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

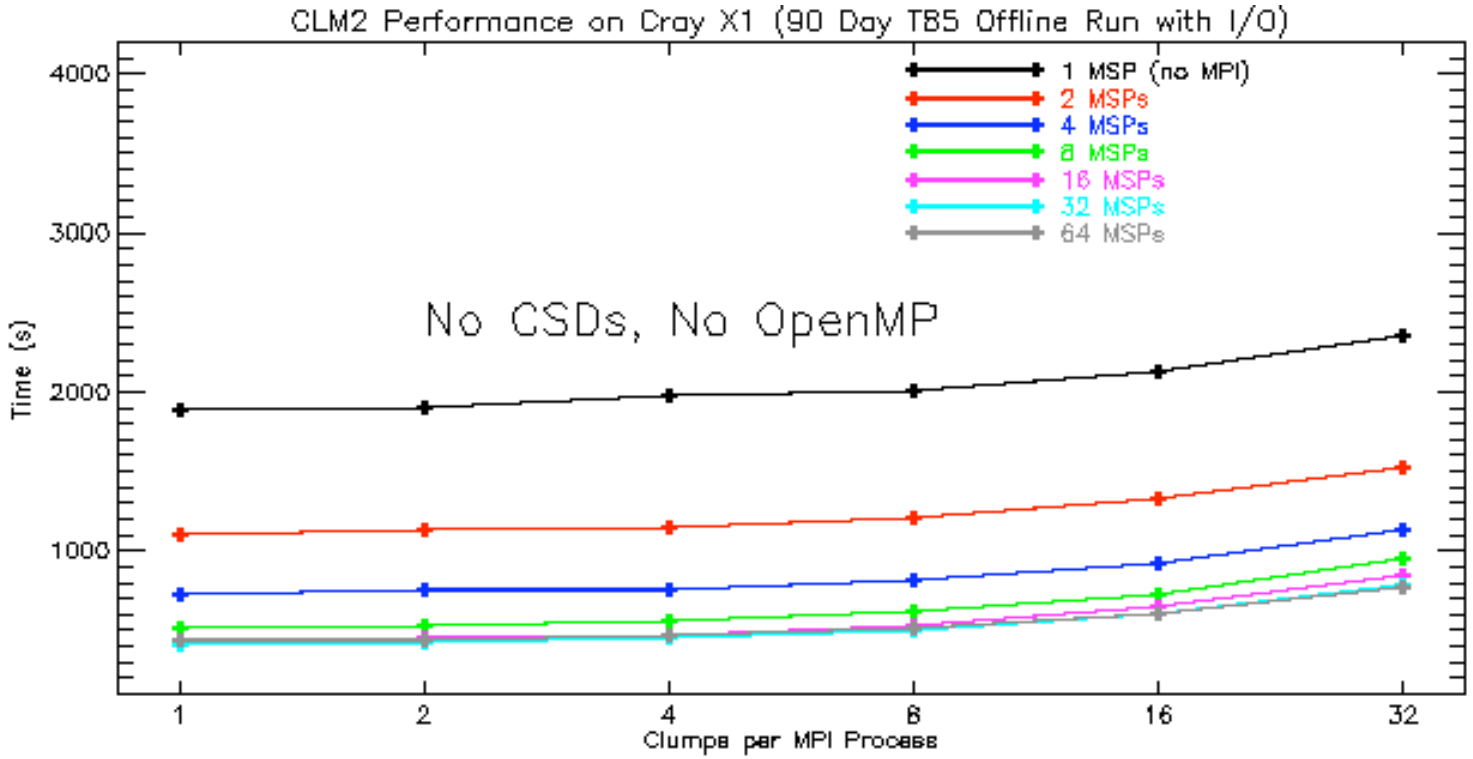
- New data structures and vectorization strategy approved by Land Model Working Group and NCAR researchers
- Created vector development branch in NCAR CVS repository
- Modified one subroutine at a time
  - Tested for correctness and performance on X1 and IBM Power4
- Cooperated with CRIEPI (Earth Simulator)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

