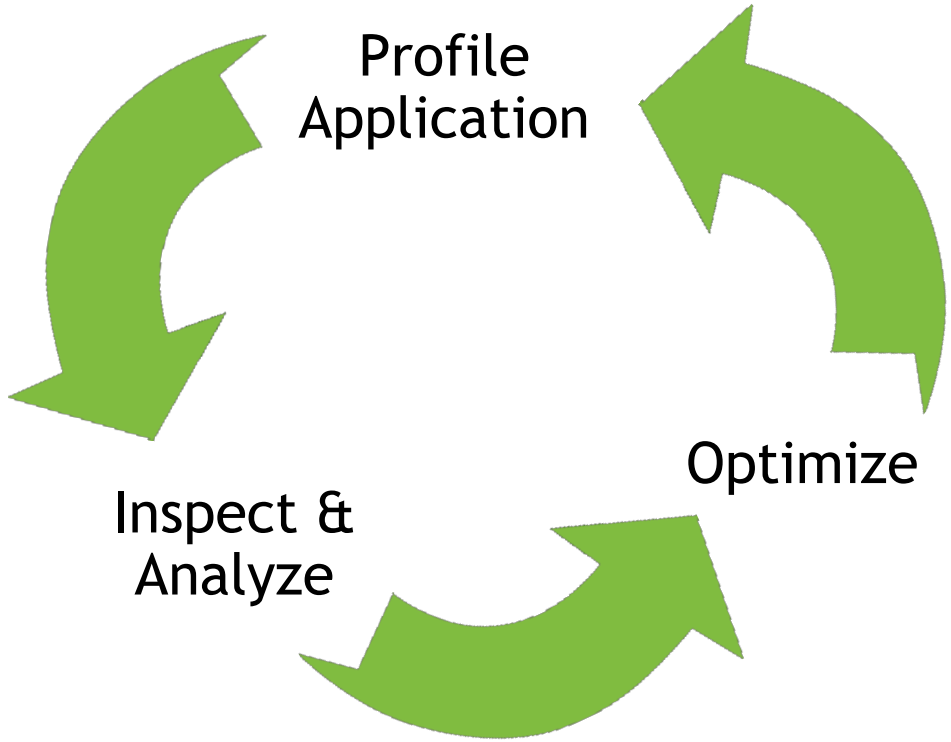
Nsight Systems – Introduction

OpenACC
More Science, Less Programming

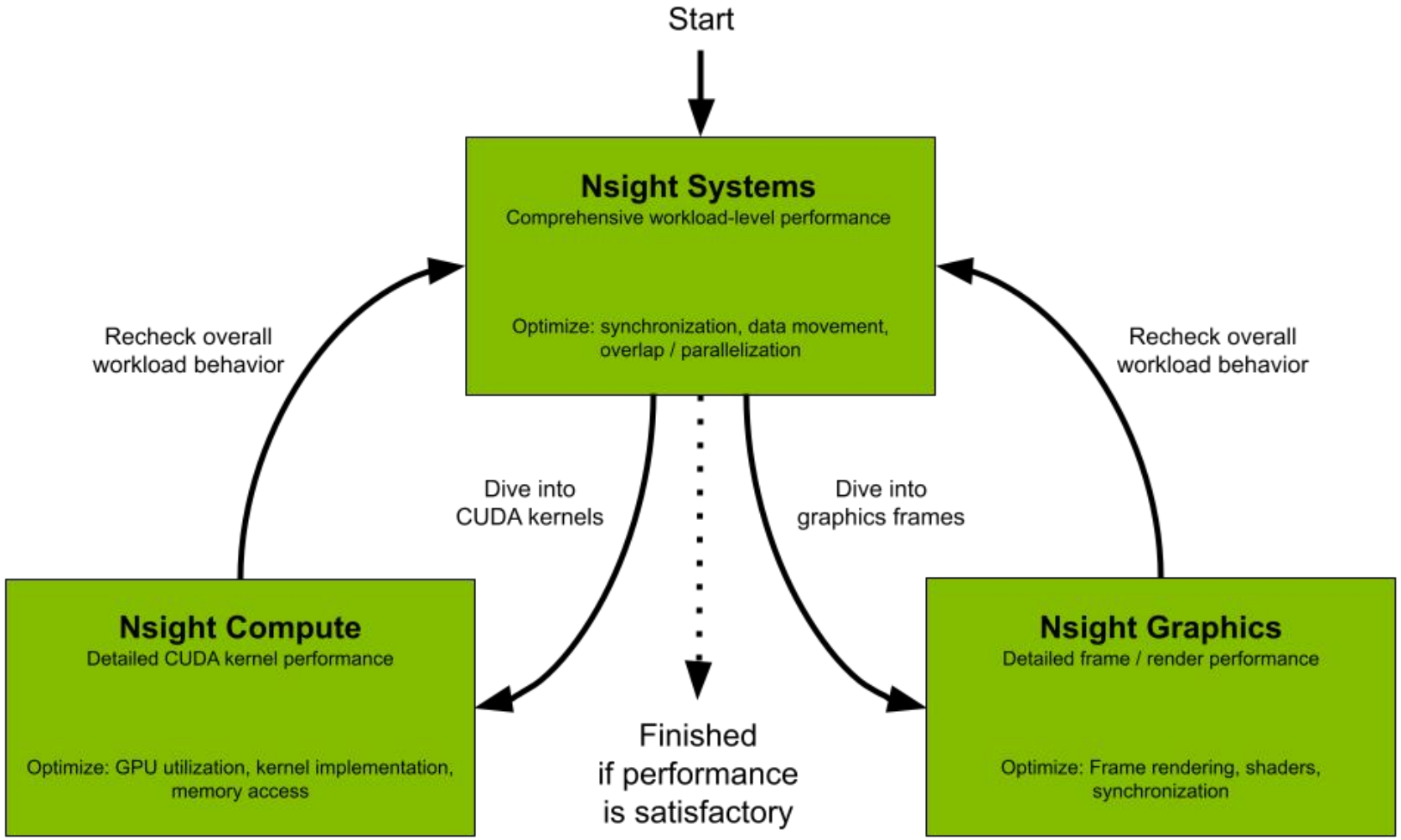
