Performance Analysis of Large-scale Simulations on Supercomputers and Clouds

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1 Overview

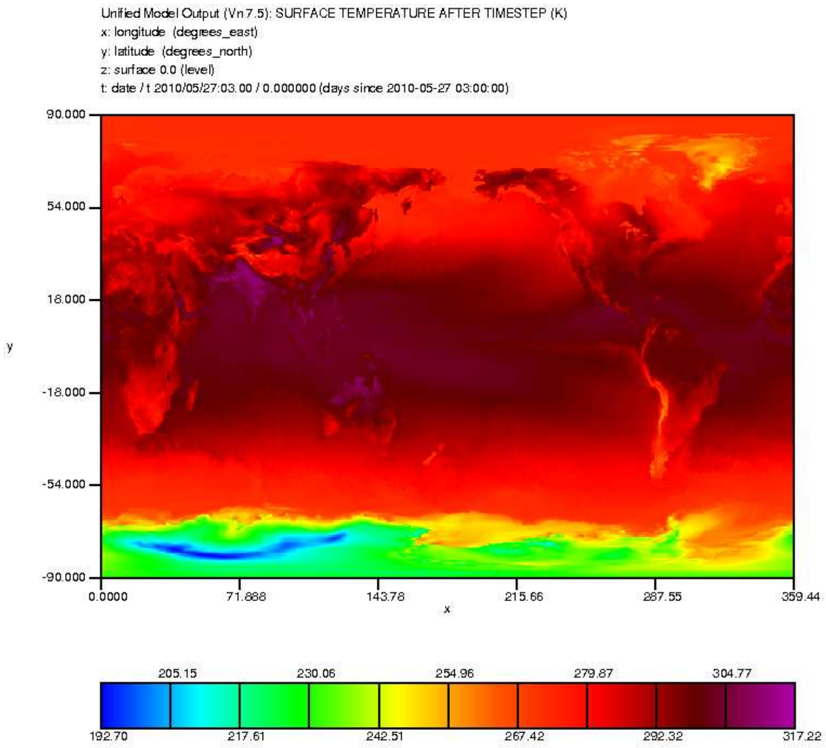
- the MetUM and Chaste projects
- supercomputers: the vayu cluster, the K supercomputer
- issues in large-scale, memory-intensive simulations
- techniques and tools for understanding scalability
  - identifying communication overhead & load imbalance, sections
  - tools: internal profilers, Integrated Performance Monitoring tool
- efficient performance analysis methodologies
  - accounting for variability of measurements; affinity effects
  - obtaining representative ‘sub-benchmarks’
- results on MetUM and Chaste on vayu
- comparison on the private and public clouds
  - motivations and setup
  - results: microbenchmarks and applications
- conclusions and future work

2 The Unified Model in Aust. Weather and Climate Simulations

- the Met Office Unified Model (MetUM, or just UM) is a (global) atmospheric model developed by the UK Met Office from early '90s
- for weather, BoM recently used a N144L50 atmosphere grid
  - wished to scale up to a N320L70 ($640 \times 481 \times 70$) then a N512L70 ($1024 \times 769 \times 70$) grid
  - operational target: 24 hr simulation in 500s on $<$ 1K cores (10-day 'ensemble' forecasts)
  - doubling the grid resolution increases 'skill' but is $\leq 8\times$ the work!
- climate simulations currently use a N96L38 ($192 \times 145 \times 38$)
- ACCESS project to run many (long) runs for IPCC
  - common infrastructure: atmosphere: UM (96 cores);
    ocean: NEMO, sea ice: CICE, coupler: OASIS (25 cores)
- next-generation medium-term models to use N216L85 then N320L70
- note: (warped) 'cylindrical' grids are easier to code but problematic . . .

3 The MetOffice Unified Model

- configuration via UMUI tool creates a directory with (conditionally-compiled) source codes + data files (for a particular grid)
    - main input file is a ‘dump’ of initial atmospheric state (1.5GB for N320L70)
    - ‘namelist’ files for ≈ 1000 run-time settable parameters
    - in operational runs, periodically records statistics via the STASH sub-system
- partition evenly the EW & NS dimensions of the atmosphere grid on a $P \times Q$ (MPI) process grid



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4 Unified Model Code Structure and Internal Profiler

