Idaho National Engineering and Environmental Laboratory

RELAP5-3D Architectural Developments in 2004

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Outline

- *Motivation for architectural improvements*
- *Completion of parallel conversion*
- *Completion of PVM*
- *Vectorization work*
- *Conversion to Fortran 90*
- *Summary*

Motivation for Architectural Improvements

- *Longevity*
- *Modernization*
- *Simplification*
  - *Reduced development time*
  - *Reduced maintenance costs*
  - *Faster debugging*
  - *Increased reliability*
- *Code run speed*

Completion of Parallel Conversion

- *Reason for conversion to OpenMP directives*
  - *Older form of parallel uses direct calls to the KAI library which is no longer maintained.*
  - *OpenMP is available on all major vendor platforms*
    - *Built into many compilers*
- *Previous work*
  - *Convert parallel in hydrodynamic subprograms*
  - *Convert parallel in heat structure subprograms*
- *Current task: Convert parallel in neutron kinetics*

Parallel Kinetics Task Summary

- *Kinetics parallelized via domain decomposition*
  - *Axial levels are grouped into subdomains*
    - *One parallel thread for each subdomain*
  - *Algorithm causes different answers when the # of subdomains or the grouping changes.*
- *All calls to KAI library calls were converted to OpenMP*
- *Environmental variable that activates/deactivates parallel for kinetics*
- *Almost all test cases all run properly*
  - *Problem with Cartesian, Krylov with 64-bit integers*

Parallel Maintenance & Development

- *Parallel is difficult to develop and maintain and it is easy to break.*
- *A parallel tool was developed during this task to help develop and maintain parallel.*
    - *By itself, this is not sufficient to maintain parallel.*
- *Training and study is needed to work on parallel code.*
- *Tutorial on OpenMP parallel programming will be taught later in the seminar.*
    - *All RELAP5-3D code developers should attend.*

RELAP5-3D Vectorization Task

- *A recent trend in HPC is a return to vector computing*
  - *Federal government initiative*
- *INEEL is vectorizing its codes for use on its Cray SV1 computers*
  - *INEEL funded task to improve RELAP5-3D vector performance.*
- *Performance analysis of RELAP5-3D*
  - *neither PHANTV nor PHANTJ vectorizes.*
  - *Both are in top 5 in execution time percentage.*