OPEN HACKATHONS

Typical Optimization Workflow



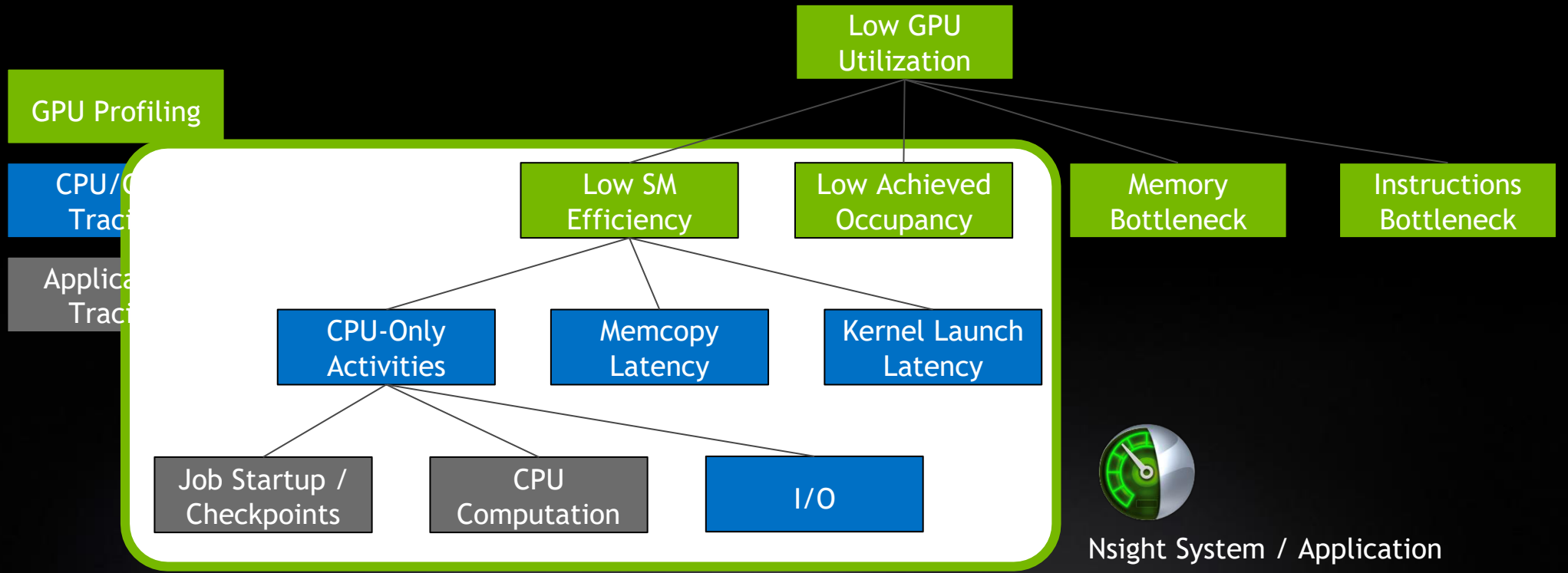
Iterate until desired performance is achieved