Vectorization results

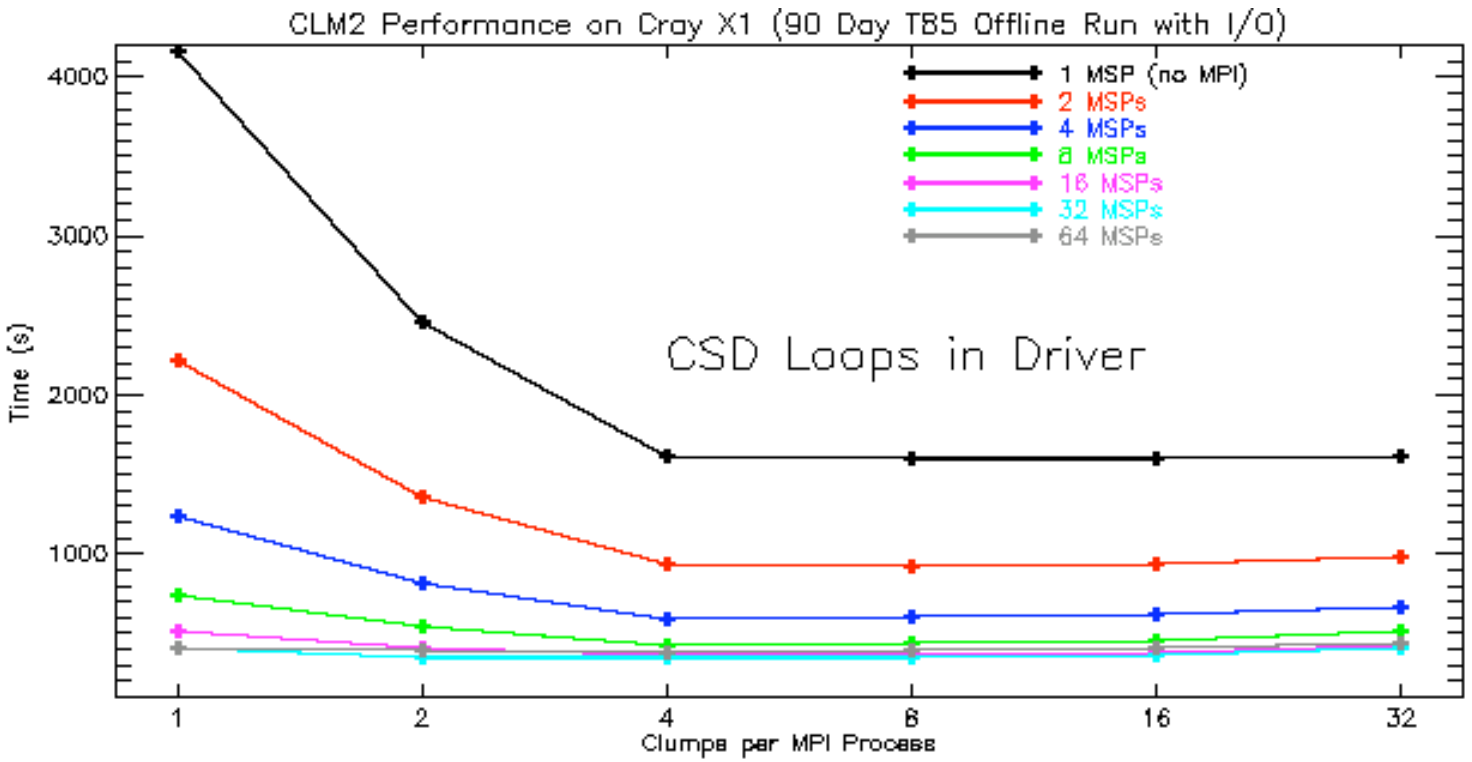
- Completed in October 2003
- CLM3.0 faster than CLM2.1
  - Improved 25.8x on X1
  - Improved 1.8x on IBM Power4
  - Smaller memory footprint
  - Simpler history updates
  - Simpler and fewer scatter/gathers

