Multiscale ocean modelling Bridging the gap between global changes and local impacts

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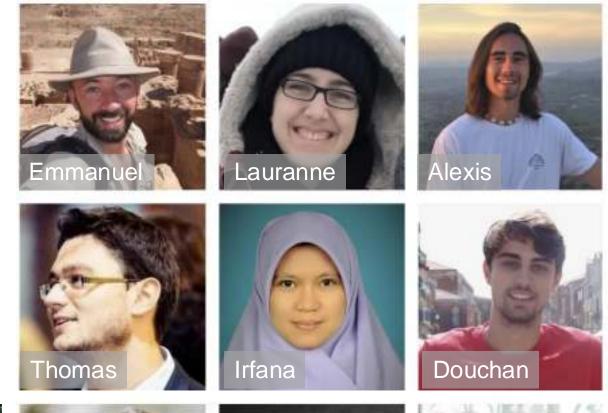
UCLouvain, Belgium





SLIM people

- 2 academics
- 2 post-doc researchers
- 11 PhD researchers
- www.slim-ocean.be





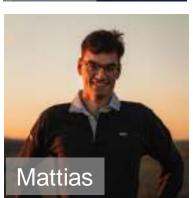






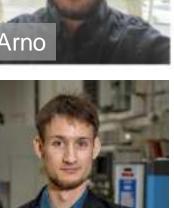








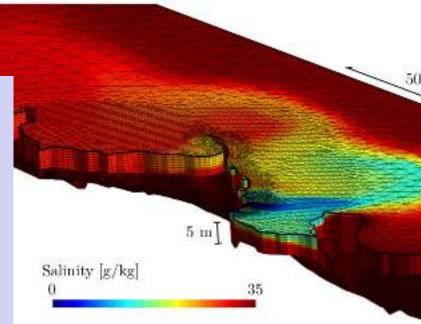


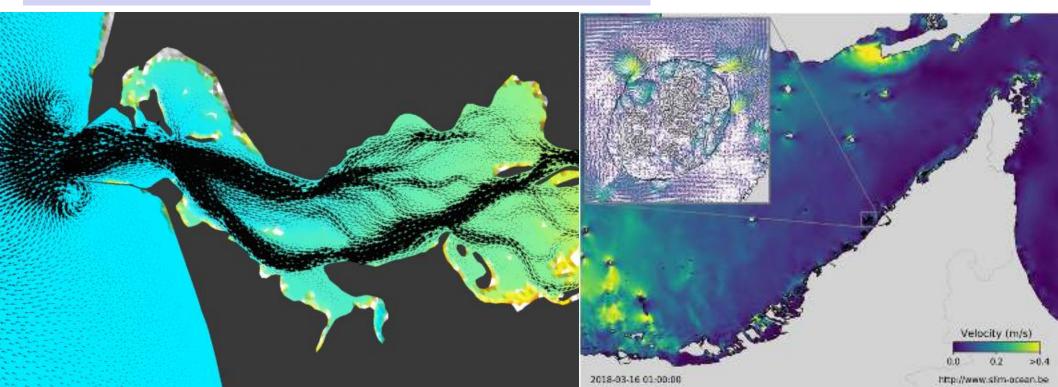


Miguel

SLIM in a nutshell...

- Unstructured meshes \rightarrow variable resolution
- Discontinuous Galerkin finite element method
- Different hydrodynamic models
 - SLIM1D for river flows
 - SLIM2D for shallow barotropic flows with W&D
 - SLIM3D for hydrostatic baroclinic flows
- Coupled with the coastal wave model SWAN
- Coupled with different transport models
 - Eulerian: sediments, water age, water quality, ...
 - Lagrangian: coral larvae, plastic debris, seagrass propagules, turtle hatchlings, oil spills, ...
- Hydrodynamic models run on GPUs.

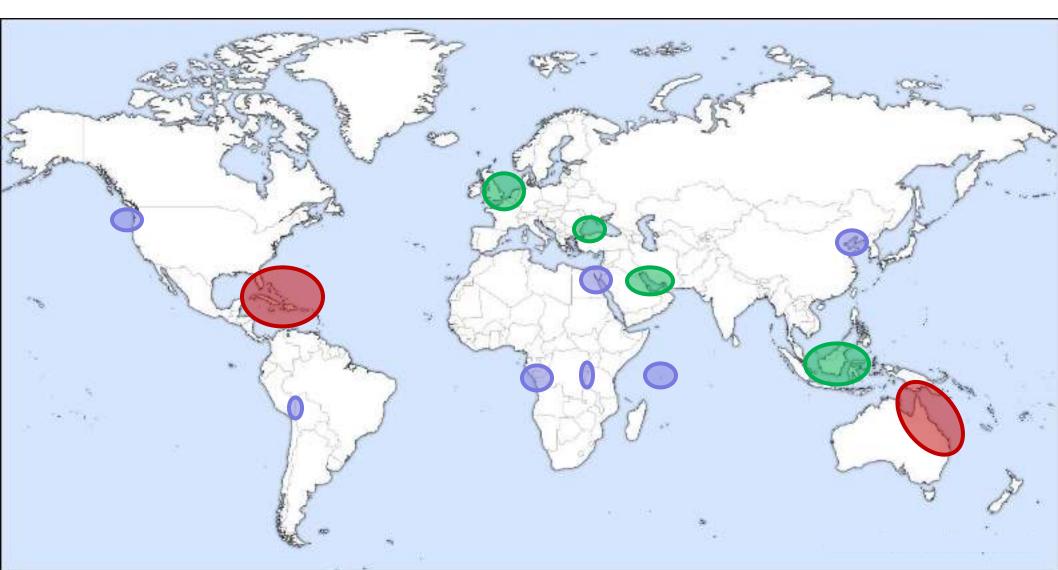




SLIM in the world...

