# Debugging and optimizing Idefix

the art of hunting segfaults and NaNs

#### Before we start

#### Bigfoot environment

- To connect to bigfoot and choose your team, follow the tutorial in « env/ Readme.md » of the idefix-days repo
- All of the steps described here are available in tutorials/debugging/ readme.md of the idefix-days repo. You can directly copy-paste the commands from there.

## What you will learn

- Use Idefix\_DEBUG to trace where you are in the code
- Use Kokkos debugging features (Kokkos Bound checks, Kernel logger),
- Use debuggers
- The most common mistakes<sup>TM</sup>
- Asynchronous error reporting on GPUs
- Use kokkos profiling tools to look at performances

#### A CPU-domain segmentation fault

- go to tutorials/debugging/problem1 (it is the sod tube problem)
- Compile and run
- Surprise!

#### A CPU-domain segmentation fault

- Add Idefix\_DEBUG=ON to your configuration (using cmake or ccmake) & recompile & run
  - The error happens in Setup::InitFlow after SyncToDevice() (cool!)
- Use gdb to debug the code and backtrace the problem

```
[nix-shell:~/workdir/days2023/tutorials/debugging/problem1]$ gdb ./idefix
GNU gdb (Debian 10.1-1.7) 10.1.90.20210103-git
Copyright (C) 2021 Free Software Foundation, Inc.
License GPLv3+: GNU GPL version 3 or later <a href="http://gnu.org/licenses/gpl.html">http://gnu.org/licenses/gpl.html</a>
This is free software: you are free to change and redistribute it.
There is NO WARRANTY, to the extent permitted by law.
Type "show copying" and "show warranty" for details.
This GDB was configured as "x86_64-linux-gnu".
Type "show configuration" for configuration details.
For bug reporting instructions, please see:
<https://www.gnu.org/software/gdb/bugs/>.
Find the GDB manual and other documentation resources online at:
    <http://www.gnu.org/software/gdb/documentation/>.
For help, type "help".
Type "apropos word" to search for commands related to "word"...
Reading symbols from ./idefix...
(gdb) run
```

```
----> DataBlockHost::DataBlockHost(DataBlock)...
---> ...returned
----> DataBlockHost::SyncToDevice()...
Program received signal SIGSEGV, Segmentation fault.
0x00007ffff7c1329c in __strlen_evex () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
(gdb) bt
#0 0x00007ffff7c1329c in __strlen_evex () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
#1 0x00007ffff7b07d39 in __printf_buffer () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
#2 0x00007ffff7b08401 in __vfprintf_internal () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
   0x00007ffff7bc3c43 in __fprintf_chk () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
   0x00000000005404d2 in Kokkos::Impl::SharedAllocationRecord<void, void>::decrement(Kokkos::Impl::SharedAllocationRecord<void, void>*) ()
   0x0000000004396dd in Kokkos::Impl::SharedAllocationTracker::~SharedAllocationTracker (this=0x7fffffff7318, __in_chrg=<optimized out>)
   at /home/lesurg/src/idefix/src/kokkos/core/src/impl/Kokkos SharedAlloc.hpp:419
#6 Kokkos::Impl::ViewTracker<Kokkos::View<double****, Kokkos::LayoutRight, Kokkos::Device<Kokkos::Serial, Kokkos::HostSpace>, Kokkos::Experimental::EmptyViewHealth
acker (this=0x7fffffff7318, __in_chrq=<optimized out>) at /home/lesurg/src/idefix/src/kokkos/core/src/impl/Kokkos_ViewTracker.hpp:39
#7 Kokkos::View<double****, Kokkos::LayoutRight, Kokkos::Device<Kokkos::Serial, Kokkos::HostSpace>, Kokkos::Experimental::EmptyViewHooks>::~View (this=0x7fffff
     <u>_in_chrg</u>=<optimized out>) at /home/lesurg/src/idefix/src/kokkos/core/src/Kokkos_View.hpp:1266
   DataBlockHost::~DataBlockHost (this=0x7fffffff7230, __in_chrg=<optimized out>) at /home/lesurg/src/idefix/src/dataBlock/dataBlockHost.hpp:25
           0000051e33a in Setup::InitFlow (this=this@entry=0x7ffffffff758f, data=...) at /home/lesurg/workdir/days2023/tutorials/debugging/problem1/setup.cpp:47
#10 0x00000000041205a in main (argc=<optimized out>, argv=<optimized out>) at /home/lesurg/src/idefix/src/main.cpp:126
```

• The problem is definitely in DataBlockHost and Idefix is crap... Or?

