

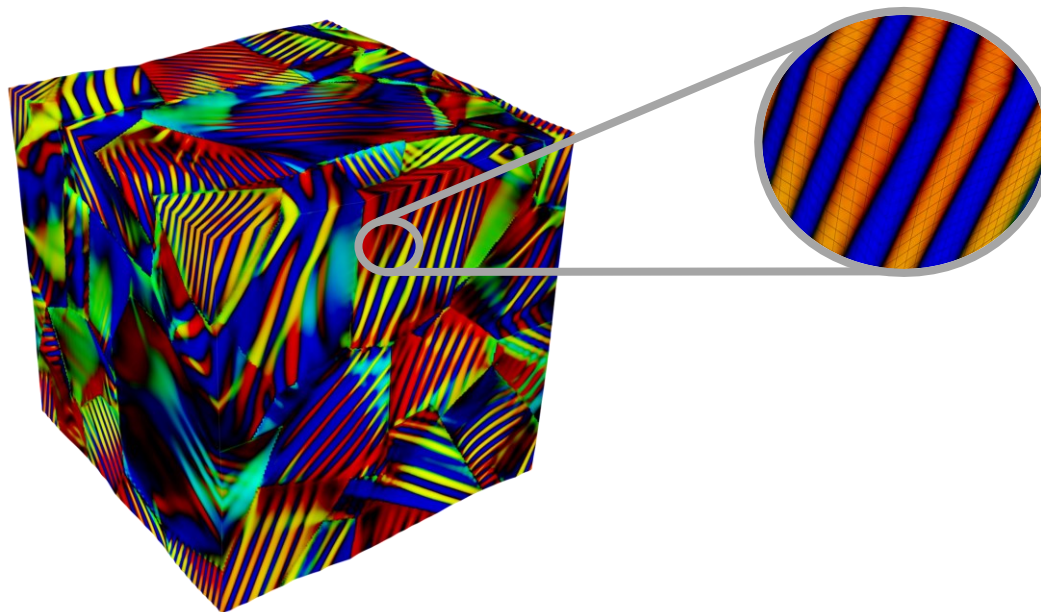


PROGRAMME
DE RECHERCHE
NUMÉRIQUE
POUR L'EXASCALE

Restitution Brainstorming Coddex, Dyablo version in situ

Laurent Colombet, Arnaud Durocher

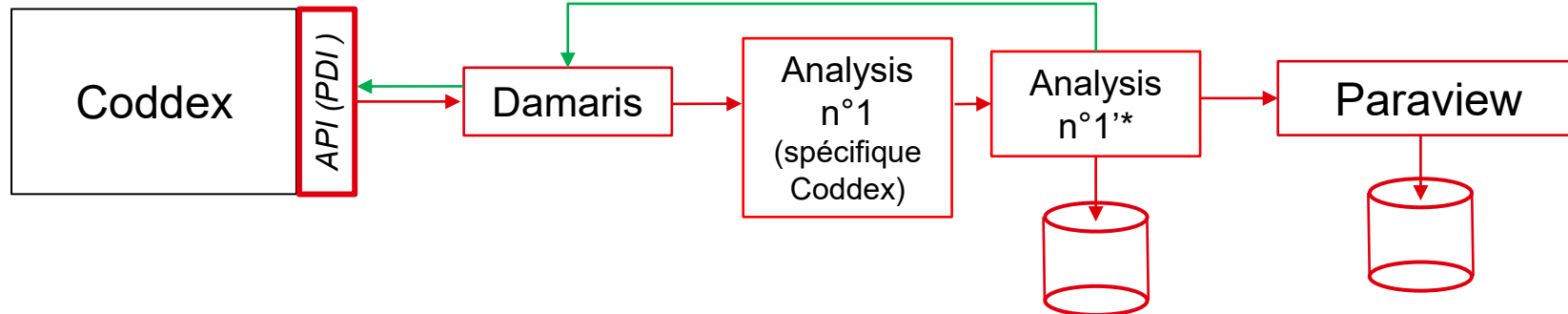
Coddex



WP1 :

- **Develop an I/O analysis component (I/O orchestrator) to ensure data consistency and manage the in-memory data pipelining problem**
 - Anyway, the in-situ infrastructure has to be in place first
 - Unsure about who is going to do this
 - It may be related to the work with Gysela? We need to think more about this

Automatic « Freeze » and « Release » not enough time to write to disk (e.g., temporary system freeze)

