TECA 2.0

HPC Toolkit for Extreme Climate Analysis, v2.0

Recent advances

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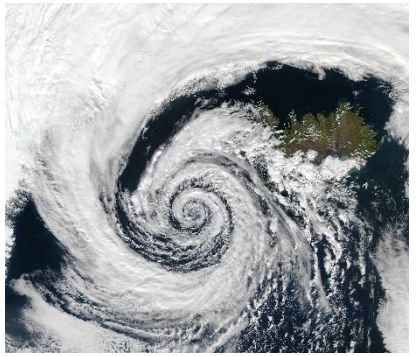
TECA 1.0 Recap

- TECA 1.0
  - 3 completely disparate command line programs
  - much in common/duplicated code
  - R&D code
  - Had major successes with these codes
    - Running 20 yrs archive in 1 hour on 750k cores on MIRA
    - Large runs on Edison
    - Numerous journal and conference pubs



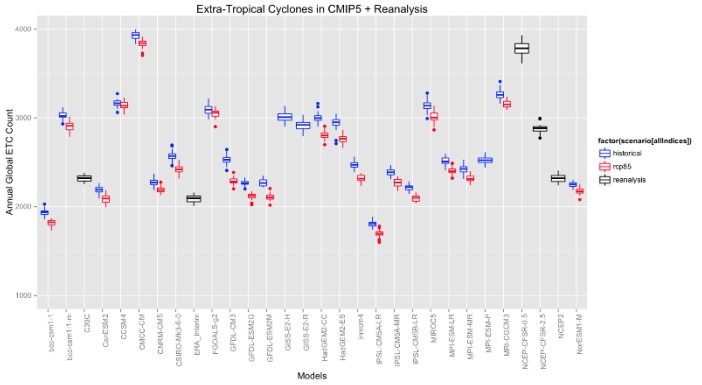


fig credit Prabhat et al AGU 2015

TECA 2.0

- Take the commonality amongst TECA 1.0 apps and design a framework to be shared by all
- Build on lessons learned from TECA 1.0 hero runs
- Port the TECA 1.0 apps to the 2.0 framework
- Transition code to many core architecture
- Design tenets
  - Performance
  - Usability
  - Modularity/code reuse
  - Reliability
- map-reduce pattern
- Parallel I/O, NetCDF CF 2, Satellite, VTK, etc
- Numerous analysis operators

On tap for the 2.0 release (Q1 ‘16)

- **Datasets**
  - 2/3D Cartesian mesh
  - Table
- **IO**
  - NetCDF CF-2 reader
  - table writer (xls, csv, bin)
  - Cartesian mesh writer (VTK)
- **Operators**
  - AR detector
  - TC/ETC Cyclone detectors
  - L2 norm
  - mask
  - connected components
  - programmable algorithm
  - Cartesian mesh regrid
  - Cartesian mesh subset
  - table map-reduce
  - temporal average
  - vorticity
- **Apps**
  - AR detect
  - TC detect
  - ETC detect

2.0 Framework

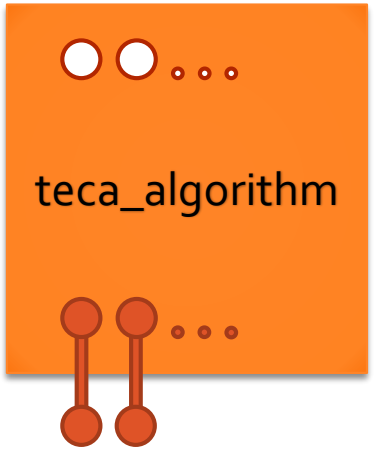
- based upon the pipeline design pattern
  - Extensibility
  - Modularity
  - Flexible, supports a variety of parallelization strategy
  - Efficiency, supports data sharing(threads) and caching
  - Easy to use, with out any in-depth knowledge (more later)
  - Parallelization can largely be hidden from end user