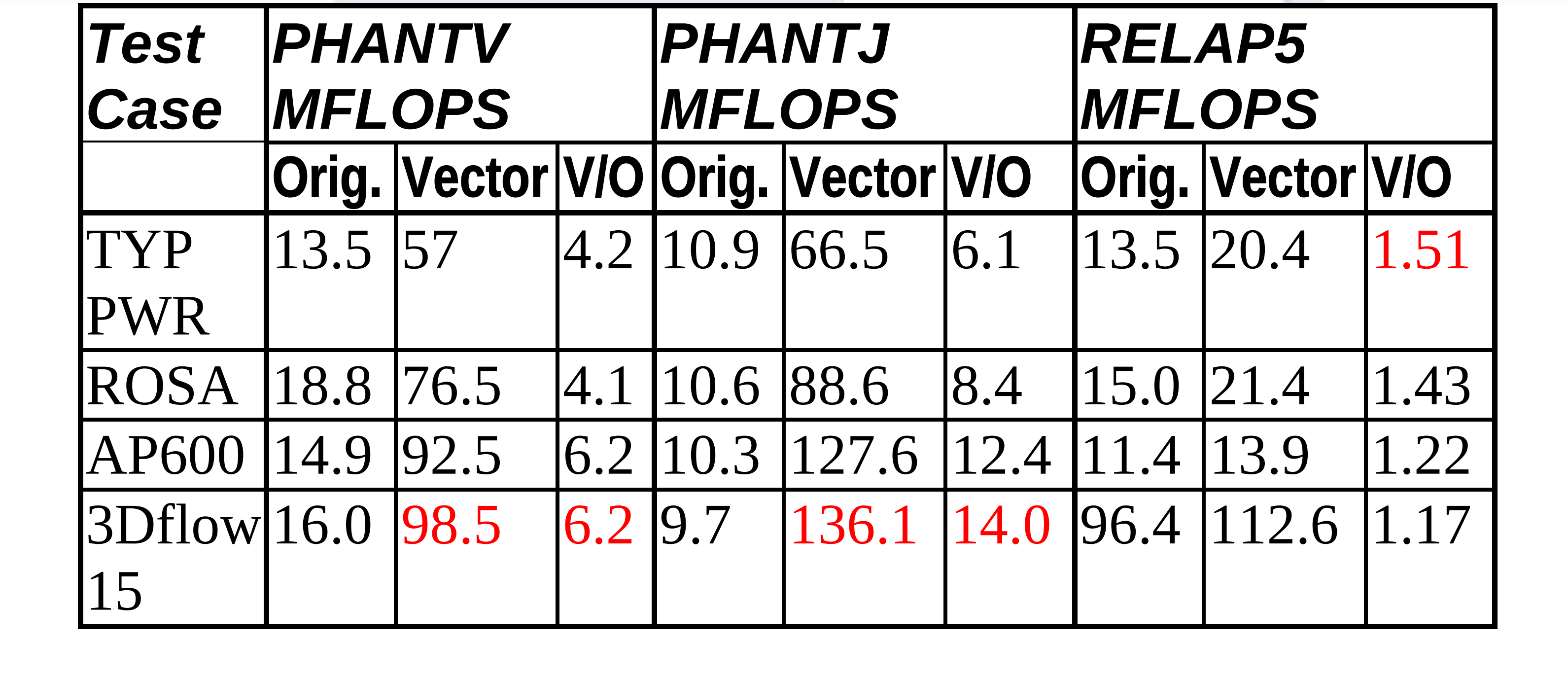
PHANTV and PHANTJ analysis

- *PHANTV & PHANTJ: have huge loops that do not vectorize:*
    - *DO-11, DO-111, DO-10*
- *These had multiple vector inhibitors:*
    - *Subroutine calls, improper module use*
    - *Variable length inner loops*
    - *Backward GO TO*
    - *Actual & false recursion*
    - *If-tests too deeply nested*
    - *Loop too long: PHANTJ is effectively 7100 lines!*

Solutions to Vectorization Problems

- *Inline subroutine calls*
- *Compile modules as “inlinable” & have no allocatables*
- *See paper for handling variable length inner loops*
- *Move recurrence relations outside loop and store results in temporary arrays for use in loop.*
- *Turn coding within backward Go To into subroutine*
- *Eliminate if-tests with use of logical variables*
- *Combat “loop too long” with use of both concurrent directive and aggressive compiler flag.*

Vectorization Speed-up



Test Case	PHANTV MFLOPS			PHANTJ MFLOPS			RELAP5 MFLOPS		
	Orig.	Vector	V/O	Orig.	Vector	V/O	Orig.	Vector	V/O
TYP PWR	13.5	57	4.2	10.9	66.5	6.1	13.5	20.4	1.51
ROSA	18.8	76.5	4.1	10.6	88.6	8.4	15.0	21.4	1.43
AP600	14.9	92.5	6.2	10.3	127.6	12.4	11.4	13.9	1.22
3Dflow 15	16.0	98.5	6.2	9.7	136.1	14.0	96.4	112.6	1.17

- *Speed is measured in MFLOPS*
- *Lesser RELAP5-3D speed-up in big problems; solver uses most of the time*

Value of Converting to Fortran 90

- *Greater machine independence*
  - *Use Fortran 90 library of intrinsic functions*
- *Ability to run any size problem*
  - *Replacement of FA-array with allocatable arrays*
- *Modernization*
  - *Conversion to derived types*
  - *Use of whole array operations*
- *Longevity*
  - *Replace any Fortran 66 & 77 constructs that may be illegal in Fortran 2000.*

Progress on Fortran 90 Conversion

- *Developed program that converts comdecks into Fortran 90 modules.*
  - *Tested & debugged.*
  - *Used to convert 3 internal FA files to modules.*
- *Developed program that converts array access into derived type access.*
  - *Tested & debugged.*
  - *Successfully applied to many RELAP5 subroutines.*
- *Conversion of many subroutines completed by hand.*
  - *Includes applying FORSTRUCT to reorganize code.*

Summary

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- *Completion of PVM*
- *Vectorization work*
- *Conversion to Fortran 90*