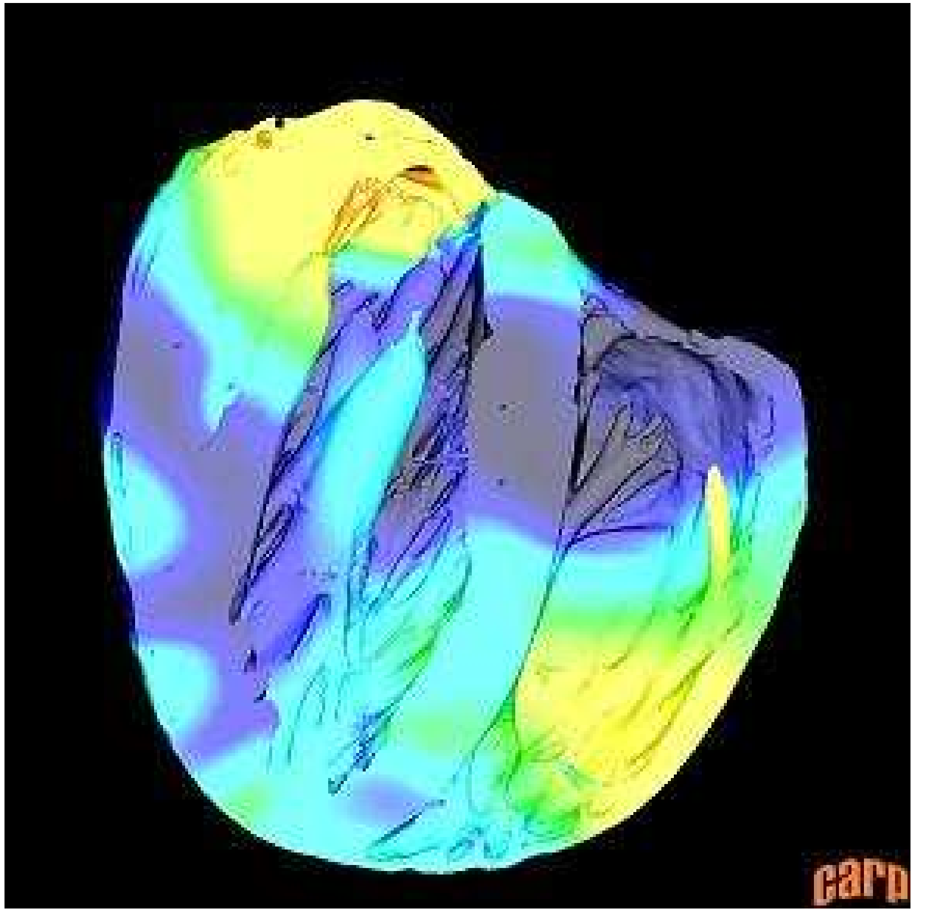
- codes in Fortran-90 (mostly F77; ≈ 900 KLOC) with cpp (include common blocks, commonly used parameter sub-lists, etc)
- main routine `u_model()`, reads dump file & repeatedly calls `atm_step()`
  - dominated by Helmholtz P-T solver (GCR on a tridia. linear system)
- internal profiling module can be activated via 'namelist' parameters
  - has 'non-inclusive' +'inclusive' timers (≈ 100 of each)
  - the top-level non-inclusive timer is for `u_model()`;
    sum of all non-inclusive timers is time for `u_model()`
  - reports number of calls and totals across all processes, e.g.

```
   ROUTINE                MEAN    MEDIAN       SD   % of mean      MAX   ...
1 PE_Helmholtz          206.97    206.98     0.05       0.02%   207.02   ...
3 ATM_STEP               36.39     38.53     9.46      25.99%    44.60   ...
4 SL_Thermo              25.38     26.60     3.45      13.58%    31.15   ...
5 READDUMP               24.18     24.36     1.12       4.62%    24.37   ...
...
```

  - due to global sync. when a timer starts, can estimate load imbalance

5 The Chaste Cardiac Simulation Project

- Chaste: software infrastructure for modelling the electro-mechanical properties of the heart
- large system of C++ code, many dependencies
- also has internal profiler
- required resolution necessitates parallelization via MPI
- most computationally-intensive part is solution of a large sparse linear system once per timestep
- workload uses a high resolution rabbit heart (Oxford University) (2 $\times$ 1 GB files – 4 million nodes, 24 million elements)



6 The Vayu Cluster at the NCI National Facility

- 1492 nodes: two 2.93 GHz X5570 quad-core Nehalems (commissioned Mar 2010)
- memory hierarchy: 32KB (per core) / 256KB (per core) / 8MB (per socket); 24 GB RAM
- single plane QDR Infiniband: latency of 2.0μs & 2600 MB/s (uni-) bandwidth per node

- jobs (parallel) I/O via Lustre filesystem
- jobs submitted via locally modified PBS; (by default) allocates 8 consecutively numbered MPI processes to each node
  - typical snapshot:

    ```
    1216 running jobs (465 suspended), 280 queued jobs, 11776 cpus in use
    ```
  - estimating time and memory resources accurately is important!
- allocation for our work was a few thousand CPU hours, max. core count 2048 . . .

7 Issues in Large-scale Memory-Intensive Simulations

- simulations of scientific interest run over many timesteps
  - ‘realistic’ benchmarks are resource-intensive: may be difficult on a ‘premiere facility’
  - variability of results problematic for accurate performance analysis
- resolution for state-of-the-art science pushes memory limits, even on a ‘premiere facility’
  - Chaste on 4M node mesh needs more memory than N320L70 atmosphere!
  - running MetUM on vayu required:
    - removing limit on stack size
    - redefining internal message buffer size (< 8 cores)
    - ‘pinning’ more (1 GB) physical memory for Infiniband (> 900 cores)
    - specifying memory limit to be physical (rather than virtual) (> 900 cores, wide process grid aspect ratios)

