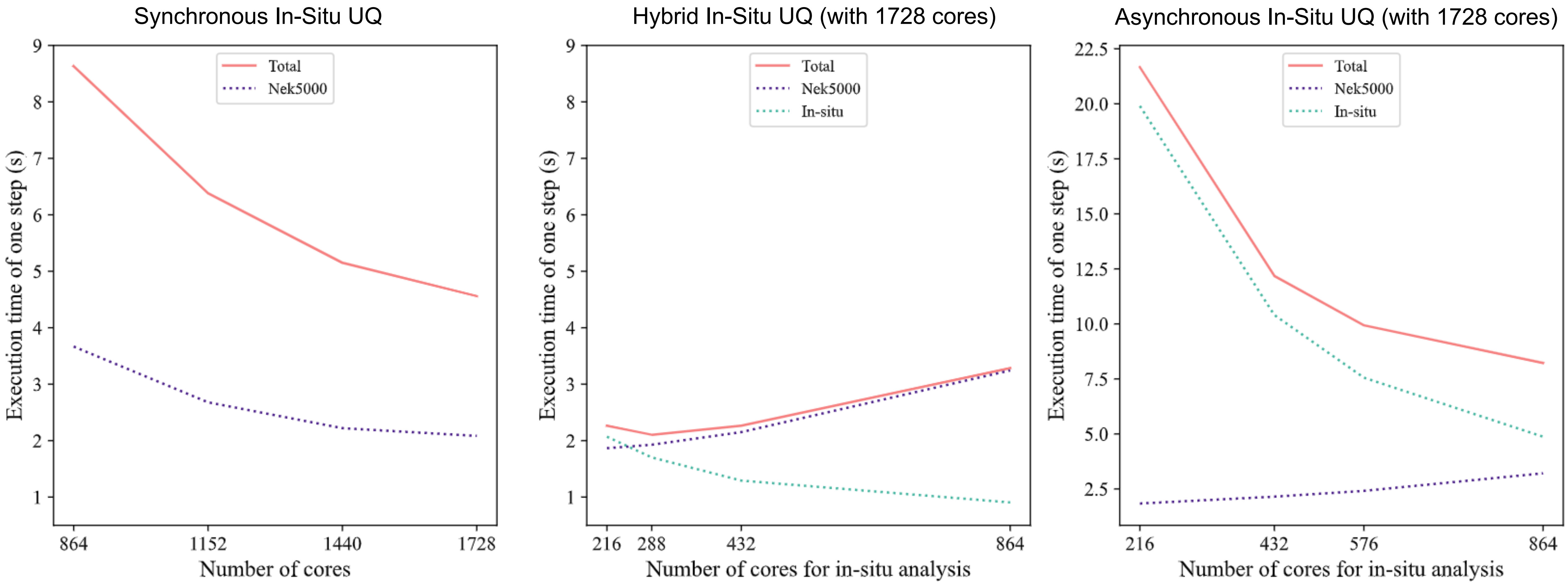
CPU-based Nek5000 with In-Situ Uncertainty Quantification (UQ)

[1]



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Summary

Approaches

- The synchronous in-situ approach: simulation waits until data process finished
- The asynchronous in-situ approach: simulation sends data to separate computing resources and continues, while data are processed concurrently
- The hybrid in-situ approach: the first part of data process is synchronous; the second part of data process is asynchronous.

Case study

- The synchronous in-situ data compression is preferred because of its low computational cost.
- 45GB VTK file for each in-situ step is avoided by in-situ techniques.
- The asynchronous in-situ image generation is preferred because of the optimal computing resource allocation to minimize the overhead from the MPI collective communication.
- The hybrid in-situ uncertainty quantification is preferred because of the more efficient computing resources usage

Outlook

- In-situ tasks to GPU based simulation
- In-situ tasks to exasacle simulation
- Performance model of in-situ techniques
- Dynamic computing resources allocation

HORIZON 2020
EuroHPC Joint Undertaking
This project has received funding from the European Union's Horizon 2020 JTI-EuroHPC research and innovation programme, with grant Agreement number: 956748 — ADMIRE — H2020-JTI-EuroHPC-2019-1

Thank you for your attention!

Understanding the Impact of Synchronous, Asynchronous, and Hybrid In-Situ Techniques in Computational Fluid Dynamics Applications

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