- Great Barrier Reef, Australia
- Florida Reef Tract, Bahamas, USVI
- Scheldt, North Sea
- Danube, Black Sea
- Arabian/Persian Gulf
- Indonesia

- Columbia River
- Lake Titicaca
- Congo River
- Lake Tanganyika
- Seychelles
- Northern Red Sea
- Bohai Sea













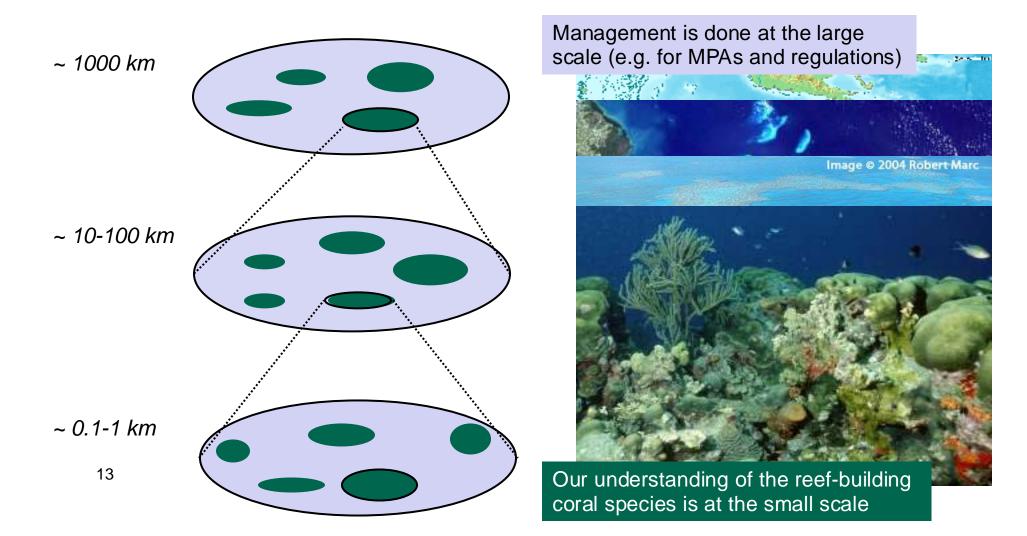






- > 3000 reefs in the GBR
- From 0.01 to 100 km²
- Cover <0.1% of the ocean surface but home to >25% of all marine species

Like most marine environments, the GBR is a large multi-scale system



2-way interactions between the small and large scales

500 km

250

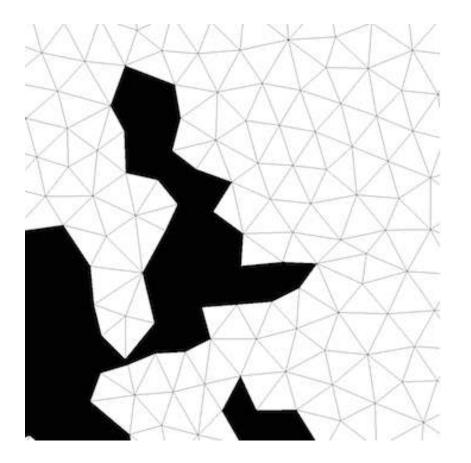
Different processes, at different scales, interact together

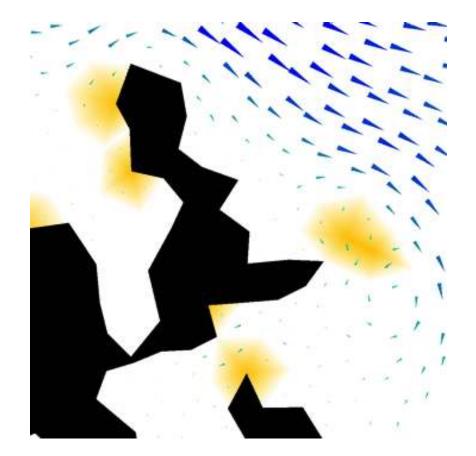
• The large-scale currents from the Pacific are deflected by the reefs.

• The small-scale flow features around the reefs, like eddies, are driven by the interplay between the tides, the wind and the large-scale currents.

• A model of the GBR should represent these different processes and their interactions from 1000's km to 10's m.

Getting the right resolution, at the right place is really important...