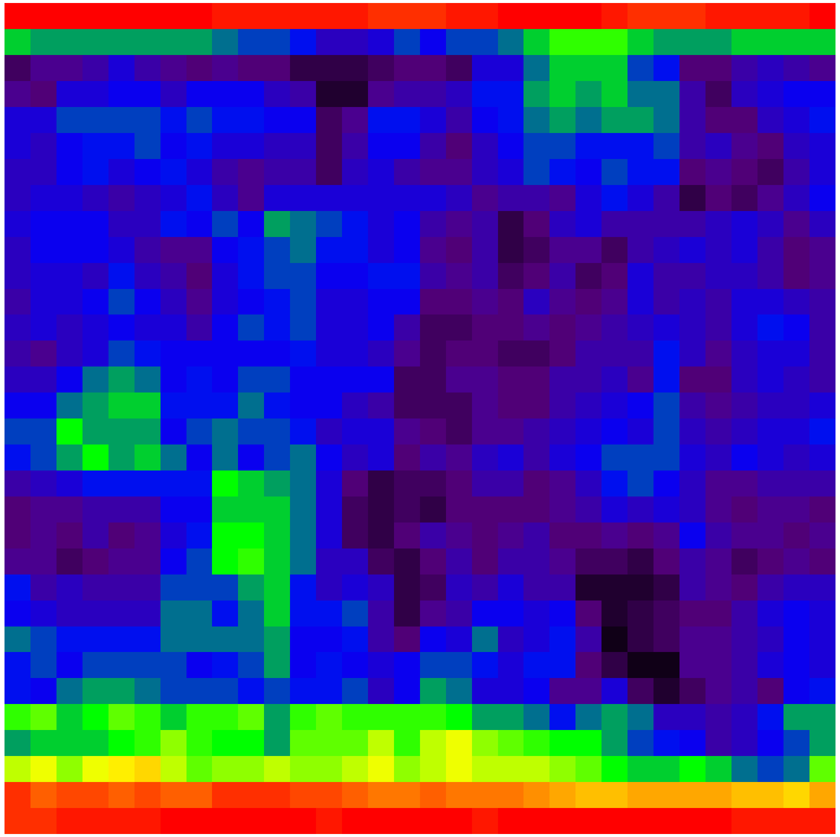
8 Techniques for Understanding Scalability: Communication Overhead and Load Imbalance

- measure time spent in communication library (MPI) separately
  - ideally, break-down per different communication operations (2 major categories: point-to-point and *collective*)
  - and (major categories of) buffer size
- load imbalance is more tricky to measure
  - differences in computation times across processes
  - *and/or* differences in times taken at barriers
    - i.e. the averaged time (over each process) spent in barriers, minus the estimated overhead of barriers (when perfectly balanced)
    - ideally, should do this for other collectives as well (e.g. small all-reduce operations)
  - note: problems are not solvable by a faster network! must be addressed at the application level

9 Case Sudy: Load Imbalance Across Cores in MetUM (32×32 process grid)

- over 'warmed period'; Red = 0%, Black = 15% of run-time
- from time spent in barriers within UM internal profiler
  - large value indicates a lighter load

  Note that this will be an underestimate!
- clear indication of especially latitudinal variations
- solution: less regular data distribution to take load off the polar areas



10 Tech. for Understanding Scalability: Section-Based Analysis

- consider latitudinal load imbalance in global atmosphere simulation
  - simulation at each timestep proceeds in a number of ‘sections’ polar filtering, thermal radiative transfers, convection, advection, etc
  - some require more work in high latitude, others in lower
- understanding of issues can be sharpened if considered separately
  - in particular, aggregate load imbalance is better estimated from weighted sum of per-section imbalances (triangle inequality)
- e.g. in the MetUM `atm_step()` routine:

```
If (Ltimer) Call timer ('PE_Helmholtz',3) ! 3: start non-inclusive timer
! code to call main PE_Helmholtz routine
...
If (Ltimer) Call timer ('PE_Helmholtz',4) ! 4: end non-inclusive timer
```

by calling at a barrier at the start of each (!) timer, can estimate per-section load imbalance by using variation in total times

11 Tools for Understanding Scalability

- desirable properties of any tool collecting scalability-related data
  - have minimum impact on computation time and memory footprint
  - communication vs. computation time breakup, load imbalance
    - provide further information indicating likely causes (i.e. hardware event counts: e.g. cache misses)
  - breakdown of these over component parts of the computation ,
- range from internal profilers to the heavy-weight SunStudio `collect`
  - the works! Pertinent sections derived automatically from the subroutine call-graph – combined with MPI & hardware event count profiling
- Integrated Performance Monitoring tool (IPM) in middle of the range
  - supports profiling of the MPI library and hardware event counters
  - support sections easily from internal profiler, e.g. from MetUM `timer()`:

```
if (timer_type == 3)  call mpi_pcontrol(+1, current_timer_name)
if (timer_type == 4)  call mpi_pcontrol(-1, current_timer_name)
```