#### A CPU-domain segmentation fault

#### RULE I: A segmentation fault always shows up after it actually happens

Sometimes, it can be 1000s of lines later

- Most likely problem: overflow of an array
- Need a way to check that the indices are always consistent with the array size: Kokkos\_ENABLE\_DEBUG\_BOUNDS\_CHECK!

```
[nix-shell:~/workdir/days2023/tutorials/debugging/problem1]$ cmake $IDEFIX_DIR -DKokkos_ENABLE_DEBUG_BOUNDS_CHECK=ON
-- Setting default Kokkos CXX standard to 17
-- The project name is: Kokkos
-- Using internal gtest for testing
[nix-shell:~/workdir/days2023/tutorials/debugging/problem1]$ make -j 8
[ 1%] Linking CXX static library libkokkossimd.a
[ 1%] Built target AlwaysCheckGit
 [ 3%] Linking CXX static library libimpl_git_version.a
[nix-shell:~/workdir/days2023/tutorials/debugging/problem1]$ gdb ./idefix
GNU gdb (Debian 10.1-1.7) 10.1.90.20210103-git
Copyright (C) 2021 Free Software Foundation, Inc.
                                                                                                                     NOT a segmentation fault,
 For help, type "help".
 Type "apropos word" to search for commands related to "word"...
                                                                                                                      but an exception raised by Kokkos!
 Reading symbols from ./idefix...
 (gdb) run
 terminate called after throwing an instance of 'std::runtime_error'
  what(): View bounds error of view DataBlock_x0 ( 504 < 504 )
 Program received signal SIGABRT, Aborted.
 0x00007fffff7b35a8c in __pthread_kill_implementation () from /nix/store/wpgrc564ys39vbyv0m50qxmq8dvhi7cc-glibc-2.37-8/lib/libc.so.6
                                                                                                                                                    line # is different
 (gdb) bt
 #10 Setup::InitFlow (this=this@entry=0x7ffffffff758f, data=...) at /home/lesurg/workdir/days2023/tutorials/debugging/problem1/setup.cpp:35
```

#### A CPU-domain segmentation fault

Conclusions

- The error is in the loop bounds in InitFlow (should be <, not <=)
- Good idea to check your code using
   Kokkos\_ENABLE\_DEBUG\_BOUNDS\_CHECK (even if it works!)
- When the system detects a segmentation fault, it is usually too late, the error happened before
- Use a debugger (IIdb on macs, gdb on linux, cuda-gdb on nvidia, see later)
- Note the importance of IdefixArray labels when debugging, and idfx::pushRegion().

#### A GPU-domain segmentation fault

- go to tutorials/debugging/problem2 (thermal diffusion problem)
- Configure it for CPU (cmake without any option will do), run it
- Same on GPU...