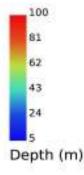


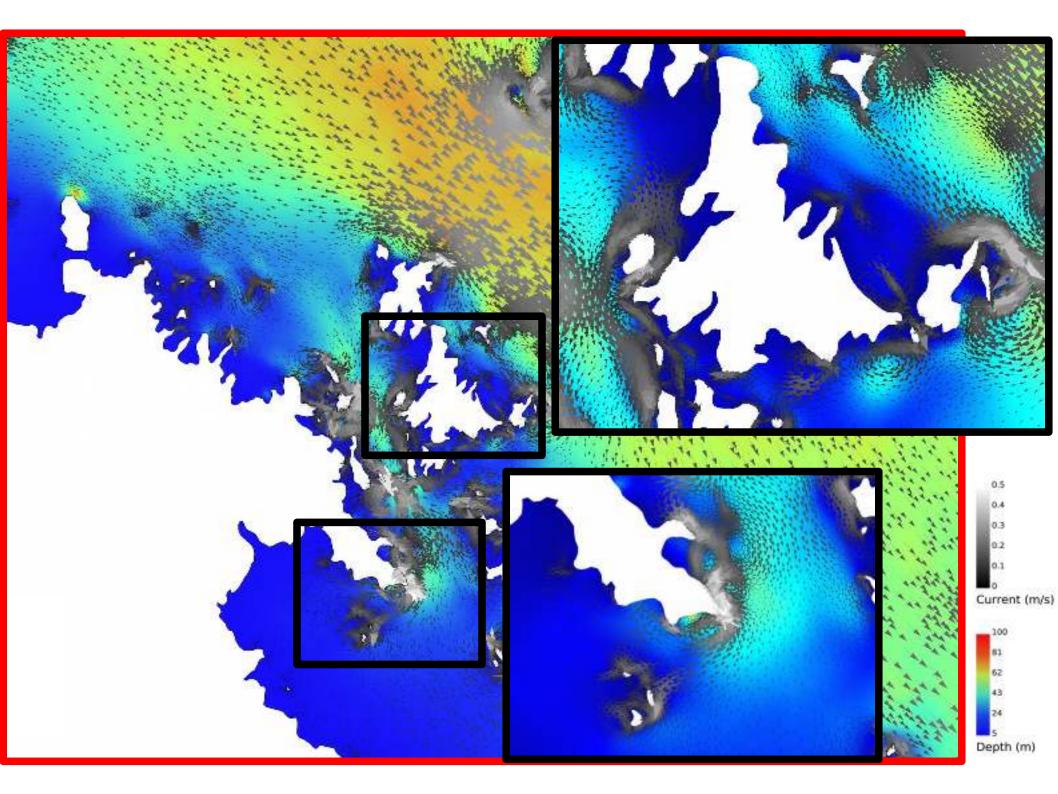


Using a multi-scale ocean model, we can reproduce this complex dynamics

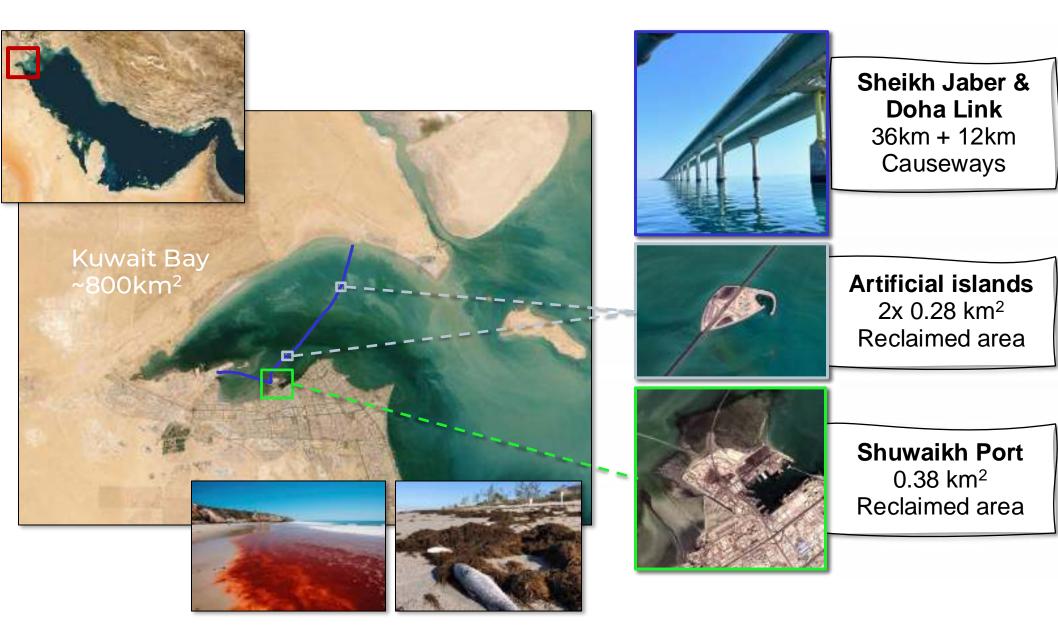


0.5 0.4 0.3 0.2 0.1