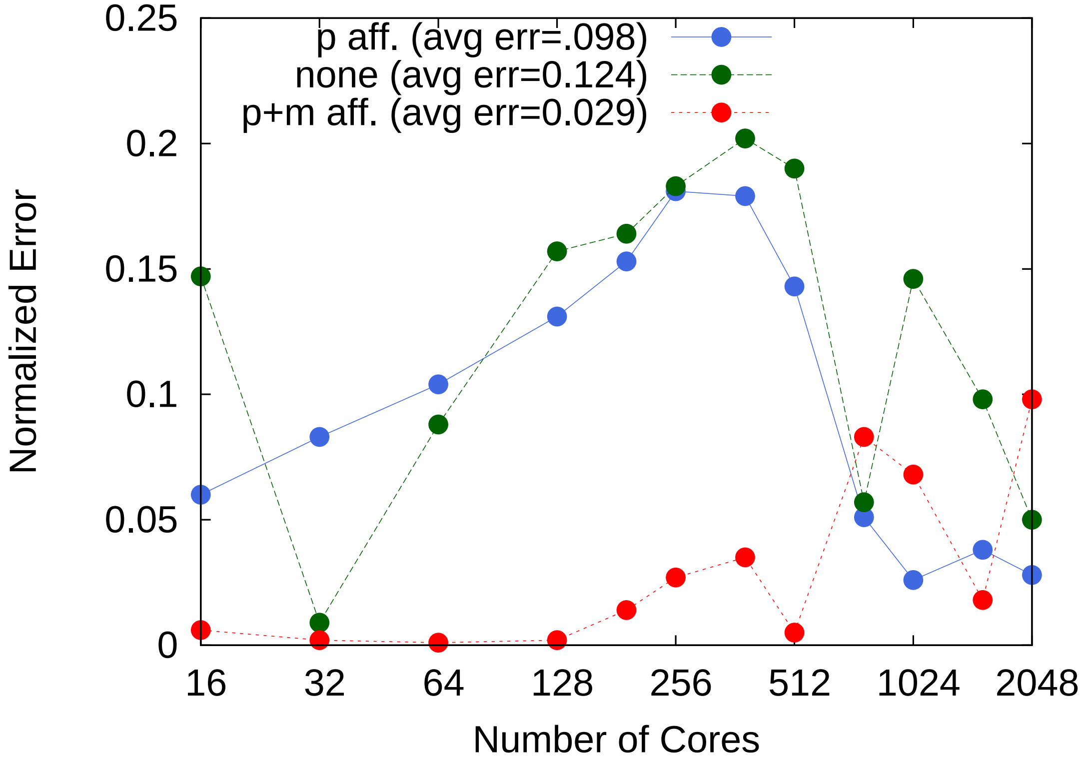
12 Methodologies: Minimizing Measurement Variability

- to analyze large-scale and long-running simulations over 1000's of cores, potentially need vast computing resources!
- compounded with fact that repeated experiments on a facility may give significant variability: many need to run many times!
- on a cluster such as vayu:
  - each node has 2 quad-core sockets; 8 processes given to each node

  the following effects were found to be important:
  - process affinity: once a node is assigned to a core, ensure that it stays there
  - NUMA affinity: memory used by a process must only be allocated on the socket of the core that it is bound to
- input/output requires (on vayu) access to the shared Lustre file system
  - exposes experiments to other users' using the file system
  - remains an open problem!

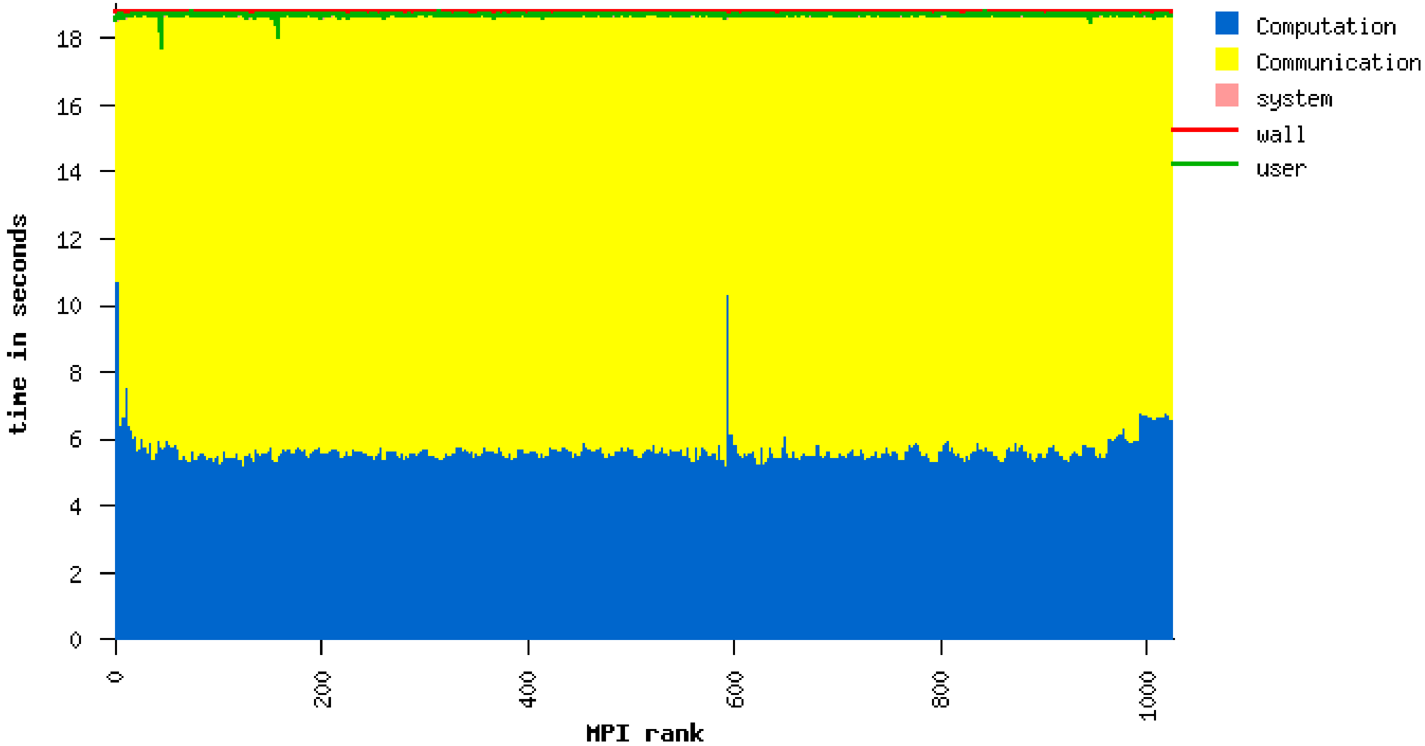
13 Case Study: Effect of Affinity on Variability of MetUM

- use the normalized error from the average $\frac{\Sigma_{i=1}^{n}|t_i - \bar{t}|}{n\bar{t}}$
- noting number of measurements ($n = 5$) only sufficient to observe general trends
  - no clear correlation of error and number of cores
  - process affinity reduces variability by 20%
  - NUMA affinity reduces this further by a factor of 4!