NVIDIA Performance Analysis Tools



PROFILING GPU APPLICATION

Focusing System Operation



Nsight System / Application Tracing

NVIDIA

PROFILING GPU APPLICATION

Focusing GPU Computing

GPU Profiling

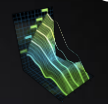
CPU/GPU Tracing

Application Tracing

Low GPU Utilization

- Low SM Efficiency
- Low Achieved Occupancy
  - Too few threads
  - Register limit
  - Large shared memory
  - …
- Memory Bottleneck
  - Cache misses
  - Bandwidth limit
  - Access pattern
  - …
- Instructions Bottleneck
  - Arithmetic
  - Control flow
  - …

NVIDIA (Visual) Profiler / Nsight Compute



NVIDIA Supports them with cuDNN, cuBLAS, and so on

System-Wide Application Tuning

Maximize your GPU Investment

Locate optimization opportunities

- Visualize millions of events on a timeline
- See gaps of unused CPU and GPU time

Balance your workload across multiple CPUs and GPUs

- CPU utilization and thread state
- GPU streams, kernels, memory transfers, etc.
- NIC performance metrics & tracing of network libraries

Multi-platform support

- Linux, Windows and Mac OS X (host-only)
- x86-64, Power9, ARM server, Tegra (Linux & QNX)