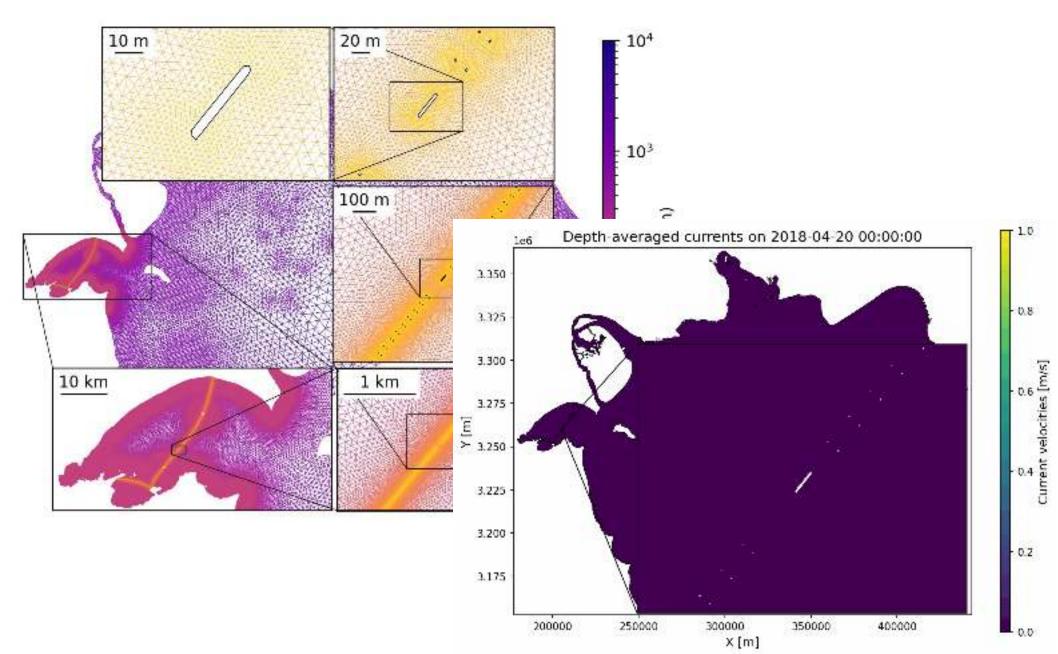




The same applies to artificial structures instead of reefs



The multiscale nature of the flow again requires a multiscale model

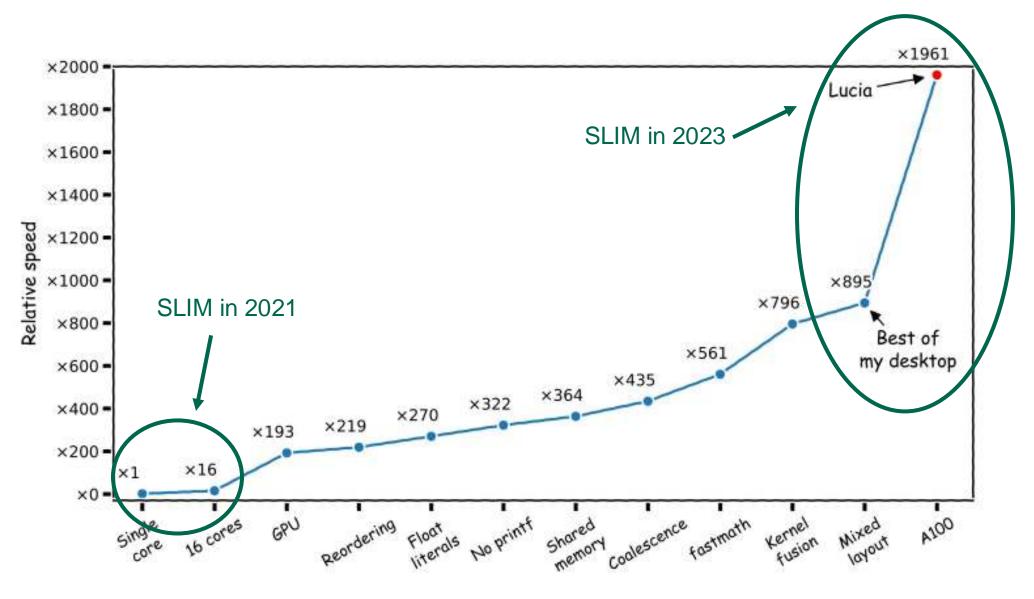


Increasing resolution is however not enough...