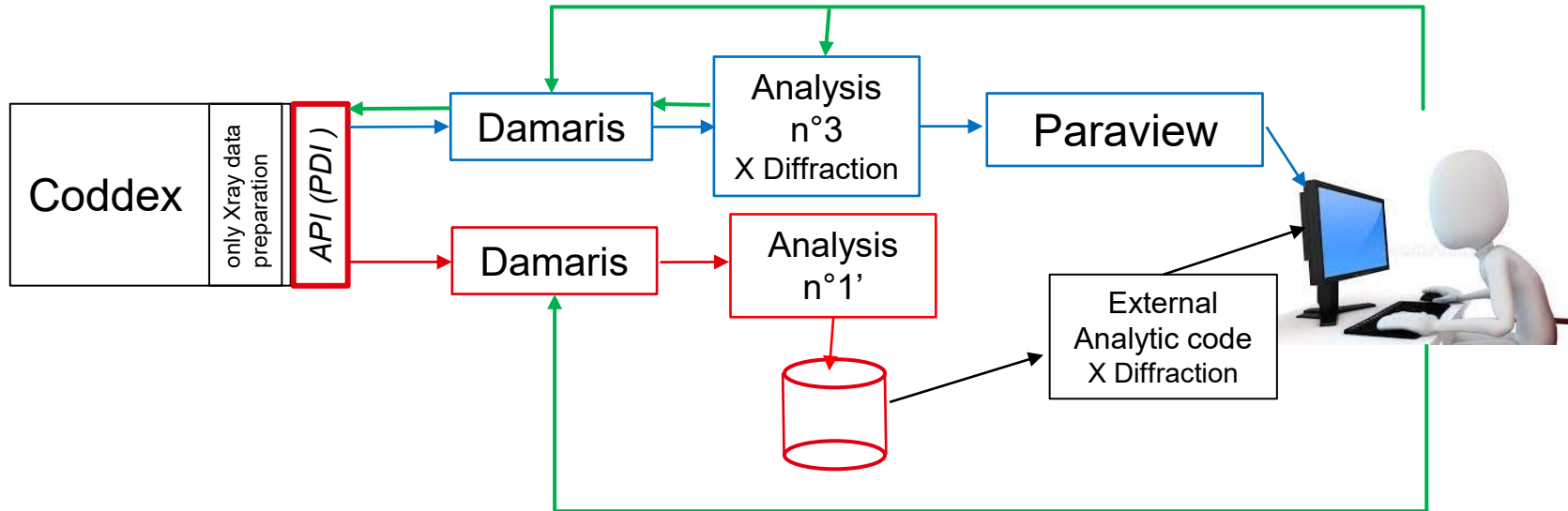


**analysis specific to IO management*

WP2 :

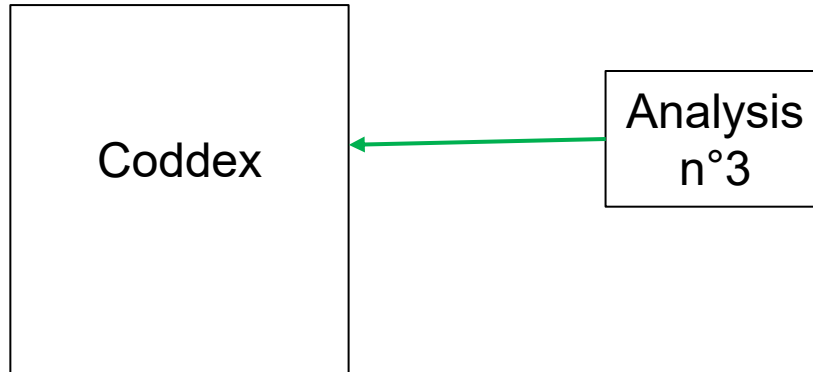
- When exploring results interactively in order to find the parameters for a method to be used in in situ analysis, is it possible to “freeze” the sending of data to this analysis?

« Freeze » sending data but Coddex (and other analytics) continue to run
or « Release » : resend data **with new parameters**