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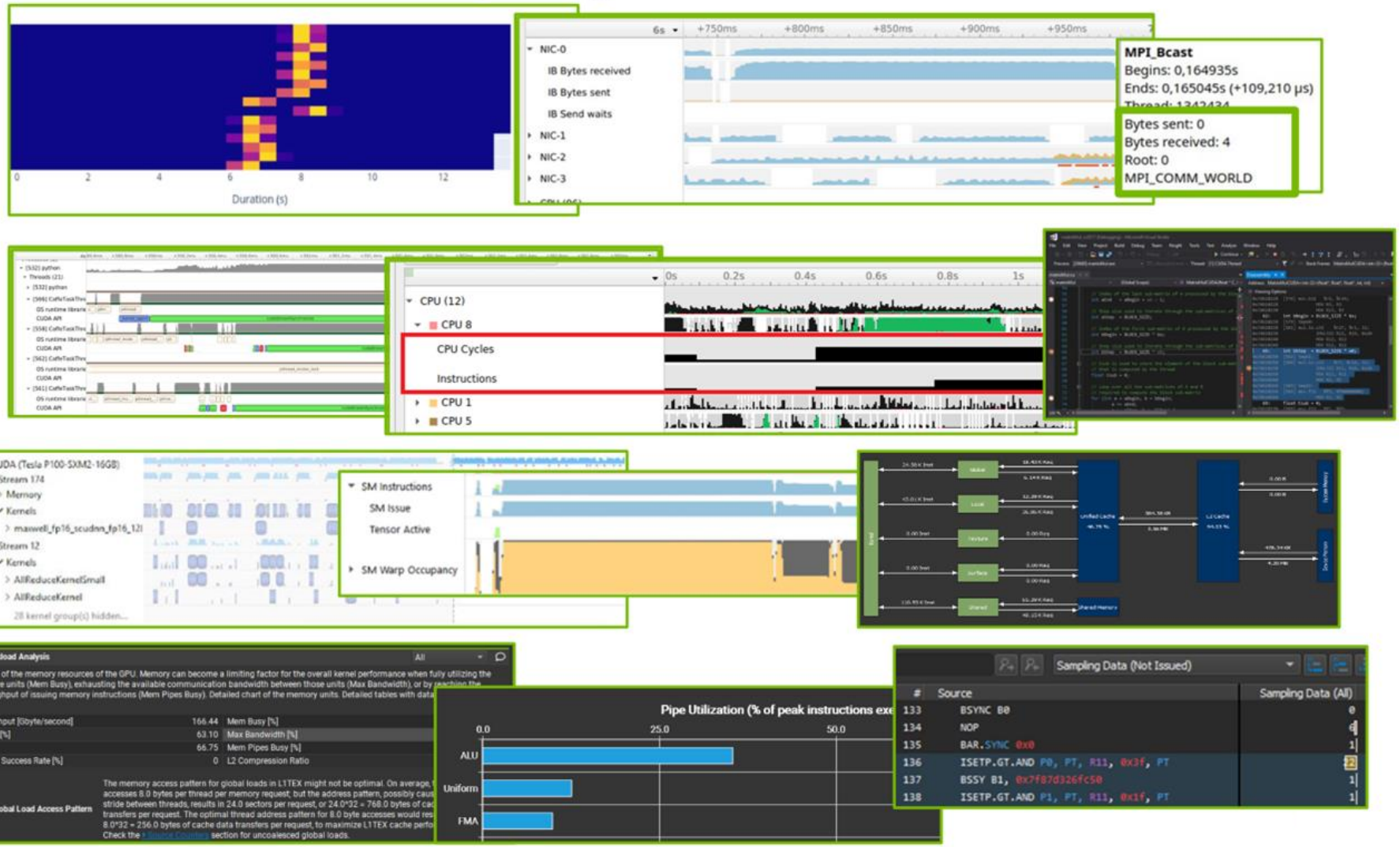
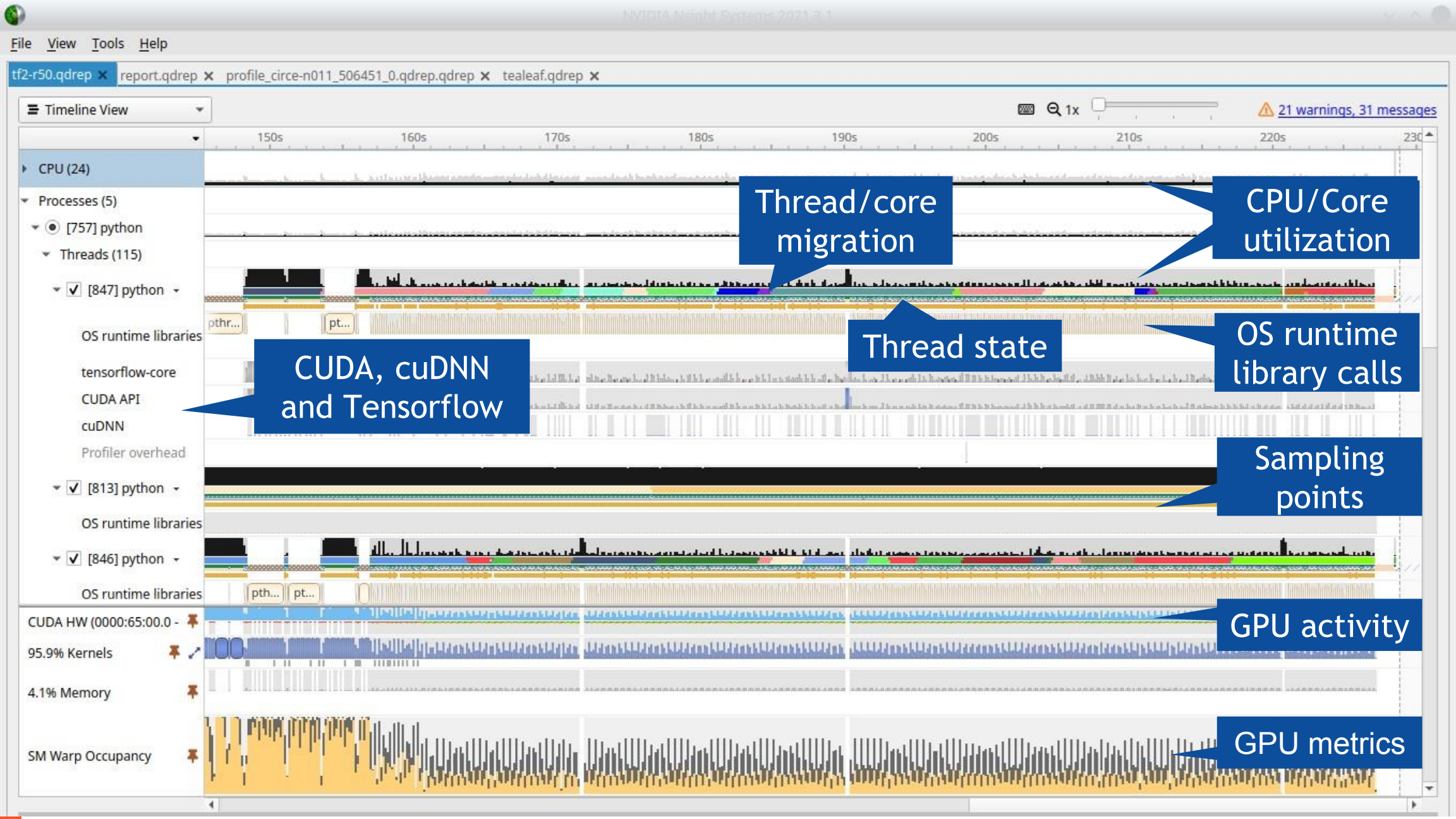
From the Macro to the Micro