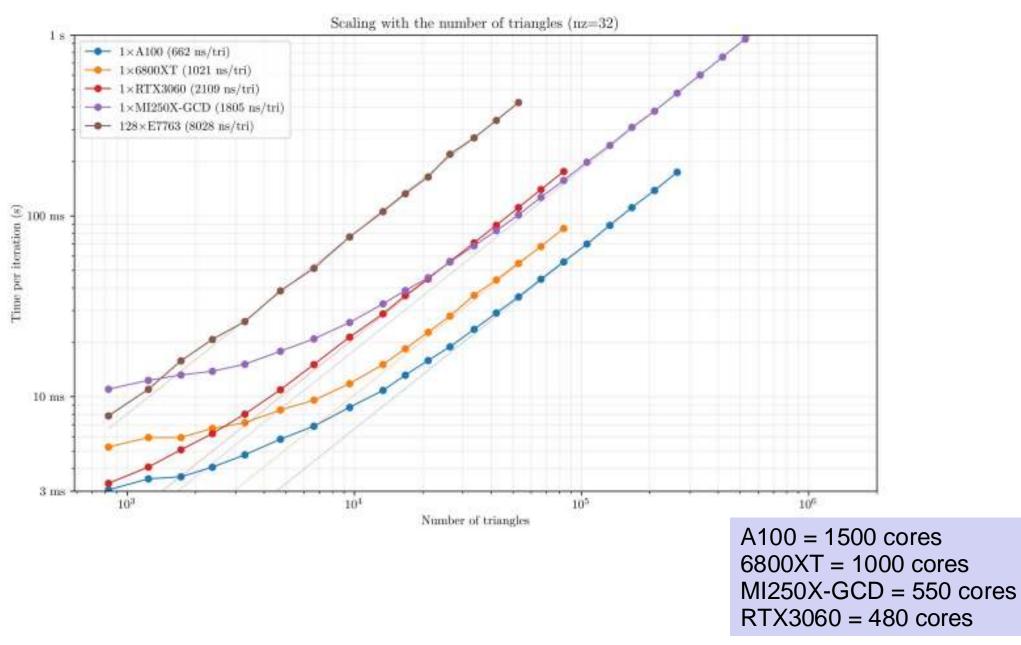
- As we increase the resolution, we have to reconsider the physical assumptions underlying our model.
- A 2D depth-averaged model is often not sufficient to capture the dynamics of marine flows, which are often driven by density gradients and hence **3D**.
- As the mesh resolution becomes of the order of water depth, non-hydrostatic effects can no longer be neglected neither.

- ⇒ We hence have to consider models with a more complex physics
- ⇒ Move from a multi-scale to a multi-physics modeling paradigm.

To do that, we had to completely rewrite our model to run on GPUs...



Single-GPU performance of the 3D model



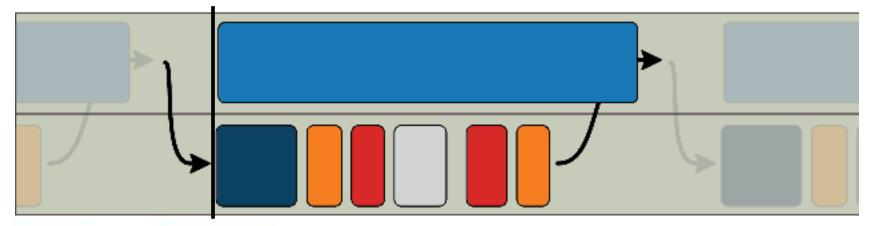
Scaling to multiple GPUs

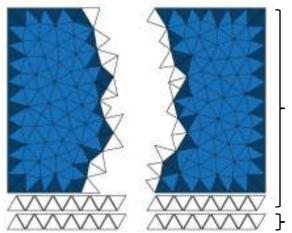
Naïve approach : Compute, then communicate

- Works very well on CPUs where the computation is very slow compared to communications
- Completely unusable with GPUs : The computation time is way too short

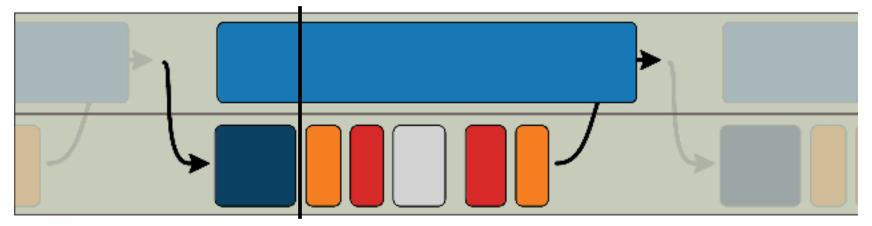
Better approach : Overlap communication and computation

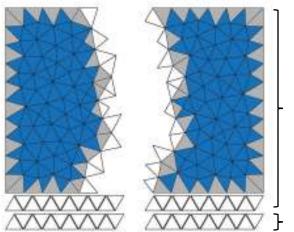
- Requires splitting the computation : boundaries VS interior
- On GPUs, requires multiple 2 streams and explicit synchronization for good performance



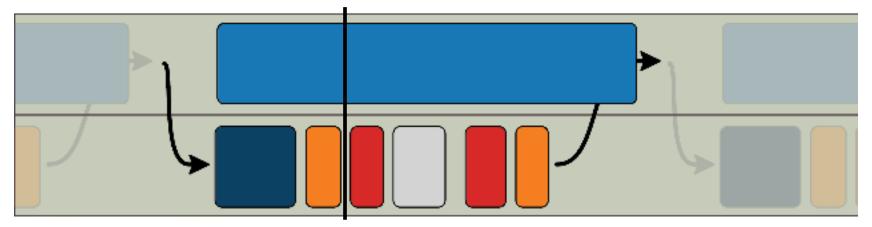


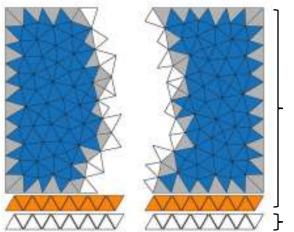
1. Launch the computation on the boundary