(for 'warmed time' of PS24/N512L70)

14 Effect of (no) NUMA Affinity – Exposed by IPM Profiles



- MetUM N320L70 (no STASH) output, 32×32 process grid
- no NUMA affinity: groups of 4 processes (e.g. socket 0) – spikes in compute times
- other runs: spikes occur on differing numbers & positions of nodes

15 Methodologies: Obtaining Representative Sub-Benchmarks

- standard 24 hour atmosphere benchmarks used by BoM are deemed to represent 10-day operational runs
- how much of this actually needs to be done for an accurate and representative performance analysis?
- basic idea: reduce number of iterations and select representative iterations for extrapolation for a larger simulation
  - works well when simulation's computational profile is *time-invariant*
- cardiac simulation is more problematic:
  - simulations of interest comprise applying an electric stimulation (e.g. 0.25 ms) and awaiting response over a longer interval (e.g. 30 ms)
  - depolarization are repolariztion wavefronts travel back and forth across the model over the response time
- in such cases, detailed performance analysis is required across all potentially different intervals to see if computational profiles (significantly) change

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16 Validation of Sub-benchmark Methodology - MetUM

- methodology: run for 3 hours, taking the 12 iterations on hours 2–3 ('warmed period') as representative
- projected run time for 24 hour operational job (960 cores) is:

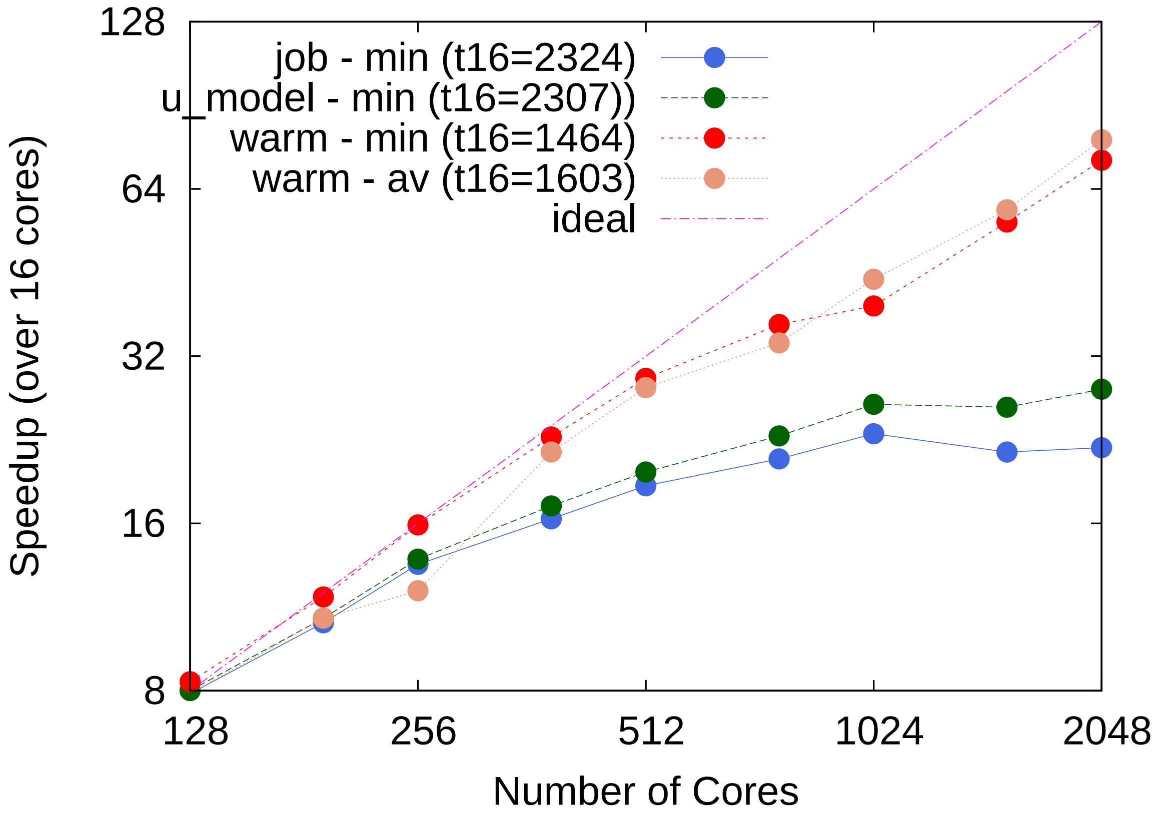
$$t' = (t - t_{2:24}) + 11.5 t_{2:3}$$

run	t	$t_{2:24}$	$t_{2:3}$	t'	anomalies
N512L70	527	39.12	6.5	524.3	–
N320L70 – 1	224	163.8	13.7	214.8	iter. 59 (7.9s)
N320L70 – 2	237	174.9	14.9	233.6	iter. 134 (4.2s)