Putting it all together




File View Tools Help
tf2-r50.qdrep
report.qdrep
profile_circe-n011_506451_0.qdrep.qdrep
tealeaf.qdrep
Timeline View
1x
21 warnings, 31 messages
150s
160s
170s
180s
190s
200s
210s
220s
CPU (24)
Processes (5)
[757] python
Threads (115)
[847] python
OS runtime libraries
tensorflow-core
CUDA API
cuDNN
Profiler overhead
[813] python
OS runtime libraries
[846] python
OS runtime libraries
CUDA HW (0000:65:00.0 -
95.9% Kernels
4.1% Memory
SM Warp Occupancy
Thread/core migration
CPU/Core utilization
Thread state
OS runtime library calls
CUDA, cuDNN and Tensorflow
Sampling points
GPU activity
GPU metrics

Command Line Interface (CLI) Statistics and Export to SQLite, JSON, etc.

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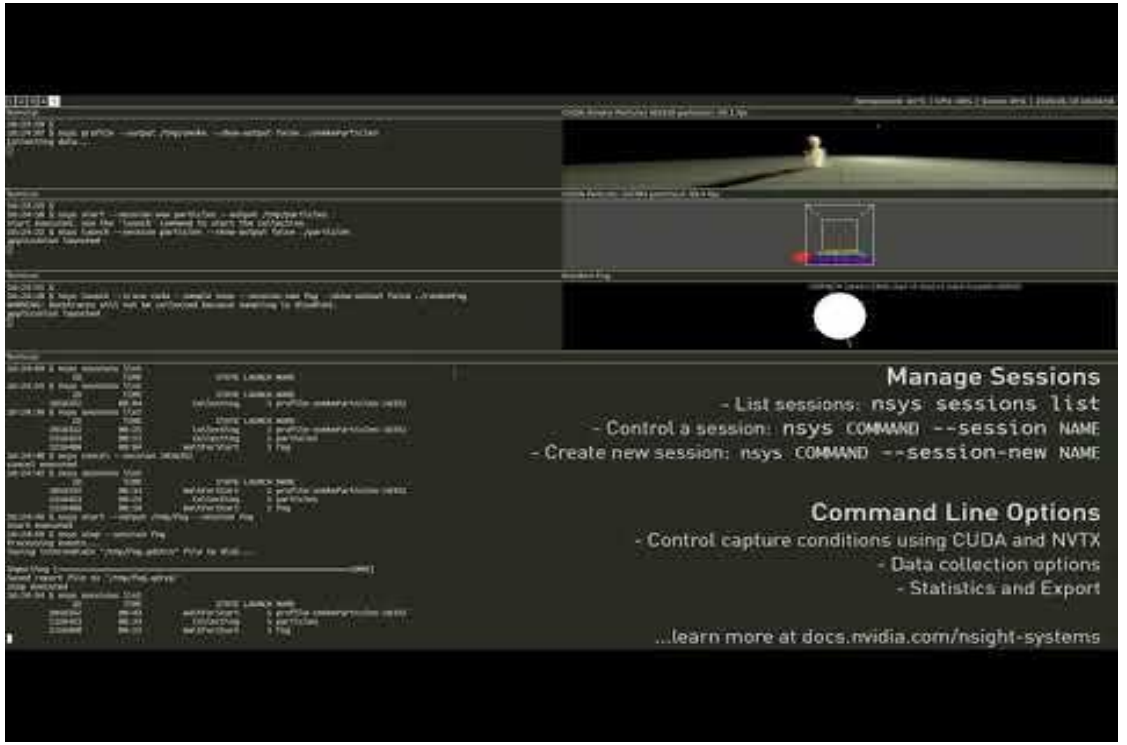
Command Line Interface

