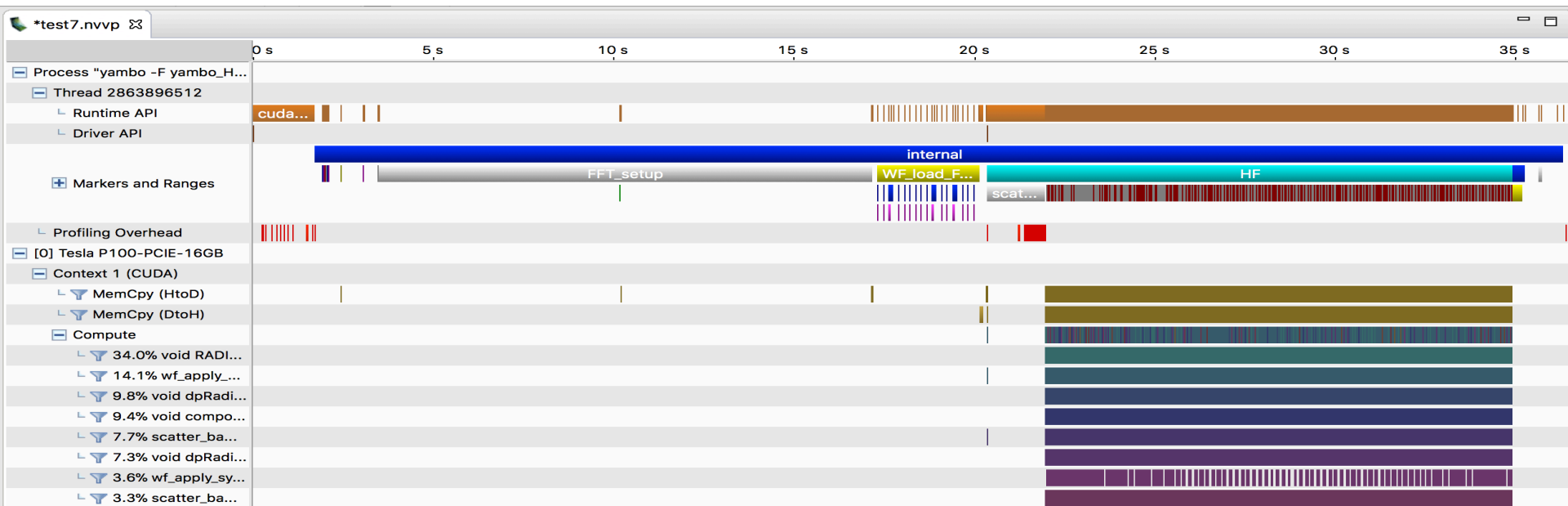# YOGA: Yambo on GPU

Pietro Bonfa', Massimiliano Fatica,
Andrea Ferretti, Anton Kozhevniko,
Ivan Marri, Everett Phillips, Josh Romero,
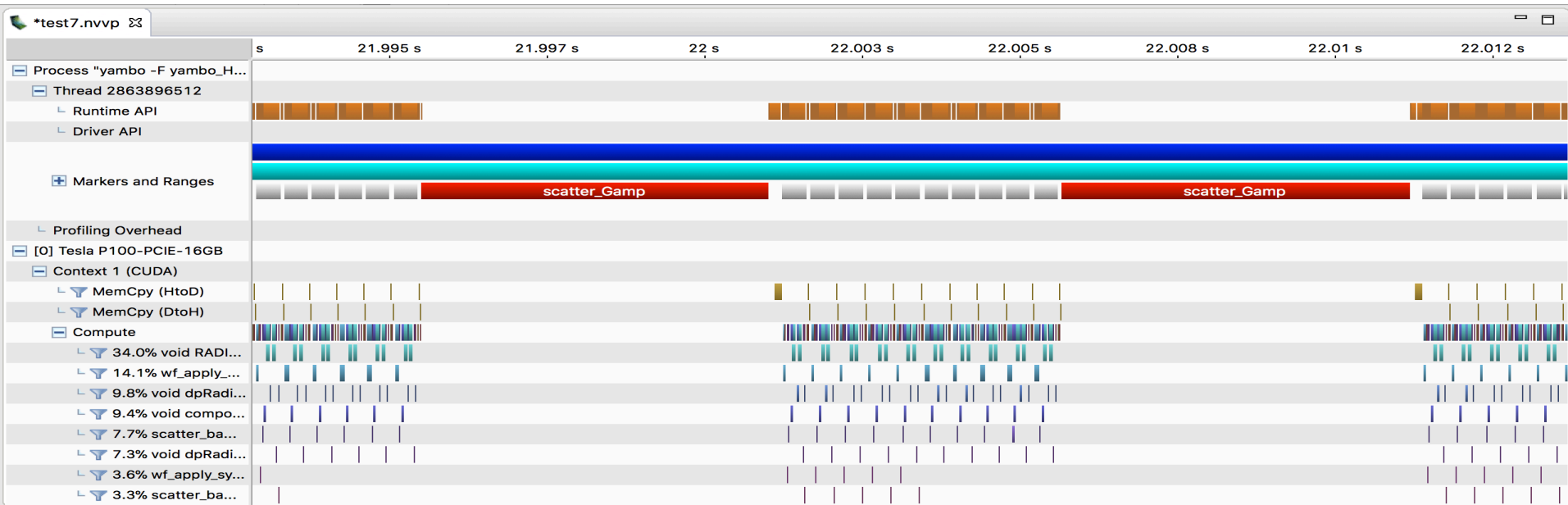
Status

