Adventures in Vectorizing the Community Land Model

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CLM data model

- Grid cells
  - Same horizontal grid as CAM
- Land units
  - Percentages of grid cell, not contiguous region
  - Soil properties, landcover types (lakes, glaciers)
- Columns
  - Soil states, fluxes with atmosphere
- Plant functional types (PFTs)
  - Compete for column resources
CLM vectorization history

- CLM 2.1 introduced “vector-hostile” data structures
- Experiments with simple vector data structure presented at CUG 2003
- CLM re-implemented with compromise data structure over last year
- Ongoing performance optimization
CLM 2.1 challenges

• High-level loops over columns
• Deep call stacks passing single-column arguments
• Very short inner loops
  – PFTs (currently length 1, 1-20 in future)
  – Soil and snow levels (single digits negligible work)
• Data structure…
CLM 2.1 data structures

• Nested user-defined types
  – Embedded pointers to sub-types
  – Arrays of pointers to sub-levels
  – Pointers up to parent level
  – Scalar quantities

• Subroutine structure
  – Pass single column argument, "c"
  – Declare (many!) local pointers
  – Associate local pointers with contents of "c"
  – Compute with local pointers as shorter aliases
CUG 2003 CLM experiment

I did this! Other authors did everything else.

- Implemented new data structures for one major physical process
- No user-defined types
- Major types become modules
  - Grid cells, land units, columns, PFTs
- "Flatten" remaining types
  - Scalar variables become 1D arrays
  - Arrays add a leading dimension
- Illustrated need for filters (index arrays) to replace if statements
CLM3.0 data structures

- Arrays of derived types → derived types with (pointers to) arrays
- Retained type hierarchy
  - One instance of each type
- Clumps and filters
- Required major rewrite of CLM
Clumps for data decomposition

• Independent grid cells (coupled through atmosphere)
• Grid cells distributed cyclically into “clumps”
• Clumps distributed cyclically among processes
• Clumps sized for:
  – Cache blocking
  – Vector length
  – Load balancing
  – Shared-memory parallelism
    (OpenMP and/or CSD)
Filters for vectorization

- Implemented as index arrays
- Group columns and PFTs based on relevant physical processes
  - Snow/non-snow, lake/non-lake, bare soil
  - PFTs that use dynamic vegetation
- Some filters created once
- Dynamic filters for snow/non-snow and vegetation
CLM3.0 driver

• Each MPI process loops over clumps
  – OpenMP or CSD parallelism
  – Using both would require two loops

• Arguments passed to physics routines:
  – Clump bounds for relevant levels of type hierarchy (grid cell, land unit, column, PFT)
  – Relevant filters

• Inner loops over clump elements
  – Sometimes filtered
  – Clump arrays implemented with pointers requiring “!dir$ concurrent”
Vectorization process

• New data structures and vectorization strategy approved by Land Model Working Group and NCAR researchers
• Created vector development branch in NCAR CVS repository
• Modified one subroutine at a time
  – Tested for correctness and performance on X1 and IBM Power4
• Cooperated with CRIEPI (Earth Simulator)
  – Provided prototype code
  – Received compiler listings and suggestion from Dave Parks of NEC
Vectorization results

• Completed in October 2003
• CLM3.0 faster than CLM2.1
  – Improved 25.8x on X1
  – Improved 1.8x on IBM Power4
  – Smaller memory footprint
  – Simpler history updates
  – Simpler and fewer scatter/gathers
Performance comparisons

- Stand-alone CLM3.0 (though plots say CLM2)
- 90 simulated days at T85 resolution
- 1, 2, 4, 8, 16, 32, 64 MSPs
- 1, 2, 4, 8, 16, 32 clumps per MPI process
- Different shared-memory parallelism
  - Automatic multistreaming only
  - CSDs in driver
  - OpenMP in driver (with automatic multistreaming)
• Scales to 32 MSPs
• One clump per process works best
• Again, scales to 32 MSPs
• Need at least four clumps per process
  – One for each SSP
- Scales to 64 MSPs (16 MPI processes)
- Four MSPs per MPI process
  - Need at least four clumps
OpenMP vs. CSD

CLM2 Performance on Cray X1 (90 Day TB5 Offline Run with I/O)

- CSD Loops (dashed)
- OpenMP Loops (solid)
- 4 Clumps per process

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OpenMP vs. CSD, rematch

• CSDs removed January 6
• Restored April 27 because CCSM won’t use OpenMP on X1
  – Multiple-binary MPI on X1 requires every process uses same number of threads
  – POP not threaded
• OpenMP & CSD?
Trey’s conclusions

- Arrays of type hierarchies are bad for performance
  - Inhibit dependence analysis (and thus vectorization)
  - Reduce spatial locality
- Types with pointers to arrays require directives
  - Less safety, may camouflage real dependencies
  - Cray Fortran compiler allows allocatables (but others don’t yet)
- Lessons for language design
  - Changing a data structure can cause profound code churn
  - The “filter” concept needs integrated support