- The Nsight Systems CLI provides several different commands
  - Basic profiling session
    `nsys profile ./app`
  - Interactive sessions (scriptable)
    `nsys start|launch|stop|cancel`
    `nsys session list`
    `nsys status|shutdown`
  - Statistics and export
    `nsys stats|export`
    (export to sqlite, hdf, text, json, info)



YouTube: Nsight Systems - Command Line Sessions Feature spotlight

CLI Profiling - Some Useful Switches

- API tracing
- `-t, --trace=cuda,nvtx,osrt,opengl`
- `(cublas,cusparse,cudnn,mpi,oshmem,ucx,openacc,openmp,vulkan,none)`
- Overwrite existing report
- `-f, --force-overwrite=[true|`**`false`**`]`
- Summary statistics (profile output on command line)
- `--stats=[true|`**`false`**`]`
- Report file name
- `-o, --output=report#`
  `(patterns for hostname, PID and environment variables)`

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CLI Profiling - Some Useful Switches

- Callstack sampling
  - `-s, --sample=[`**`cpu`**`|none]`
  - `--sampling-period=`*number of CPU Instructions Retired events*
  - `-b, --backtrace=[`**`lbr`**`|fp|dwarf|none]`
  - `--samples-per-backtrace={`**`1`**`..12}`

    (The number of CPU IP samples collected for every CPU IP sample backtrace collected.)

- Set the paranoid level: "`sudo sh -c 'echo 1 >/proc/sys/kernel/perf_event_paranoid`'
- CUDA memory usage
  - `--cuda-memory-usage=[true|`**`false`**`]`
- (Use `nsys profile --help` for a list of available options.)

CLI Profiling - MPI Programs

- **Single Node**
- `nsys profile [nsys_args] mpirun [mpirun_args] your_executable`
- ⇨ This creates one report file.

- **Multiple Nodes**
- `mpirun [mpirun_args] nsys profile [nsys_args] your_executable`
- Set output report name with `-o report_name_%q{OMPI_COMM_WORLD_RANK}`
- (for OpenMPI, `PMI_RANK` for MPICH and `SLURM_PROCID` for Slurm)

- ⇨ This creates one report file per MPI rank.

Profile only specific ranks. ⇨

```
#!/bin/bash
# OMPI_COMM_WORLD_LOCAL_RANK for node local rank
if [ $OMPI_COMM_WORLD_RANK -eq 0 ]; then
  nsys profile -t mpi "$@"
else
  "$@"
fi
```

CLI Profiling - Additional Output

```
WARNING: The command line includes a target application therefore the CPU context-switch scope has been set to process-tree.
Collecting data…
  … APP OUTPUT …
Processing events...
Saving temporary "/tmp/nsys-report-2b96-9038-d0bd-2600.qdstrm" file to disk...

Creating final output files...
Processing [==========================================================100%]
Saved report file to "/tmp/nsys-report-2b96-9038-d0bd-2600.nsys-rep"
Report file moved to "/final/destination/report.nsys-rep"
```

Temporary data is written to **/tmp/nvidia/nsight_systems** by default. Set **TMPDIR** to specify another location.

CLI Stats Output

- CUDA API, kernels and memory operations (by time and by size)
- OS runtime
- NVTX

NVTX Push-Pop Range Statistics:

Time(%)	Total Time (ns)	Instances	Average	Minimum	Maximum	Range
80,0	16.193.376.534	21.268	761.396,0	6.823	2.438.848	MPI:MPI_Waitall
18,0	3.680.937.672	8.072	456.013,0	1.726	1.932.681	MPI:MPI_Allreduce
0,0	88.587.708	4	22.146.927,0	21.714.183	22.579.671	MPI:MPI_Init
0,0	57.888.066	21.268	2.721,0	1.319	297.466	MPI:MPI_Isend
0,0	24.282.234	21.268	1.141,0	872	16.931	MPI:MPI_Irecv
0,0	8.793.048	4	2.198.262,0	2.181.292	2.215.232	MPI:MPI_Finalize
0,0	3.814.158	28	136.219,0	2.302	1.265.786	MPI:MPI_Barrier
0,0	266.630	32	8.332,0	832	104.980	MPI:MPI_Reduce