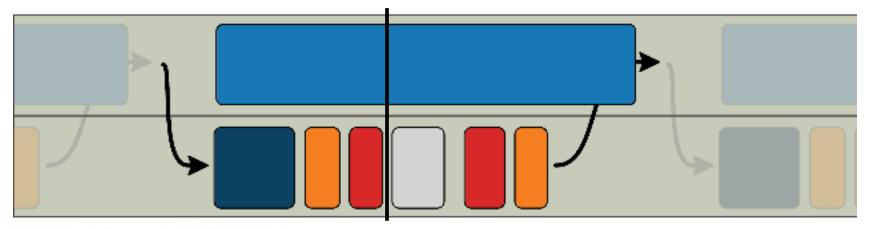


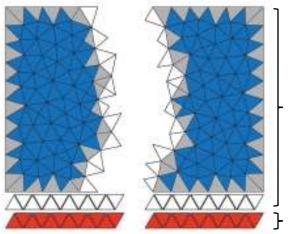
- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer



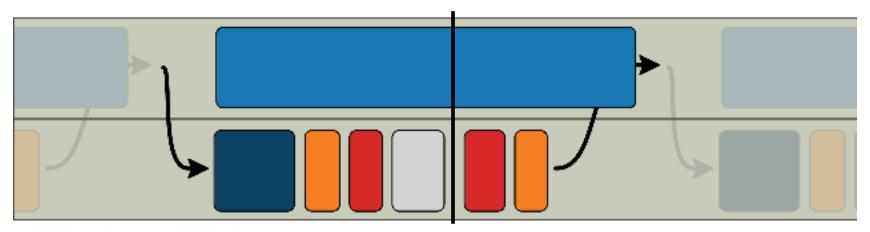


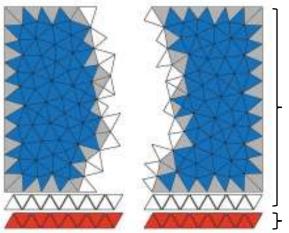
- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU



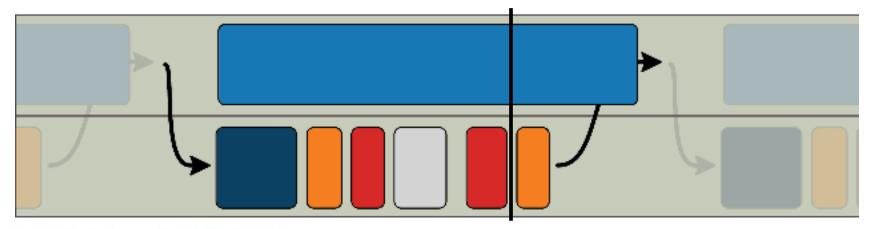


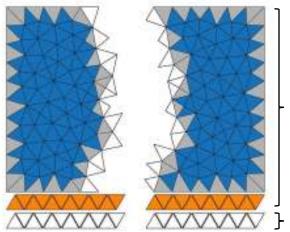
- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU
- 4. Communicate with MPI



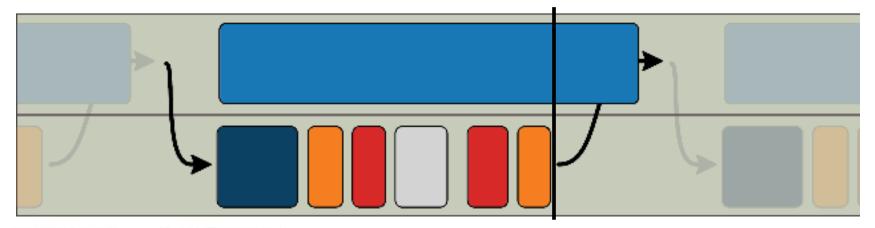


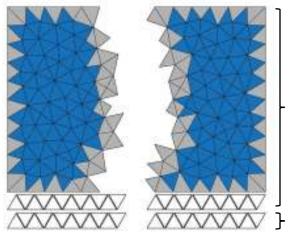
- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU
- 4. Communicate with MPI
- 5. Copy back to the GPU





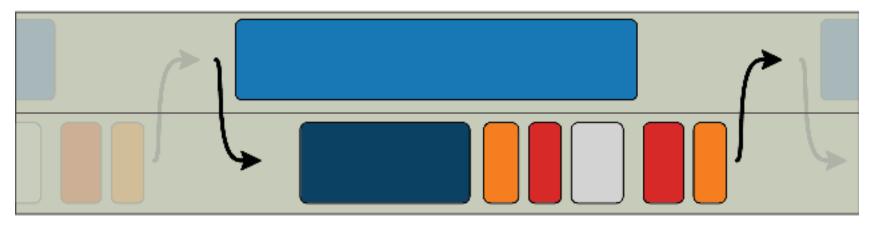
- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU
- 4. Communicate with MPI
- 5. Copy back to the GPU
- 6. Unpack the arriving data