CPU

GPU (AMD/Rocm)

```
Input: Compiled with DOUBLE PRECISION arithmetic.
Input: DIMENSIONS=3.
Input: COMPONENTS=3.
Grid: full grid size is
         Direction X1: periodic -0.5....500....0.5
                                                       periodic
        Direction X2: periodic 0....1....1
                                               periodic
        Direction X3: periodic 0....1....1
                                              periodic
Hydro: solving HD equations.
Hydro: Reconstruction: 2nd order (PLM Van Leer)
Hydro: EOS: ideal with gamma=1.4
RiemannSolver: hllc (HD).
Thermal Diffusion: ENEABLED with constant diffusivity kappa=0.1.
Thermal Diffusion: uses an explicit time integration.
TimeIntegrator: using 2nd Order (RK2) integrator.
TimeIntegrator: Using adaptive dt with CFL=0.8 .
main: Creating initial conditions.
Dump: Write file n 0...done in 0.000445219 s.
Main: Cycling Time Integrator...
                                             cycle |
                                                            time step | cell (updates/s)
TimeIntegrator:
                           time |
                   0.000000e+00
TimeIntegrator:
                                                         1.000000e-10
                                                                                    N/A
                                                 0 |
                                                                            5.962295e+05
TimeIntegrator:
                   1.377961e-05 |
                                                100
                                                         1.378061e-06
                   2.912137e-03 |
                                                         3.884597e-05
TimeIntegrator:
                                                                            7.541577e+05
                                                200
TimeIntegrator:
                   6.796734e-03 |
                                                         3.884597e-05
                                                                            7.966867e+05
                                                300
TimeIntegrator:
                   1.068133e-02 |
                                                400 |
                                                         3.884597e-05 |
                                                                            8.155215e+05
```

```
Input: Compiled with DOUBLE PRECISION arithmetic.
Input: DIMENSIONS=3.
Input: COMPONENTS=3.
Input: Kokkos HIP target ENABLED.
Grid: full grid size is
                                                        periodic
        Direction X1: periodic -0.5....500....0.5
        Direction X2: periodic 0....1....1
                                                periodic
        Direction X3: periodic 0....1....1
                                                periodic
Hydro: solving HD equations.
Hydro: Reconstruction: 2nd order (PLM Van Leer)
Hydro: EOS: ideal with gamma=1.4
RiemannSolver: hllc (HD).
Thermal Diffusion: ENEABLED with constant diffusivity kappa=0.1.
Thermal Diffusion: uses an explicit time integration.
TimeIntegrator: using 2nd Order (RK2) integrator.
TimeIntegrator: Using adaptive dt with CFL=0.8 .
Main: Creating initial conditions.
Memory access fault by GPU node-2 (Agent handle: 0x5569bc244030) on address 0x5569bc983000. Reason: Unknown.
Aborted
```

#### A GPU-domain segmentation fault

same as case I: start with Idefix\_DEBUG

```
Thermal Diffusion: ENEABLED with constant diffusivity kappa=0.1.
Thermal Diffusion: uses an explicit time integration.
                                                                                                                                         Our initial conditions
TimeIntegrator: using 2nd Order (RK2) integrator.
TimeIntegrator: Using adaptive dt with CFL=0.8 .
Main: Creating initial conditions.
> Setup::Initflow...
----> DataBlockHost::DataBlockHost(DataBlock)...
----> ...returned
 ----> DataBlockHost::SyncToDevice()...
                                                                                                                                         Our internal boundaries
----> ...returned
> ...returned
> Boundary::SetBoundaries...
----> Boundary::UserDefInternalBoundary...
                                                                                                                                         So, it is in the periodic boundary
----> Boundary::EnforceBoundaryDir...
    ----> Boundary::EnforcePeriodic...
                                                                                                                                         conditions implemented in Idefix?!
 terminate called after throwing an instance of 'std::runtime_error'
 what(): cudaMemcpyToSymbol(Kokkos::Impl::g_device_cuda_lock_arrays, &Kokkos::Impl::g_host_cuda_lock_arrays, sizeof(Kokkos::Impl::CudaLockArra
ErrorIllegalAddress): an illegal memory access was encountered /home/lesurg/src/idefix/src/kokkos/core/src/Cuda/Kokkos_Cuda_KernelLaunch.hpp:63
Traceback functionality not available
```

Enable Kokkos kernel logger:

export KOKKOS\_TOOLS\_LIBS=\$KOKKOS\_TOOLS\_DIR/debugging/kernel-logger/libkp\_kernel\_logger.so ... and execute again idefix

```
---> Boundary::UserDefInternalBoundary...

KokkosP: Executing parallel-for kernel on device 33554433 with unique execution identifier 323

KokkosP: Boundary::SetBoundaries

KokkosP: Boundary::UserDefInternalBoundary

KokkosP: InternalBoundary

KokkosP: InternalBoundary

terminate called after throwing an instance of 'std::runtime_error'

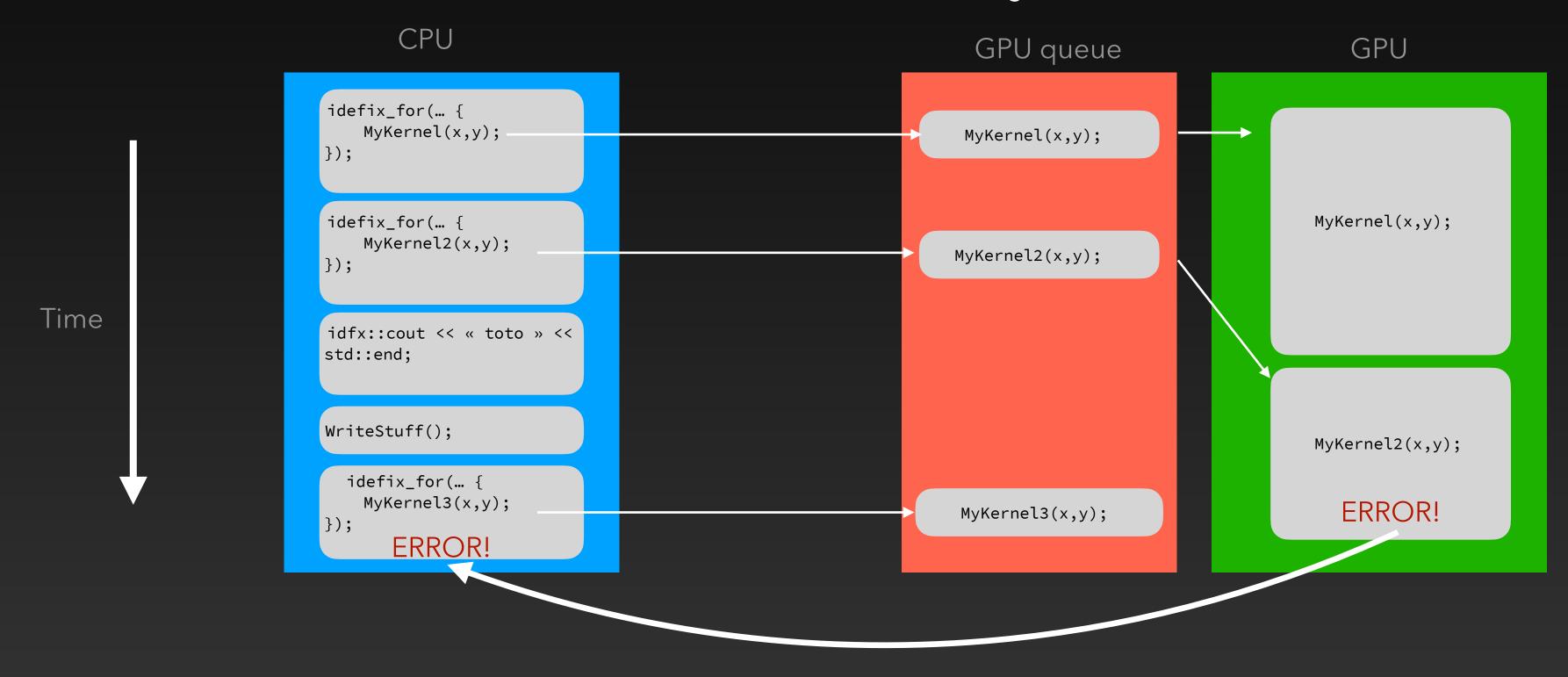
what(): cudaDeviceSynchronize() error( cudaErrorIllegalAddress): an illegal memory access was encountered /home/lesurg/src/idefix/src/kokkos/core/src/Cuda/Kokkos_Cuda_Instance.cp
p:150

Traceback functionality not available

Aborted
```

#### A GPU-domain segmentation fault

• The problem with GPU execution is called « non blocking dispatch »: each idefix\_for (=« kernel ») is sent to the GPU for it to be executed, but there is no guarantee it has been executed when the call to idefix\_for ends on the CPU! (similar to non-blocking MPI instructions)



• Kokkos kernel logger forces synchronisation between CPU & GPU by introducing Kokkos::fence at the end of each idefix\_for

#### A GPU-domain segmentation fault

Origin of the problem

RULE III: Never use pointers to Host space in idefix\_for loops RULE III: Always shallow copy whatever you need.

Solution: shallow copy the array needed before calling idefix\_for

#### A GPU-domain segmentation fault in a C++ class

- go to tutorials/debugging/problem3 (disk+planet problem)
- Configure it for CPU (cmake without any option will do), run it
- Same on GPU...