CUDA Kernel Statistics:

Time(%)	Total Time (ns)	Instances	Average	Minimum	Maximum	Name
37,0	7.344.350.347	8.568	857.183,0	851.546	876.922	device_tea_leaf_ppcg_solve_calc_sd_new(kernel_info_t, dou
36,0	7.229.217.310	8.568	843.746,0	839.323	899.482	device_tea_leaf_ppcg_solve_update_r(kernel_info_t, double
10,0	2.050.961.573	2.010	1.020.378,0	1.005.849	1.036.569	device_tea_leaf_cg_solve_calc_ur(kernel_info_t, double, d
9,0	1.879.919.365	2.010	935.283,0	913.754	1.214.808	device_tea_leaf_cg_solve_calc_w(kernel_info_t, double*, d
5,0	1.008.596.179	1.980	509.392,0	501.469	521.756	device_tea_leaf_cg_solve_calc_p(kernel_info_t, double, do
0,0	61.606.046	30	2.053.534,0	1.176.600	2.890.541	device_tea_leaf_calc_rrn(kernel_info_t, double const*, do
0,0	38.094.843	12.336	3.088,0	1.887	13.184	void reduction<double, (REDUCTION_TYPE)0>(int, double*)

NVTX
NVIDIA Tool Extension Library

NVTX

NVIDIA Tool Extension Library

NVTX provides means to correlate the profile data with the application code.

```
#include <nvtx3/nvToolsExt.h>
…
nvtxMark("Point in time");

nvtxRangePush("Name of your code region");
// your code goes here
nvtxRangePop();

nvtxRangeId_t rid = nvtxRangeStart("Name of another code region"
// stop might be on another thread
nvtxRangeEnd(rid)
```

Add **nvtx** to the tracing options of **nsys profile**.)

NVTX

Domains and Resource Naming

```
nvtxDomainHandle_t yourDomain = nvtxDomainCreateA("My Domain");

nvtxEventAttributes_t evtAttr = {0};
evtAttr.version = NVTX_VERSION;
evtAttr.size = NVTX_EVENT_ATTRIB_STRUCT_SIZE;
evtAttr.messageType = NVTX_MESSAGE_TYPE_ASCII;
eventAttrib.message.ascii = "My Range";

nvtxDomainRangePushEx(yourDomain, &evtAttr);
// your code
nvtxDomainRangePop(yourDomain);


// #include <sys/syscall.h>
nvtxNameOsThreadA(syscall(SYS_gettid), "My Thread");
```

NVTX

Registered Strings

```
nvtxDomainHandle_t yourDomain = nvtxDomainCreateA("My Domain");
nvtxStringHandle_t yourStrHdl =
     nvtxDomainRegisterStringA(yourDomain, "My String Handle");

nvtxEventAttributes_t evtAttr = {0};
evtAttr.version = NVTX_VERSION;
evtAttr.size = NVTX_EVENT_ATTRIB_STRUCT_SIZE;
evtAttr.messageType = NVTX_MESSAGE_TYPE_REGISTERED;
eventAttrib.message.registered = yourStrHdl;

nvtxDomainRangePushEx(yourDomain, &evtAttr);
// your code
nvtxDomainRangePop(yourDomain);
```

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https://github.com/NVIDIA/NVTX

NVTX

Fortran Bindings

The NVIDIA HPC SDK Fortran compiler provides NVTX bindings.