Framework details

- Performance
  - c++11
  - Template meta programming, inlining
  - Compiler auto vectorization
- Parallelization
  - MPI
  - threads
- Portability
  - STL
  - Cross platform, from big iron to laptop, Linux, Mac, (Windows).
  - CMake
- Usability
  - Python bindings

Pipeline details

- The “teca_algorithm”
  - defines the user facing interface
  - Contains all of the internal execution logic
  - Manages data sharing/caching across updates and between threads
  - Each instance has
    - 0 or more input connections
    - 0 or more output ports
  - Egs.
    - Reader (0 inputs, 1 output)
    - Simple operator (1 input, 1 output)
    - Writer (1 input, 0 output)



Pipeline interface

Building and running pipelines

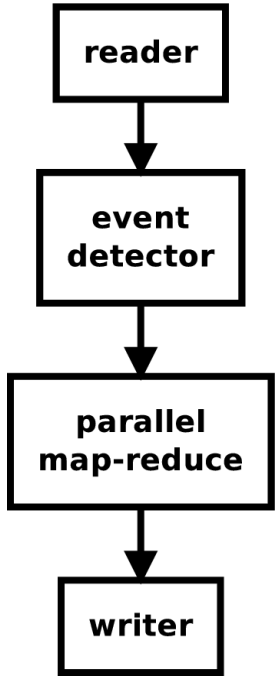
- get_output_port()
- set_input_connection(…)
- Update()

Dialing in specific settings

- set_[PROPERTY_NAME](…)

An example

```
from mpi4py import MPI
from teca_py_io import *
from teca_py_alg import *

# start the pipeline with the NetCDF CF-2.0 reader
cfr = teca_cf_reader.New()
cfr.set_files_regex('cam5_1_amip_run2\.cam2\.h2\.198[0-9].*')

# connect the tropical cyclone detector
tcd = teca_tc_detect.New()
tcd.set_pressure_variable('PSL')
tcd.set_temperature_variable('TMQ')
tcd.set_wind_speed_variable('wind_speed')
tcd.set_vorticity_variable('wind_vorticity')
tcd.set_input_connection(cfr.get_output_port())

# now add the map-reduce, the pipeline above is run in parallel using MPI+threads.
# Each thread processes one time step. the pipeline below this algorithm runs in
# serial on rank 0, with 1 thread
mapr = teca_table_reduce.New()
mapr.set_thread_pool_size(16)
mapr.set_first_step(0)
mapr.set_last_step(-1)
mapr.set_input_connection(tcd.get_output_port())

# save the detected stomrs
twr = teca_table_writer.New()
twr.set_file_name('detections_%t%.csv')
twr.set_input_connection(mapr.get_output_port())

# the commands above connect and configure the pipeline
# this command actually runs it
twr.update()
```