CPU

```
GIAVILY: ENABLED.
Gravity: G=1.
Gravity: central mass gravitational potential ENABLED with M=1
Gravity: planet(s) potential ENABLED.
TimeIntegrator: using 2nd Order (RK2) integrator.
TimeIntegrator: Using adaptive dt with CFL=0.5 .
Main: Creating initial conditions.
Vtk: Write file n 0...done in 0.00404309 s.
Dump: Write file n 0...done in 0.00463619 s.
Main: Cycling Time Integrator...
TimeIntegrator:
                                                             time step | cell (updates/s)
                           time
                                              cycle
TimeIntegrator:
                   0.000000e+00
                                                          1.000000e-03
                   1.731716e+00
TimeIntegrator:
                                                         2.277130e-02
                                                                             2.599456e+06
                                               100
TimeIntegrator:
                   4.009747e+00
                                                         2.268748e-02
                                                                             2.562011e+06
                                               200
TimeIntegrator:
                                                         2.231100e-02
                   6.259031e+00
                                                300
                                                                             2.615404e+06
TimeIntegrator:
                   8.396568e+00
                                                         2.016500e-02
                                                                             2.587613e+06
                                                400
Vtk: Write file n 1...done in 3.284987e-03 s.
Dump: Write file n 1...done in 3.255321e-03 s.
Main: Reached t=1.000000e+01
Main: Completed in 6 seconds and 483 cycles
Main: Perfs are 2.572279e+06 cell updates/second
Outputs represent 0% of total run time.
Profiler: maximum memory usage for Host memory space: 8.282364e+00 MB.
Main: Job completed successfully.
```

#### GPU (AMD/Rocm)

```
Direction X1: userdef 0.4....128....2.5
                                                       userdef
        Direction X2: periodic 0....256....6.28319
                                                       periodic
Hydro: solving HD equations.
Hydro: Reconstruction: 2nd order (PLM Van Leer)
Hydro: EOS: isothermal with user-defined cs function.
RiemannSolver: hllc (HD).
Fargo: ENABLED with user-defined velocity function.
Fargo: using standard PLM advection scheme.
PlanetarySystem: have 1 planets.
PlanetarySystem: uses analytical integration for planet location.
PlanetarySystem: uses plummer expression for planet potential.
Planet[0]: mass qp=0.001
Planet[0]: initial location dp=1
Gravity: ENABLED.
Gravity: G=1.
Gravity: central mass gravitational potential ENABLED with M=1
Gravity: planet(s) potential ENABLED.
TimeIntegrator: using 2nd Order (RK2) integrator.
TimeIntegrator: Using adaptive dt with CFL=0.5.
Main: Creating initial conditions.
Vtk: Write file n 0...done in 0.910953 s.
Dump: Write file n 0...done in 0.0223124 s.
Main: Cycling Time Integrator...
TimeIntegrator:
                                                            time step | cell (updates/s)
                           time |
                                              cycle |
                   0.000000e+00 |
TimeIntegrator:
                                                         1.000000e-03 |
                                                 0 I
Memory access fault by GPU node-2 (Agent handle: 0x558457a987e0) on address 0x558457d12000. Reason: Unknown.
Aborted
```

#### A GPU-domain segmentation fault in a C++ class

Notice the warning on GPU (not always...)

Enable kokkos-kernel-logger+IDEFIX\_GPU

-> Problem is clearly in the idefix\_for called in SoundSpeed::Compute

A GPU-domain segmentation fault in a C++ class

- What is Rcoord? what is h0?
- For the compiler, these are member variables of the SoundSpeed class
- Hence, they are transformed into this->Rcoord and this->ho
- The pointer this-> is in host space! Back to rule II and III
- Very common bug, check https://github.com/kokkos/kokkos/issues/695

### Case Study 4

#### A slow execution

- go to tutorials/debugging/problem4 (disk+planet problem, again)
- Compile & run on your favorite GPU
- Checkout the code performances (NB: expect at least 1e8 cell/sec per GPUs!)

Frigation Cycleaning Talling	e incegnatorii.				
TimeIntegrator:	time	cycle	time step   c	ell (updates/s)	
TimeIntegrator:	0.000000e+00	0	1.000000e-05	N/A	1 1
TimeIntegrator:	2.506014e-03	100	2.607530e-05	1.773492e+07	OW!
TimeIntegrator:	5.113544e-03	200	2.607530e-05	1.784479e+07	
TimeIntegrator:	7.721074e-03	300	2.607530e-05	1.788350e+07	
TimeIntegrator:	1.032860e-02	400	2.607530e-05	1.782232e+07	
TimeIntegrator:	1.293613e-02	500	2.607530e-05	1.789490e+07	