- Get a working environment on PizDaint
- Add profiler markers in YAMBO timing routines (we can now generate detailed nvprof files to analyze the timeline)
- Ported one function to the GPU, identified the next ones.
- Preparing more input cases
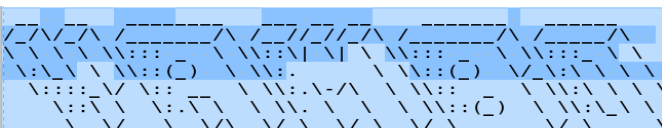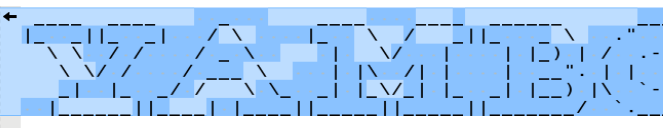- Starting to compare results between the CPU and the CUDA versions.

Profiler

Profiler

Accuracy

Version 4.4.0 Revision 16027 Hash 773ca4ddd
                MPI+CUDA Build
          http://www.yambo-code.org

Hartree-Fock Components and Corrections

K-point	Band	Eo	Ehf	DFT	HF
1.00000	1.00000	-16.30089	-28.34165	-15.18405	-27.22481
1.00000	2.00000	-9.76485	-18.85173	-13.84756	-22.93444
1.00000	3.00000	-4.73902	-12.05470	-16.17428	-23.48995
1.00000	4.00000	-4.72337	-11.17716	-12.73399	-19.18779
1.00000	5.00000	-3.78752	-10.63660	-14.55829	-21.40737

Version 4.4.0 Revision 16027 Hash 773ca4ddd
                  MPI Build
          http://www.yambo-code.org

Hartree-Fock Components and Corrections

K-point	Band	Eo	Ehf	DFT	HF
1.00000	1.00000	-16.30089	-28.34165	-15.18405	-27.22481
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1.00000	3.00000	-4.73902	-12.05470	-16.17428	-23.48995
1.00000	4.00000	-4.72337	-11.17716	-12.73399	-19.18779
1.00000	5.00000	-3.78752	-10.63660	-14.55829	-21.40737

Double precision

Version 4.4.0 Revision 16027 Hash 773ca4ddd
                MPI+CUDA Build
          http://www.yambo-code.org

Hartree-Fock Components and Corrections

K-point	Band	Eo	Ehf	DFT	HF
1.00000	5.00000	-3.78752	-10.63673	-14.55816	-21.4073
1.000000	6.000000	3.976900	6.273014	-3.628596	-1.33248

Version 4.3.0 Revision 15819 Hash ac5a4e1bd
                 Serial Build
          http://www.yambo-code.org

Hartree-Fock Components and Corrections

K-point	Band	Eo	Ehf	DFT	HF
1.00000	5.00000	-3.78752	-10.63649	-14.55805	-21.4070
1.000000	6.000000	3.976900	6.272833	-3.628388	-1.33245

Double and Single precision