- **`libnvhpcwrapnvtx.[a|so]`** has to be linked
- Documentation can be found here: https://docs.nvidia.com/hpc-sdk/compilers/fortran-cuda-interfaces/index.html#cfnvtx-runtime

```
use nvtx
…
call nvtxStartRange("YourRange")
! some Fortran code
call nvtxEndRange
```

For other compilers, write your own Fortran NVTX bindings or use existing ones, e.g. https://raw.githubusercontent.com/maxcuda/NVTX_example/master/nvtx.f90

NVTX

Automatic code instrumentation

The NVIDIA HPC SDK and GNU compilers provide an automatic code instrumentation mechanism using respectively the options **-Minstrument** and **-finstrument-functions** with the __cyg_profile_* funcs

- **C/C++ example with gcc/g++ and option `-finstrument-functions` :**

https://developer.nvidia.com/blog/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx/

- **Fortran documentation with nvfortran:**

https://docs.nvidia.com/hpc-sdk/compilers/fortran-cuda-interfaces/index.html#cfnvtx-auto

NVTX

"Python developers can either use decorators `@nvtx.annotate()` or a context manager with `nvtx.annotate(..)`"

```
import nvtx

@nvtx.annotate("f()", color="purple")
def f():
    for i in range(5):
        with nvtx.annotate("loop", color="red"):
            # Python code goes here
```

Get NVTX Python module:
`python -m pip install nvtx`

Also see this blog or the docs: https://nvtx.readthedocs.io/en/latest/index.html

PyTorch CUDA provides NVTX bindings

```
from torch.cuda import nvtx

nvtx.range_push("YourCode")
# your Python code
nvtx.range_pop()
```

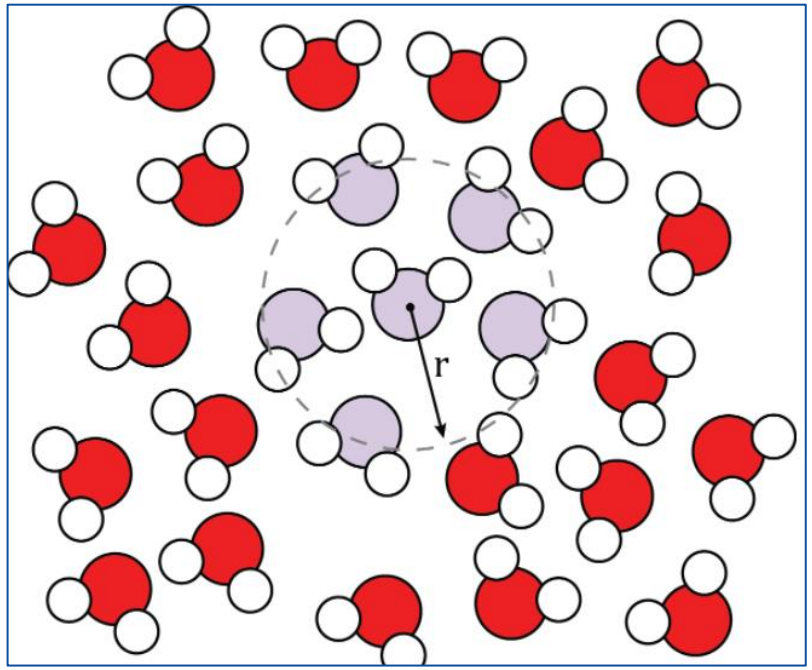
Application

APPLICATION

Molecular Simulation

RDF

The radial distribution function (RDF) denoted in equations by g(r) defines the probability of finding a particle at a distance r from another tagged particle.



RDF

Pseudo Code - C

```
for (int frame=0;frame<nconf;frame++){

            for(int id1=0;id1<numatm;id1++)
            {
                        for(int id2=0;id2<numatm;id2++)
                        {
                                    dx=d_x[]-d_x[];
                                    dy=d_y[]-d_y[];
                                    dz=d_z[]-d_z[];
                                    r=sqrtf(dx*dx+dy*dy+dz*dz);

                                    if (r<cut) {
                                                ig2=(int)(r/del);
                                                d_g2[ig2] = d_g2[ig2] +1 ;
                                    }
                        }
            }
}
```

- Across Frames
- Find Distance
- Reduction

RDF

Pseudo Code - Fortran

```
do iconf=1,nframes
  if (mod(iconf,1).eq.0) print*,iconf

  do i=1,natoms
    do j=1,natoms
                    dx=x(iconf,i)-x(iconf,j)
                    dy=y(iconf,i)-y(iconf,j)
                    dz=z(iconf,i)-z(iconf,j)

                    r=dsqrt(dx**2+dy**2+dz**2)
                    if(r<cut)then
                              g(ind)=g(ind)+1.0d0
                    endif
          enddo
  enddo
enddo
```

- Across Frames
- Find Distance
- Reduction