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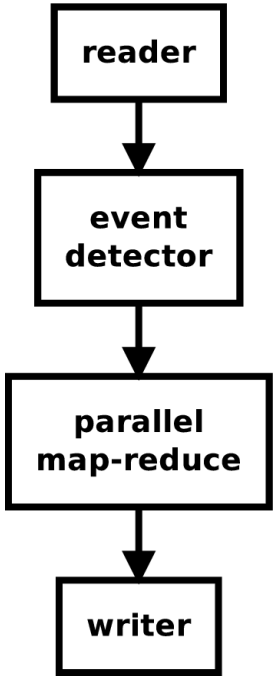
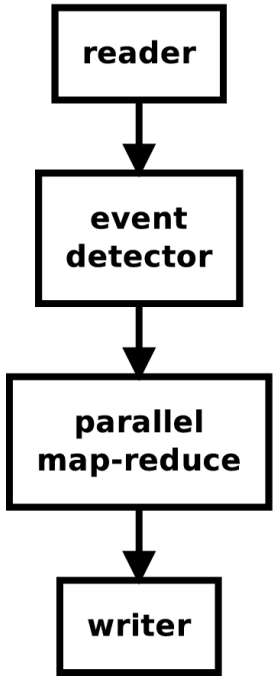
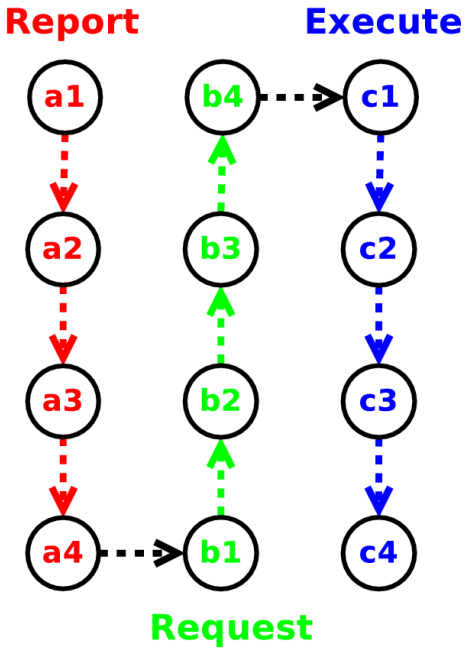
Only 2 lines of code make it parallel!



Serial execution

- 3 phases of execution
  - Report
    - Each stage reports the data it can produce
  - Request
    - For each output tell the upstream what data is needed
  - Execute
    - Make a computation, produce data, take some action, to fulfil the incoming request



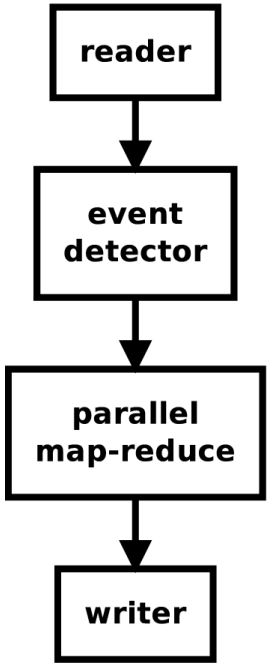


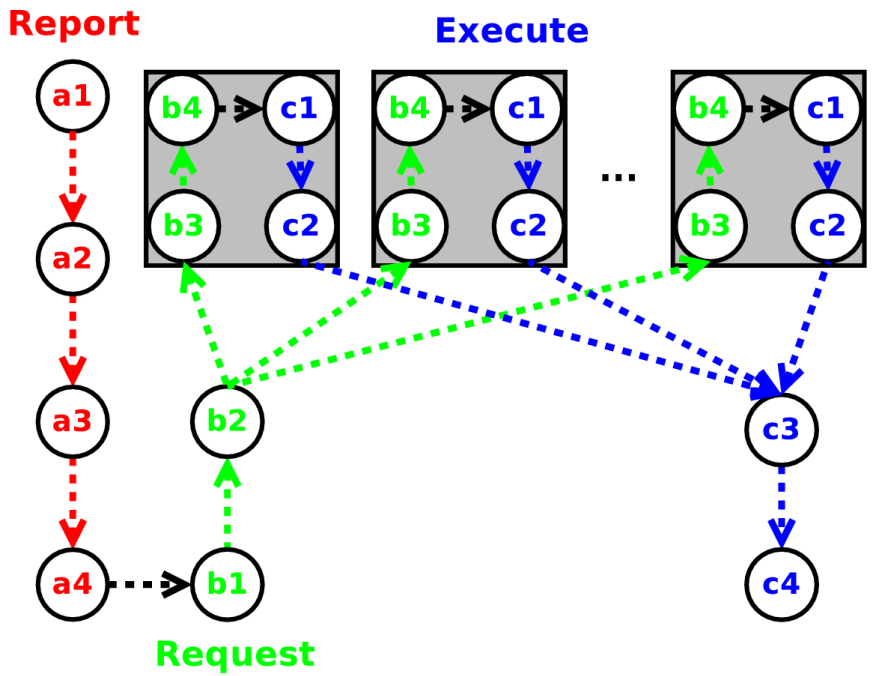
time: a1 - a4 - b1 - b4 - c1 - c4

Parallel execution

MPI+threads map-reduce

- time steps partitioned to MPI ranks
- a request is issued for each time step
- a thread pool executes the requests in parallel

