End-to-end optimization potentials in HPC applications for NWP and Climate Research

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and
Many Colleagues

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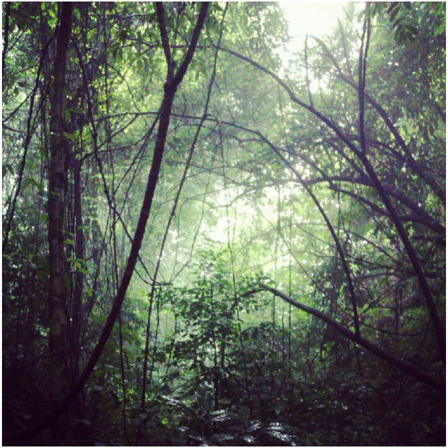
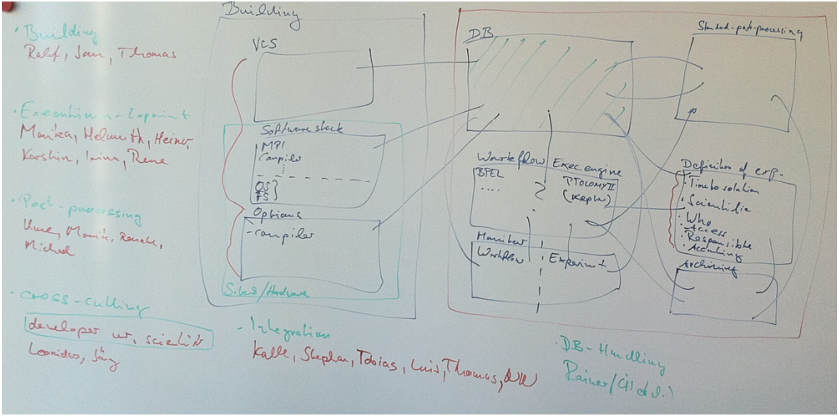


. . . or a guided tour through the jungle . . .

Joint DKRZ/MPIM initial brainstorming



Courtesy of Joachim Biercamp, DKRZ

Rationals

Why do end-to-end management?

- Scientific responsible experimentation support

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- Scientific responsible experimentation support
- *Reduce workload of all members of the numerical experimentation community . . .*

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- Title, statement of problem, and hypothesis

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- Publication of the results

The context

What is our context?

- complex, non-standardized workflows and toolchains
- various processing steps by various actors
- in climate research as well very often changing workflows

Important to note - we are not doing mainstream computing!

Target: provenance of the whole data life cycle

Focus on adding:

- primary data generation
- primary data processing

Already available to a large extent:

- data publishing
- secondary data processing
- data distribution
- further not controlable data processing

Scientists

- define experiment easily
- should organize their individual experiments workflow easily
- should be enabled to program their individual tasks
- should not care on collecting provenance data

Scientific programmers

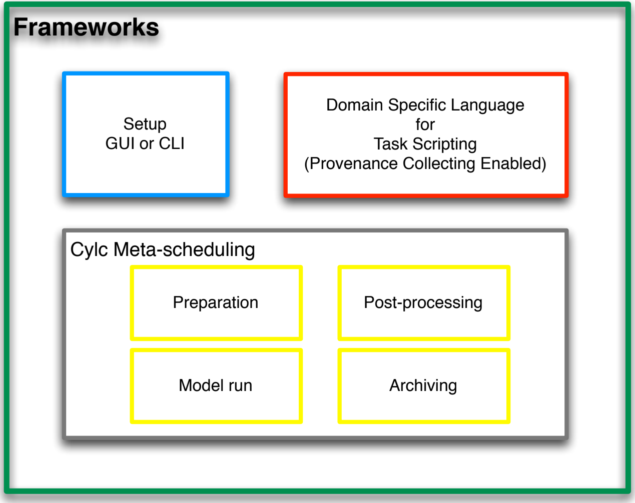
- define experiment easily
- should organize experiment workflows easily
- should be enabled to program individual tasks
- should not care on collecting provenance data

- should be enabled to query provenance data for bug tracking, performance improvements, . . .

Computing center staff

- should not care on collecting provenance data
- should be enabled to query provenance data for failure analysis, performance improvements, . . .

Components of the basic systems



Frameworks

Setup
GUI or CLI

Domain Specific Language
for
Task Scripting
(Provenance Collecting Enabled)

Cylc Meta-scheduling

Preparation

Post-processing

Model run

Archiving

Tools

Packages in use:

- python as scripting language
- postgres - provenance data collection
- subversion/git (migration to git for parts or all later, if model developers get convinced)
- cmake (migration from autotools and self-maintained makefile generator)
- Web interface for site and compiler dependencies; dependencies versioned in line with model code
- namelist migration to xml as model source code, user interfaces: a kind of namelist and a GUI.

Single task component

Scripting

- user friendly modeling language
- restartability
- exception and error handling in scientist understandable form
- full support of modern programming concepts
- use the python hype to change from shell to python

Model build requirements

Standardized, convenient, and fast tools

- out-of-source build

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- make, with hooks for actions at certain steps
- make test
- make install

Use of optimized codes: mpiesm and icon

In use

- vectorization (we never gave up on this!), hand gather, scatter, merge instead of standard conditionals, and exposing transcendentials
- nproma blocking for different architectures
- OpenMP orphaning - whole physics including radiation run in an single OpenMP directive
- MPI implementation constantly revisited including building up static load-balancing strategies
- real asynchronous parallel I/O
- invest in optimization of libraries

Maybe give up on bit-reproducability for production,
but not for development!