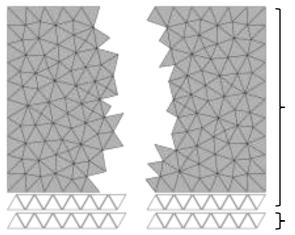




- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU
- 4. Communicate with MPI
- 5. Copy back to the GPU
- 6. Unpack the arriving data
- 7. Wait for the computation to finish and synchronize
- Interior computations: specialized for no boundaries
- Works great for big kernels



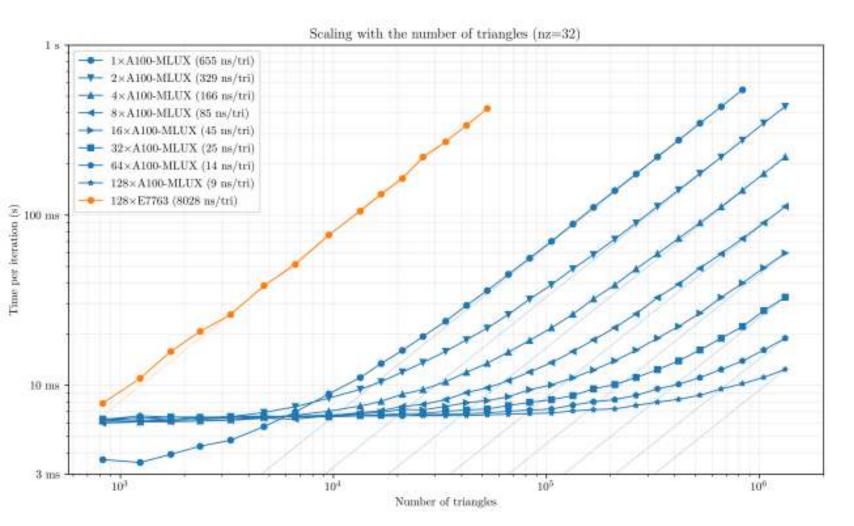




- 1. Launch the computation on the boundary
- 2. Pack the data that needs to be sent in a buffer
- 3. Copy to the CPU
- 4. Communicate with MPI
- 5. Copy back to the GPU
- 6. Unpack the arriving data
- 7. Wait for the computation to finish and synchronize
- Interior computations: specialized for no boundaries
- Works great for big kernels, but not so much for small kernels (<100µs)

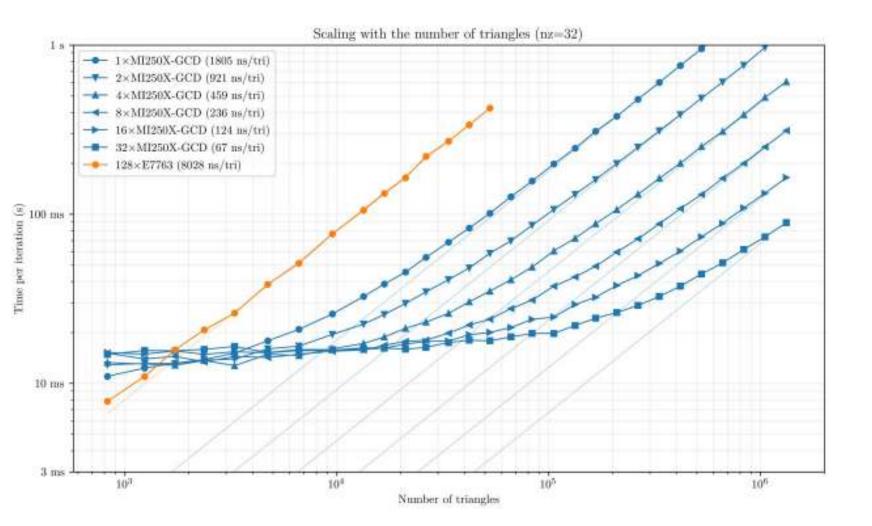


Scaling of the 3D model on A100 GPUs



- Good single-GPU performance
- Good latency on single GPU
- Ok latency for multi-GPU