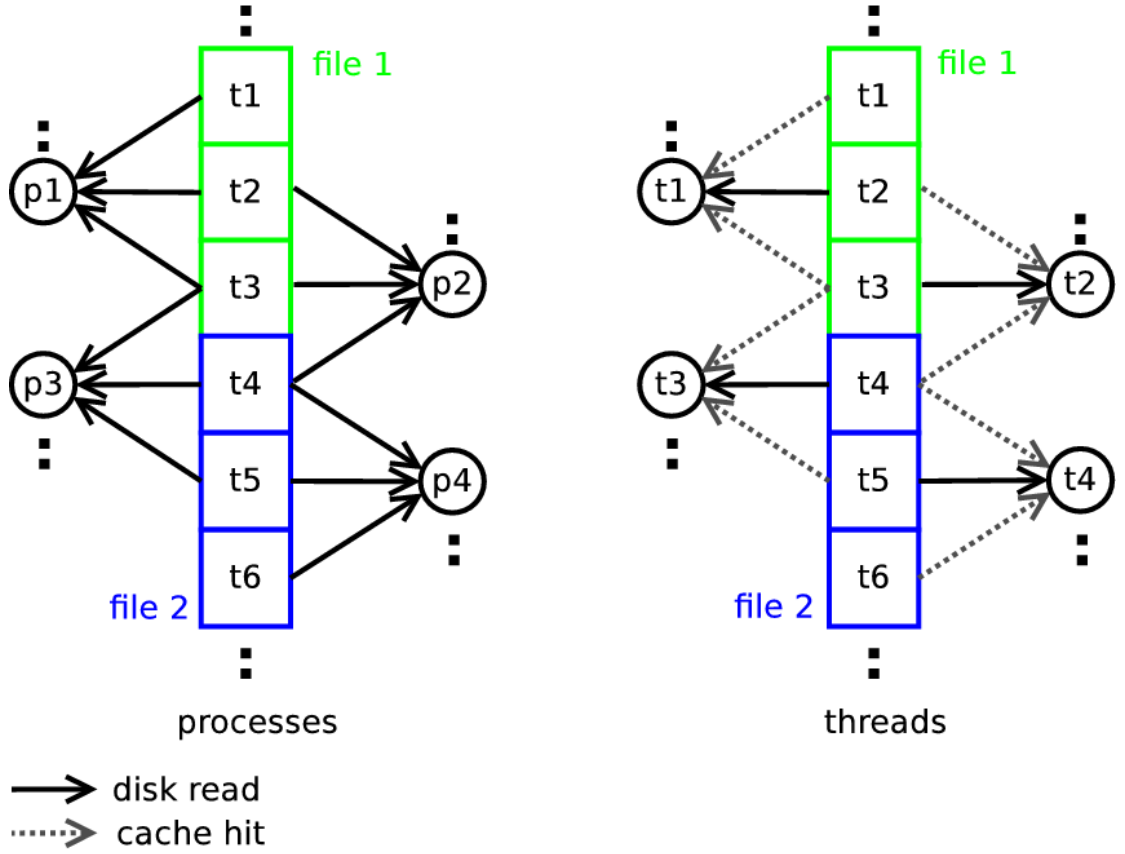




time: a1 - a4 - b1 - b4 - c1 - c4

Data sharing and I/O efficiency

- TECA 1, MPI only
  - 12 reads
  - each file opened/closed 3x
- TECA 2, MPI+threads
  - 4 reads, 8 cache hits
  - each file opened/closed 1x