Data compression

On top compression for grib2: AEC (CCSDS algorithm).

a standardization exercise

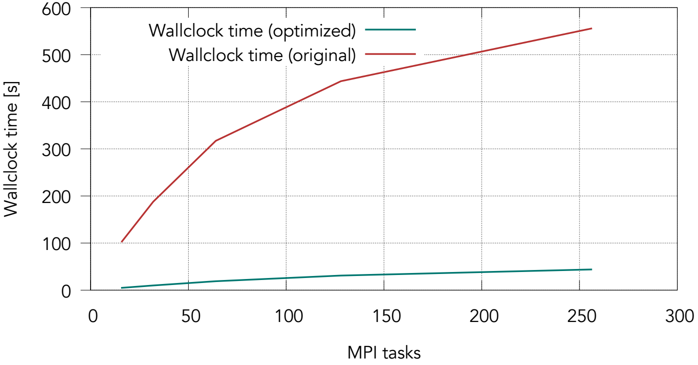
- got NASA US patent released
- reimplement from scratch to go around commercial copyright
- define grib2 template for WMO
- validate with independent software stacks (Q4 2014)

- *Average reduction in data size over 4-byte float: factor 5, and for grib2 2.5.*
- *Encoding and decoding are really, really fast.*
- *Get this ported to netcdf4 (hdf5), started but process is slow.*

Joint work of Mathis Rosenhauer, DKRZ, Shahram Najm, ECMWF,

Uwe Schulzweida, and Luis Kornblueh

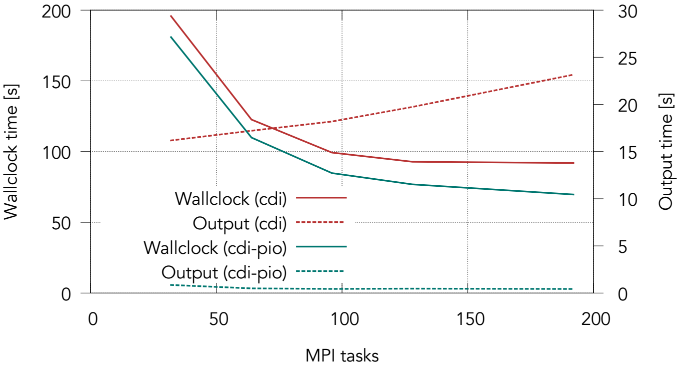
ICON ocean scaling improvements



Ocean scaling improvements: no land points, gmres restart, hybrid MPI/OpenMP, code rewrite.

Courtesy of Leonidas Linardakis

ECHAM6 scaling improvements



Change from serial (cdi) to parallel output (cdi-pio, using RDMA, I/O time on compute nodes is essentially zero).

Courtesy of Irina Fast, Thomas Jahns, DKRZ, and Deike Kleberg

Use of optimized post-processing tools

Extend and improve our toolchain (cdi and cdo)

Available

- basic optimized code
- compute intensive operators are OpenMP parallelized
- processing of data can be handled by an threaded pipelining method

Future

- data streaming instead of file storage transfer
- DAG based processing for highest possible parallel efficiency
- database information system for online data

Experiment organization

cylc - the Meta-Scheduler

- design your own distributed suites of inter-dependent cycling tasks efficient, modular, and reusable
- validate and visualize workflows on the fly
- control your running suites
- diagnose failures (easily!?)
- simplify failure recovery
- benefit from expert experience with a specialized tool for meteorological forecasting systems

Courtesy of Hilary Oliver, NIWA and contributors

A task modeling framework (provenance data collection)

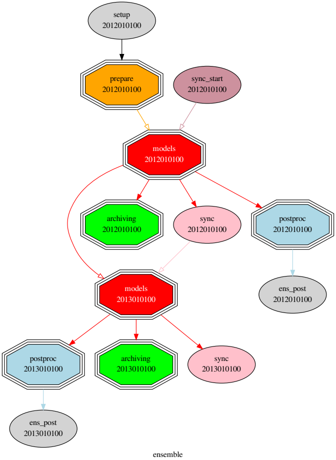
Cylc controled tasks and provenance collection

- high level programming language — python
- embedded abstraction layer for file operations
- abstract task description
- embedded provenance data collection (database stored)
- tightly connected to cylc
- connect provenance enabled workflow to ESGF data distribution

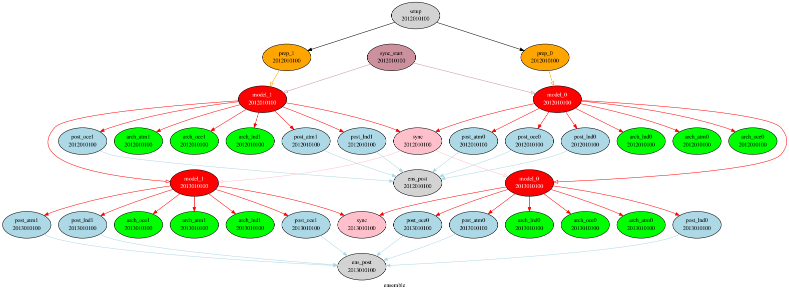
Remark: introduces complexity reduction methods to all users

Courtesy of Deike Kleberg, MPIM and Pavan Siligam, DKRZ

Ensemble overview



Ensemble detail



A cylc optimization step

- connect cylc from inside application (in C)
- use curl for submitting http/POST request to a WebServer
- POST triggers CGI as interface to cylc
- Later: server part integrated into cylc

Do not poll! It is expensive!

What is coming next?

- Primary target:
  Get an optimized worflow system working AT OUR SITE!
- Keep being conservative in model source code adaptation: concentrate on what we have
- But:
  Outsource exploration of GPU handling (CSCS) and take over necessary changes
- Constantly observe development directions
- Explore CS concepts in the easier context of post-processing
- Do:
  Tutorials and training, training and tutorials, tutorials and training, . . .