- defensive programming check: sum of 'non-inclusive' timers matched total to less than 0.1%
- to reduce overhead, 1st hour was used to determine which sections were 'important' enough to perform barriers to estimate load imbalance
  - reduced number of such barriers by a factor of 10
  - measured profiler overhead (gather data, barriers) of $< 1\%$ of 'warmed period' times

17 Results: Which Time to Take? (N512L70 + PS24)

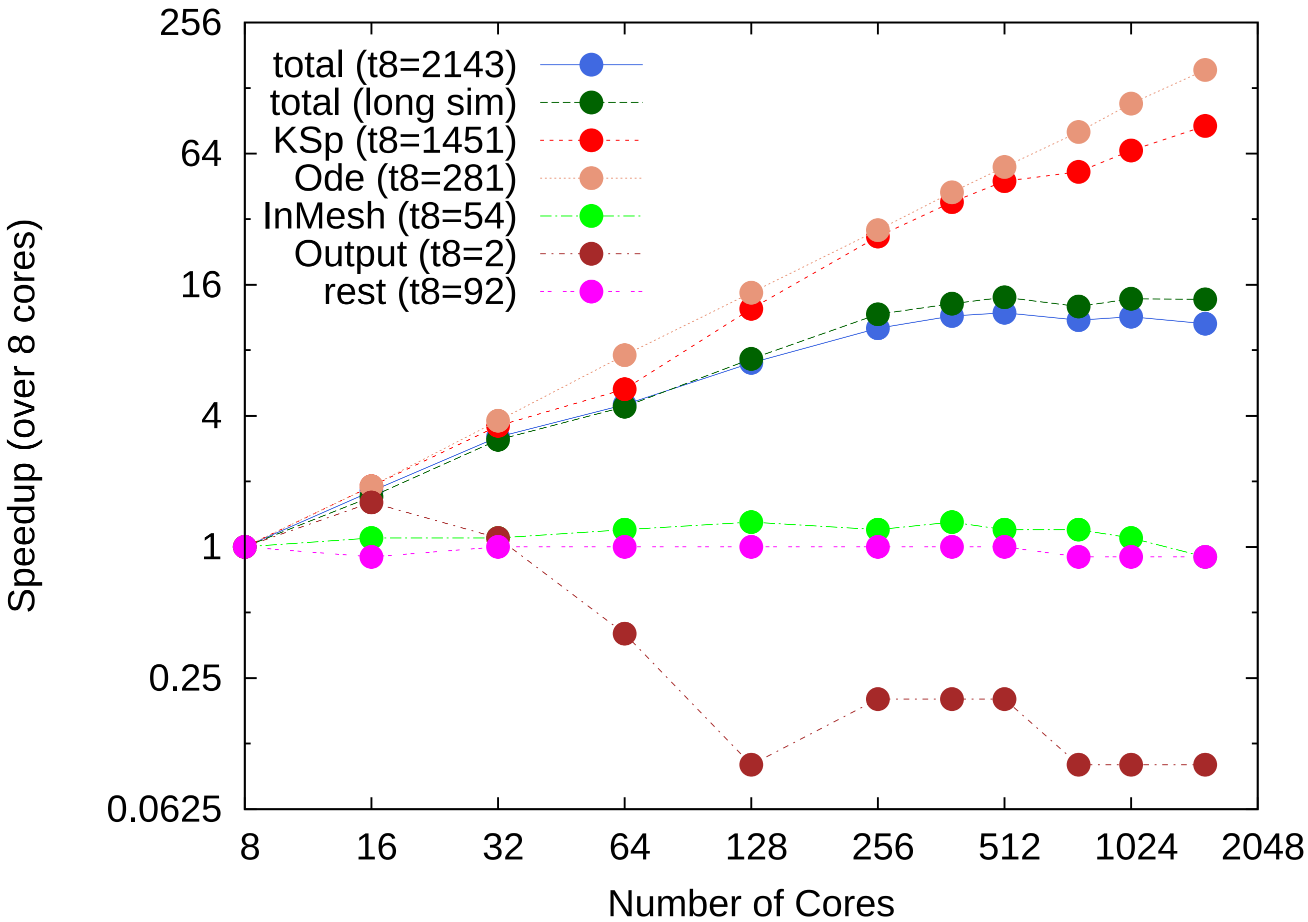
- process grids aspects between 1:1 and 1:2 chosen
- 't16' is time for 16 cores
- essentially linear scaling from 16 to 64 cores (slightly super-)
- surprisingly, average & minimum times show similar curves



- job time @ 1024 cores includes: pre-launch: 2s, launch processes: 4s, read 'namelist' files: 6s, `read_dump()`: 27s, cleanup: 1s
- message: 'warmed time' is a better predictor of the full simulation

18 Results: Section Analysis and Scaling Behavior (Chaste)

- 't8' is the time in seconds for 8 cores (due to memory constraints, could not run on less)