Python

- Address c++/template meta programming usability issue
- Leverage external universe of scientific/numeric Python tools
- 2 approaches
  - Python as “glue” for building and executing pipelines
    - native c++ performance
  - Python operators, to do computations
    - numpy performance

teca_algorithm how to, method 1

- Override 1 or more of the 3 pipeline execution phase implementations
- Write native c++ to do the computations

```
// implementations must override this method to provide
// information to downstream consumers about what data
// will be produced on each output port.
virtual
teca_metadata get_output_metadata(
    unsigned int port,
    const std::vector<teca_metadata> &input_md);

// implementations must override this method and
// generate a set of requests describing the data
// required on the inputs to produce data for the
// named output port, given the upstream meta data
// and request.
virtual
std::vector<teca_metadata> get_upstream_request(
    unsigned int port,
    const std::vector<teca_metadata> &input_md,
    const teca_metadata &request);

// implementations must override this method and
// produce the output dataset for the port named
// in the first argument. The second argument is
// a list of all of the input datasets. See also
// get_request. The third argument contains a request
// from the consumer which can spcify information
// such as arrays, subset region, timestep etc.
virtual
const_p_teca_dataset execute(
    unsigned int port,
    const std::vector<const_p_teca_dataset> &input_data,
    const teca_metadata &request);
```

teca_algorithm how to, method 2

- Provide callbacks for 1 or more execution phases to the teca_programmable_algorithm
- Any “callable”
  - c functions
  - FORTRAN functions (ISO-C Bindings)
  - c++ lambdas, functions, and objects

```
// report phase
teca_metadata
report_callback(unsigned int port,
    const std::vector<teca_metadata> &input_md)
{
    // your code goes here
}

// request phase
std::vector<teca_metadata>
request_callback(unsigned int port,
    const std::vector<teca_metadata> &input_md, const teca_metadata &req)
{
    //  your code goes here
}

// execute phase
const_p_teca_dataset execute_callback(unsigned int port,
const std::vector<const_p_teca_dataset> & in_data,
const teca_metadata &req)
{
    // your code goes here
}

// set up the programmable algorithm and connect
p_teca_programmable_algorithm alg = teca_programmable_algorithm::New();
alg->set_number_input_connections(1);
alg->set_number_of_output_ports(1);
alg->set_report_callback(report_callback);
alg->set_request_callback(request_callback);
alg->set_execute_callback(execute_callback);
alg->set_input_connection(other_alg->get_output_port());
```

teca_algorithm how to, method 3

- Pure Python solution
- Provide 1 or more callbacks
- NumPy performance

```
# a simple TECA algorithm that computes wind speed
def report_callback(o_port, rep_in):
    # add the names of the variables we could generate
    rep_in[0].append('variables', 'wind_speed')
    return rep_in[0]

def request_callback(o_port, rep_in, req_in):
    # add the name of arrays that we need to compute
    req_in['arrays'] = ['U850', 'V850']
    return [req_in]

def execute_callback(o_port, data_in, req_in):
    # pass the incoming data through
    in_mesh = as_teca_cartesian_mesh(data_in[0])
    out_mesh = teca_cartesian_mesh.New()
    out_mesh.shallow_copy(in_mesh)
    # pull the arrays we need out of the incoming dataset
    arrays = out_mesh.get_point_arrays()
    u = arrays['U850']
    v = arrays['V850']
    # compute the derived quantity
    w = np.sqrt(u*u + v*v)
    # add it to the output
    arrays['wind_speed'] = w
    # return the dataset
    return out_mesh

# add our wind speed computation
alg = teca_programmable_algorithm.New()
alg.set_report_callback(report_callback)
alg.set_request_callback(request_callback)
alg.set_execute_callback(execute_callback)
alg.set_input_connection(cfr.get_output_port())
```

Conclusion

- TECA 1 has had many successes
- In TECA 2 we are building on those successes while addressing usability and performance issues and transitioning to many core architectures.
- TECA 2 public release Q1 ’16