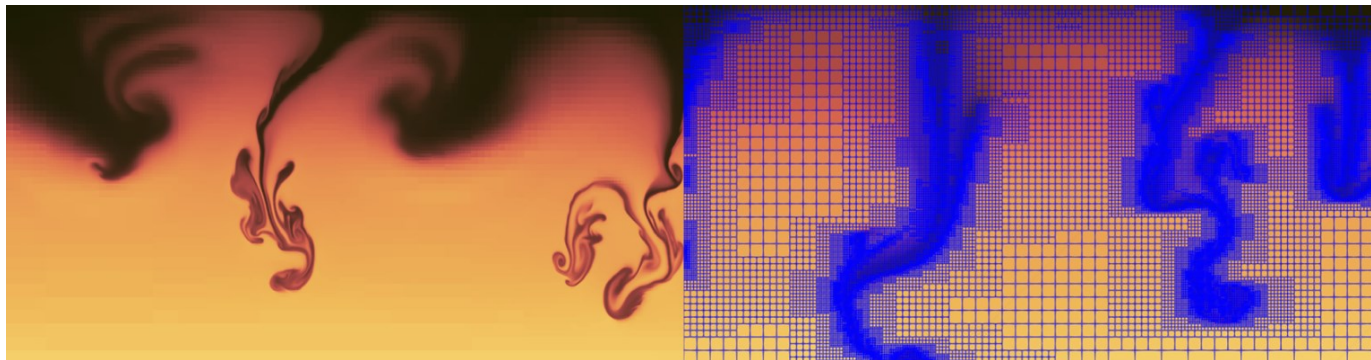
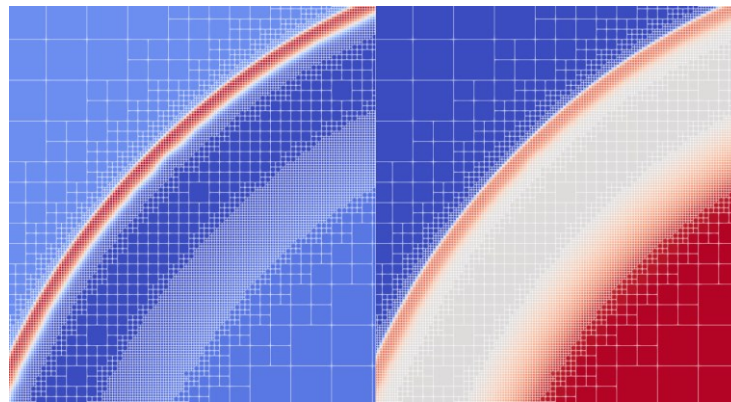
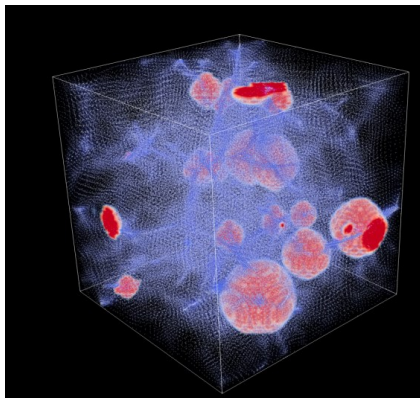
WP2 :

- From the Coddex code perspective, a priority for WP2 would be to develop the in situ scenario that allows an analysis to send feedback to the code.



WP3 :

- **How AI can “help” Coddex analyses:**
 - **Event Detection :**
 - Detecting phase transitions in a material, such as the α - γ transition in cerium
 - **Anomaly detection**
 - Help to find “non-physical” situation and trigger a specific response from Coddex
 - **Simulation-based inference (P1):**
 - Propose an initial relevant setting for the algorithm simulating X-ray diffraction
 - Learning from smaller scale simulations and generalize on larger ones



Develop new AMR data formats

Post-Doc financed by Exa-DoST

Currently in Dyablo

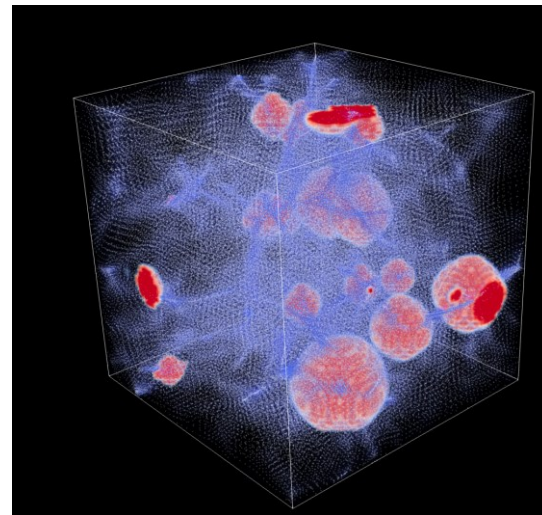
- Post-processing outputs use *Paraview Unstructured Mesh + HDF5*
 - Heavy geometry / connectivity (more disc space than actual data)
 - Slow post-processing
 - Large data loaded all at once through paraview

But makes nice images for small simulations

Wishlist for a new format dedicated to AMR

- Efficient storage of AMR grid (implicit geometry)
 - Allow efficient and fast post-processing with AMR
 - Leverage hierarchical structure (Level of detail, ...)
 - AMR-optimized algorithms (Slices, subdomains, ...)
 - Works for distributed simulations
 - Independent of simulation MPI parallelism
 - Load partial data (less RAM than full simulation)
 - Standardization : integrate with existing tools
- 18 month : nov. 2025 → 2027
 - AMR *data* format
 - Implementations : Dyablo (CEA), Samurai (Polytechnique)
 - Associated post-processing tools (?)

(few leads : Paraview HyperTreeGrid, yt, ...) **Exa-DoST expertise will be precious to help implementation**



Cosmology : 4 Mpc box with dark matter particles and ionization, image generated by paraview

Post-Doc : Sylvain JOUBE

General :

- **Collaborate through the post-doc (Financed through WP1)**
 - Co-design the data format with IO libraries / experts
 - Standardization/data format is specific to AMR : we probably have to do it on our own
 - Help him implement actual disk writes (maybe PDI)
- **We are open to provide a mini-app / benchmark with dyablo**
 - We can generate a lot of data (bench up to 2000 GPUs on AdAstra)

In-situ / AI :

Dyablo is still young and post processing / AI analysis are not ready yet

- Use-cases (post-processings, ...) will come later from physicists / dyablo applications
 - We want to make sure everything we make for IO is ready for in-situ / AI
- => Pave the way to in-situ, AI, ... by using Exa-Dost software