19 Results: Understanding Scalability Analysis via Profiling

- scalability of total time: max. 11.9 at 512 cores (from 8)
- scalability of ODE and KSp quite high; loss due to un-parallelized ‘rest’ and inversely scaling ’Output’ (using HDF5)
- execution time spent for 1024 cores

section	%t	%comm	main MPI	comments
rest	43	30	all-gather	25% time in I/O
Output	20	30	barrier	high load imbalance
InMesh	19	41	broadcast	
KSp	14	25	all-reduce (8b)	
Ode	1	18	all-reduce (4b)	
AssSys	0.8	0		slight imbalance; some I/O
AssRHS	0.5	7	waitany	high load imbalance

- note: IPM dilated the time spent in the KSp section by 50% and overall by 10%

20 Motivations for Using Clouds: a Cloud-bursting Supercomputer Facility

- supercomputing facilities provide access to state-of-the-art cluster computers
  - also provide comprehensive software stacks to support a diverse range of applications
- the supercomputing cluster is typically highly contended resource
  - users may be restricted to limited resources
  - may have long turnaround times
  - some workloads may not make good use of cluster
- $\Rightarrow$ may be better off using a private or even public cloud
  - requires easily replication of software stack on cloud resources
  - ideally, migration of jobs onto cloud would be transparent
  - recent frameworks can transparently profile HPC jobs for cloud suitability, e.g. ARRIVE-F, (and migrate VMs accordingly)

21 Experimental Cloud Setup: Systems

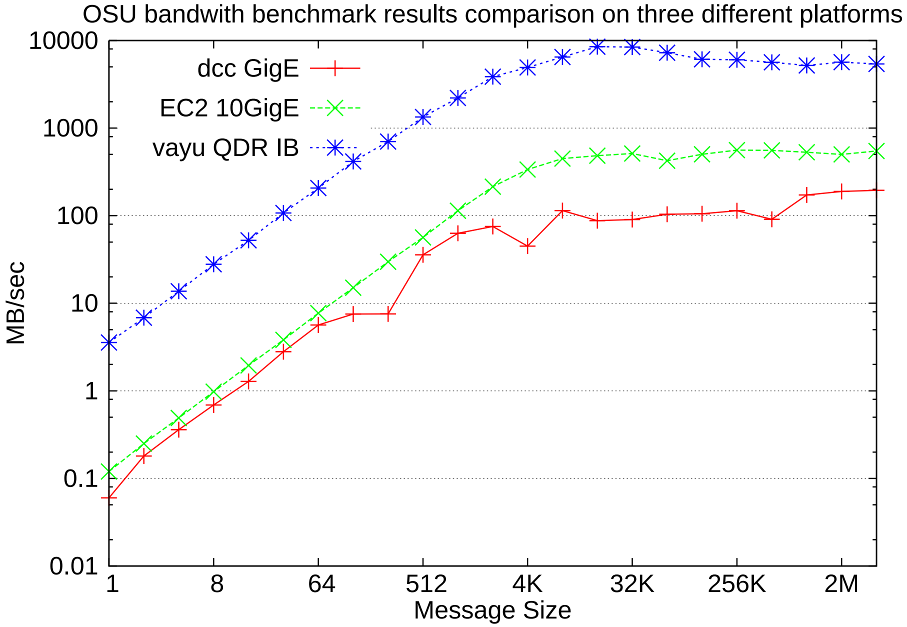
Platform		private cloud	public cloud	premiere cluster
Platform		DCC	EC2	Vayu
# of Nodes		8	4	1492
CPU	Model	Intel Xeon E5520	Intel Xeon X5570	Intel Xeon X5570
	Clock Spd	2.27GHz	2.93GHz	2.93GHz
	#Cores	8 (2 slots)	8×2	8 (2 slots)
	L2 Cache	8MB (shared)	8MB (shared)	8MB (shared)
Memory per node		40GB	20GB	24GB
Operating System		Centos 5.7	CentOS 5.7	CentOS 5.7
Virtualization		VMware ESX 4.0	Xen	–
File System		NFS	NFS	Lustre
Interconnect		1 GigE (dual)	10 GigE	QDR IB

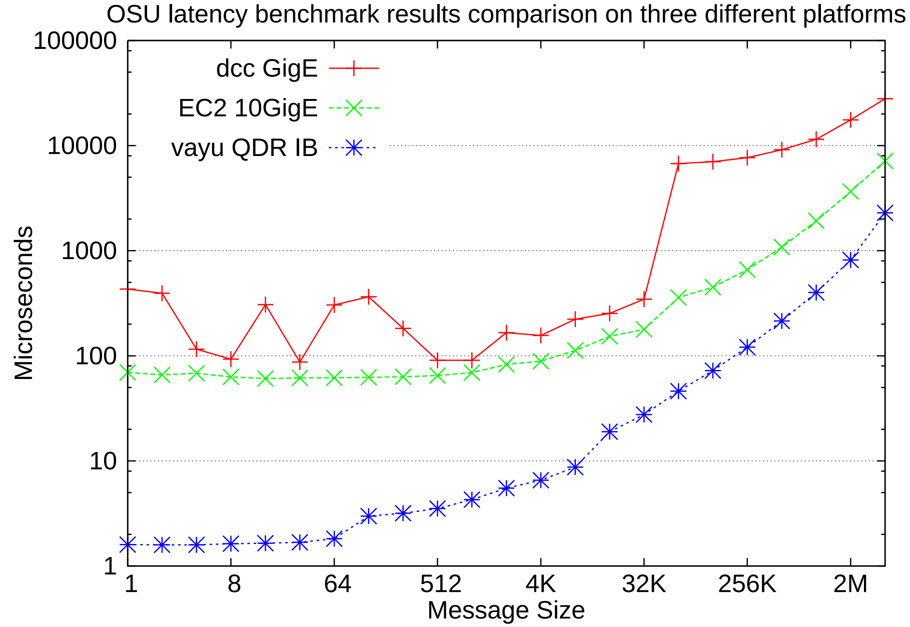
- DCC: 1 VM/node; filesystems mounted via external cluster via two QLogic channel fibre HBAs
- vayu: QDR IB used for both compute and storage