# Case Study 4 A slow execution

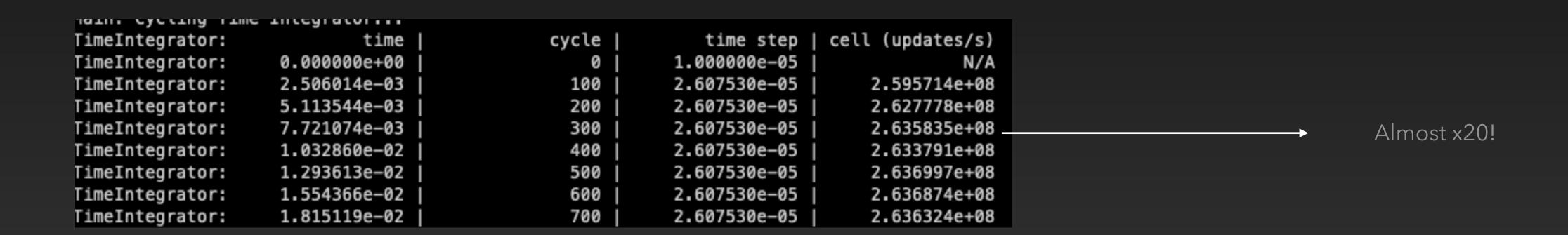
- Use the space-time-stack provided by Kokkos: export KOKKOS\_TOOLS\_DIR/profiling/space-time-stack/libkp\_space\_time\_stack.so
- No need to recompile, just re-run the same executable. Profiling is performed on the fly...

```
TOP-DOWN TIME TREE:
<average time> <percent of total time> <percent time in Kokkos> <percent MPI imbalance> <remainder> <kernels per second> <number of calls> <name> [type]
                                                                                                                                                                     Most of the time is spent in the
|-> 3.60e+01 sec 91.2% 30.1% 0.0% 0.0% 4.52e+02 772 Output::CheckForWrites [region]
    |-> 3.56e+01 sec 90.4% 30.3% 0.0% 25.1% 4.55e+02 772 UserDef::User-defined analysis function [region]
                                                                                                                                                                           user-defined analysis!
        |-> 1.63e+01 sec 41.2% 61.5% 0.0% 38.5% 9.03e+02 772 DataBlockHost::DataBlockHost(DataBlock) [region]
            |-> 2.72e+00 sec 6.9% 100.0% 0.0% ----- 772 Kokkos::View::initialization [Hydro_Uc_mirror] via memset [for]
            |-> 2.71e+00 sec 6.9% 100.0% 0.0% ----- 772 Kokkos::View::initialization [Hydro_Vc_mirror] via memset [for]
            |-> 9.13e-01 sec 2.3% 100.0% 0.0% ----- 772 Kokkos::View::initialization [Hydro_InvDt_mirror] via memset [for]
            |-> 9.08e-01 sec 2.3% 100.0% 0.0% ----- 772 Kokkos::View::initialization [DataBlock_A1_mirror] via memset [for]
            |-> 9.08e-01 sec 2.3% 100.0% 0.0% ----- 772 Kokkos::View::initialization [DataBlock_A0_mirror] via memset [for]
            |-> 9.06e-01 sec 2.3% 100.0% 0.0% ----- 772 Kokkos::View::initialization [DataBlock_dV_mirror] via memset [for]
            |-> 9.01e-01 sec 2.3% 100.0% 0.0% ----- 772 Kokkos::View::initialization [DataBlock_A2_mirror] via memset [for]
        |-> 9.61e+00 sec 24.4% 0.0% 0.0% 100.0% 0.00e+00 772 DataBlockHost::SyncFromDevice() [region]
        |-> 8.17e-01 sec 2.1% 100.0% 0.0% ----- 1544 ComputeForce [reduce]
    |-> 1.28e-01 sec 0.3% 2.2% 0.0% 97.6% 1.17e+02 1 Dump::Write [region]
    -> 9.76e-02 sec 0.2% 31.2% 0.0% 47.4% 1.95e+02 1 UserDef::User-defined variables function [region]
    -> 7.94e-02 sec 0.2% 3.0% 0.0% 97.0% 3.78e+01 1 Vtk::Write [region]
```

## Case Study 4

#### A slow execution

- The culprit is the frequency of the analysis routine in idefix.ini, which is set to 0 (i.e. every integration loop!)
- Set it to 0.01, and things get back to normal



RULE IV: always check that the performances are what you expect