Performance comparisons

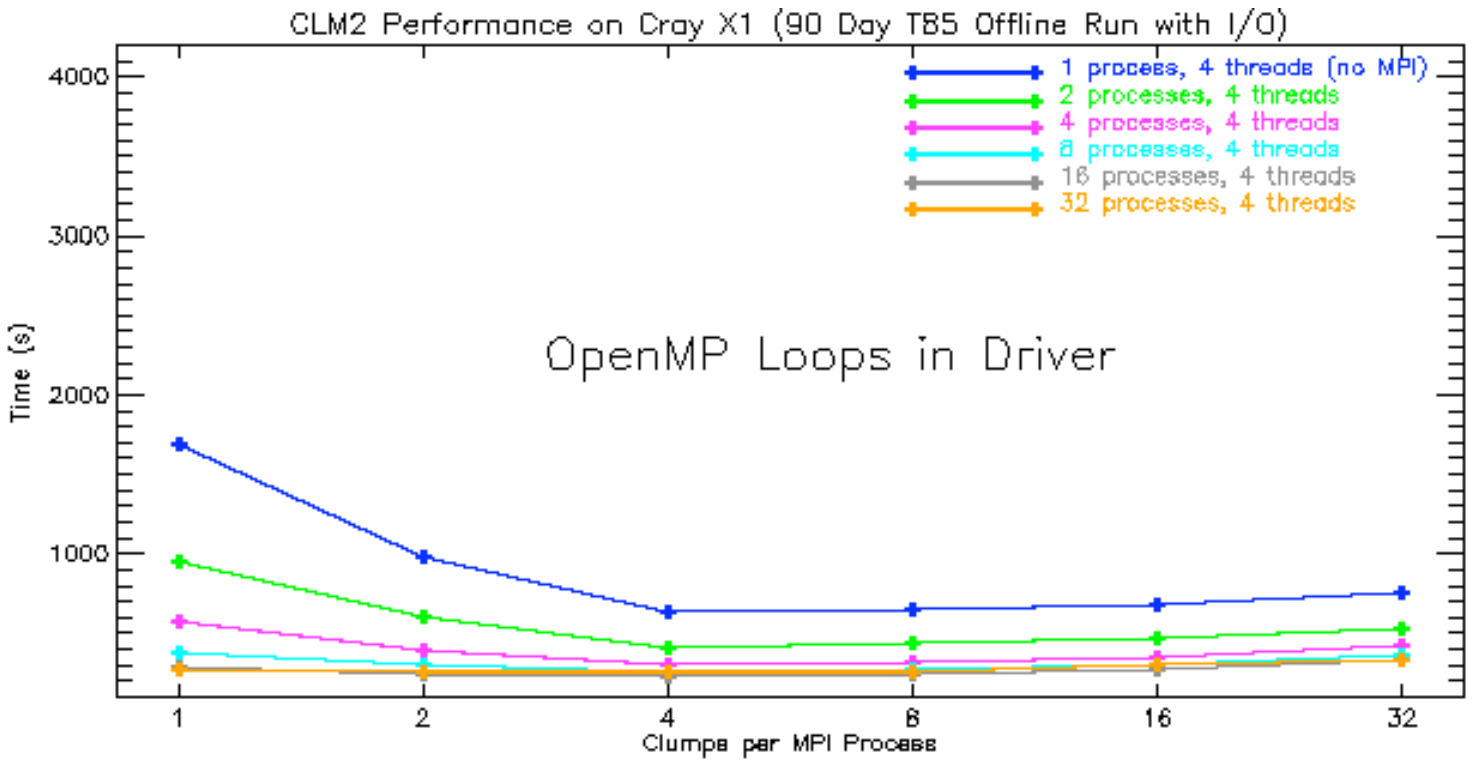
- Stand-alone CLM3.0
  (though plots say CLM2)
- 90 simulated days at T85 resolution
- 1,2,4,8,16,32,64 MSPs
- 1,2,4,8,16,32 clumps per MPI process
- Different shared-memory parallelism
  - Automatic multistreaming only
  - CSDs in driver
  - OpenMP in driver (with automatic multistreaming)