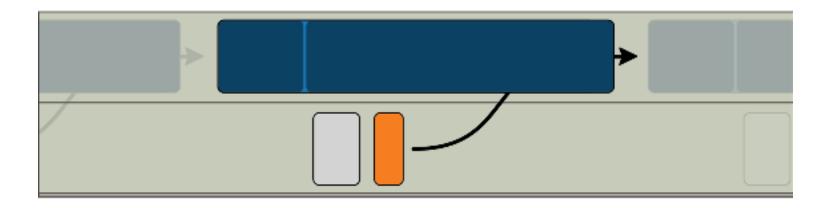
Scaling of the 3D model on MI250X GPUs



- Weaker single-GPU performance
- Higher latency
- OK-ish weak scaling

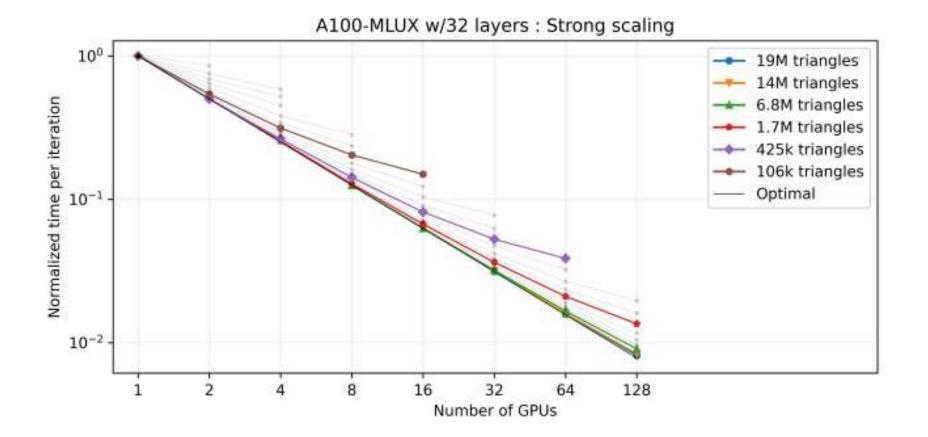
There are solutions to improve the MI250X perfs

- GPU-aware MPI
- Compute on the boundary and pack the data within the same kernel
- Launch the full computation (inside and boundary nodes) and packing on the main kernel

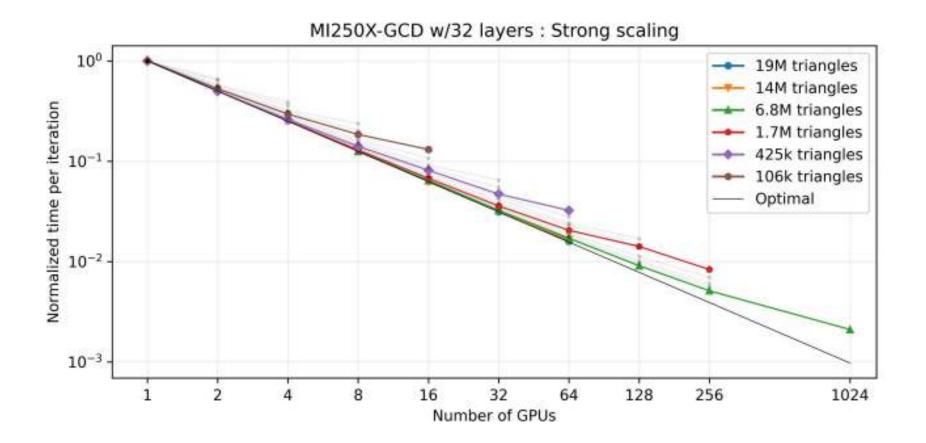


 ⇒ Leads to lower latency and better performances for AMD hardware
⇒ A bit slower on the NVIDIA hardware

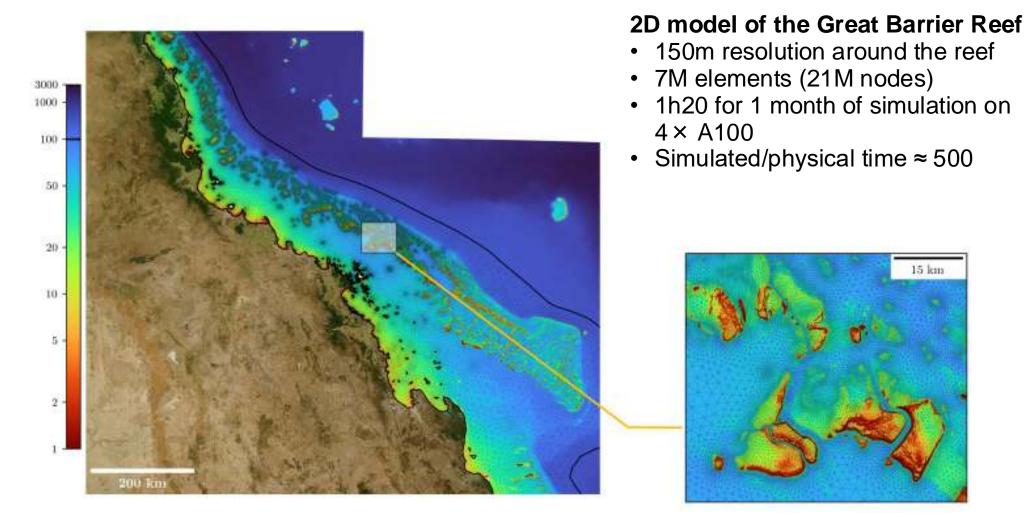
Strong scaling of the 3D model on A100 GPUs



Strong scaling of the 3D model on MI250X GPUs



And in the end, how well does it perform?



Conclusions

- Rewriting our code from scratch was a good investment!
- Simulations that used to take a few weeks now take a few hours.
- Achieving good strong scaling on 100's of GPUs opens the door to very ambitious simulations.
- Minimizing latency however remains an issue that requires hardware-specific solutions.
- The next step for us is to adapt the physics of the model to the new resolutions that we can now achieve...

Many thanks to LUMI-BE and EuroHPC for granting us access to those fast tools!