- Scales to 32 MSPs
- One clump per process works best

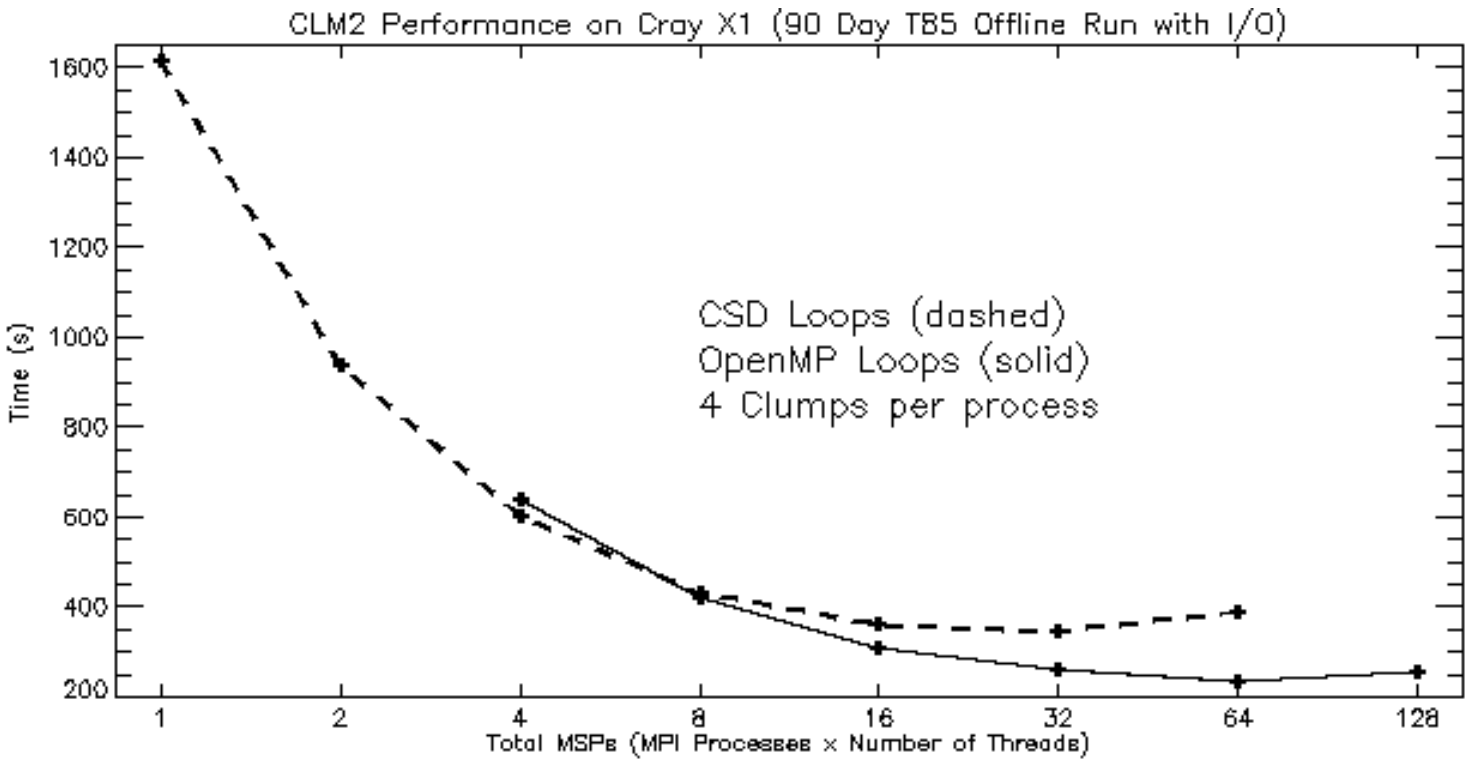


- Again, scales to 32 MSPs
- Need at least four clumps per process
  - One for each SSP



- Scales to 64 MSPs (16 MPI processes)
- Four MSPs per MPI process
  - Need at least four clumps

OpenMP vs. CSD



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