22 Cloud Setup: Software

- EC2: StarCluster instance to automate the build, configuration & management of HPC compute nodes
- vayu `/apps` directory: system-wide compilers, libraries, and application codes
  - user environment is configured via `module` package
- rsync `/apps` and user home/project directories onto the VM to replicate stack
  - minimizes interference of existing stack on the clouds
  - only occasionally needed to recompile for the clouds
- benchmarking software
  - OSU MPI communication micro-benchmarks: bandwidth and latency
  - NAS Parallel Benchmark MPI suite 3.3, class B
    - 5 kernels & 3 pseudo-applications derived from CFD applications

23 Cloud Results: Communication Micro-benchmarks



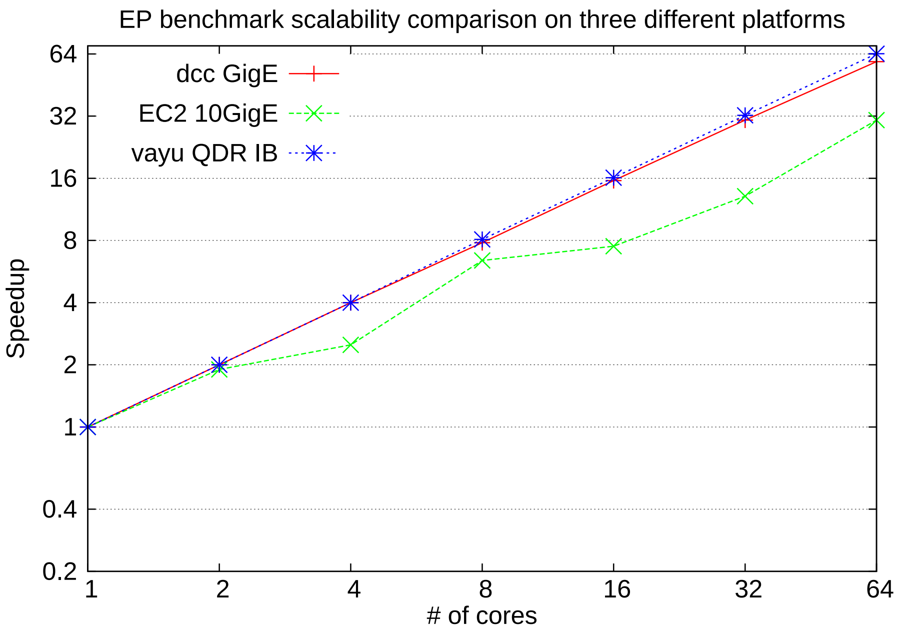


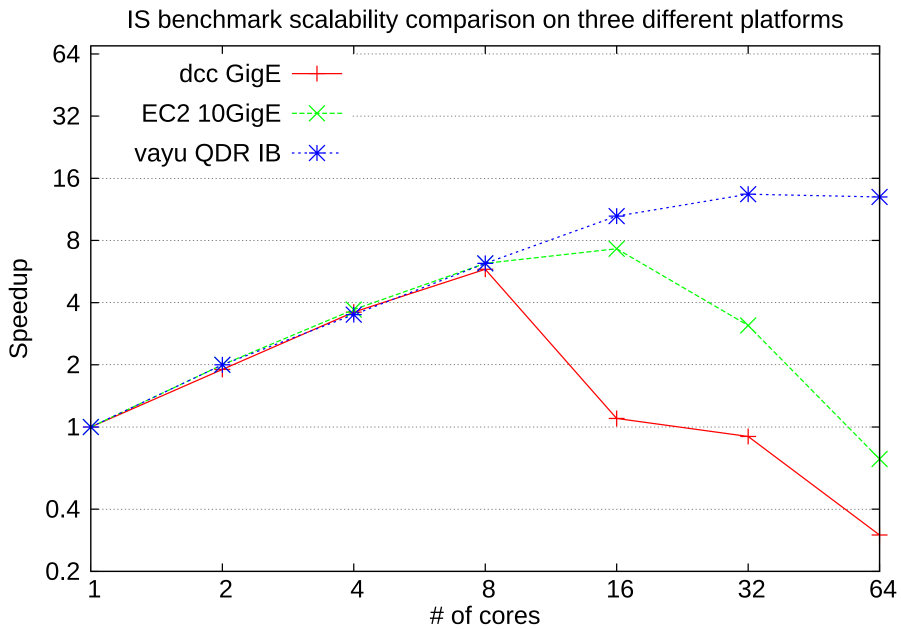
OSU MPI bandwidth tests (MB/s vs message size)

OSU MPI latency tests (time (μs) vs message size)

- trends as expected per theoretical specifications: more than one order of magnitude better performance on vayu
- fluctuations on DCC suspected from CPU scheduling by hypervisor

24 Cloud Results: NAS Parallel Benchmarks (I)





EP.B speedup, 1 to 64 cores IS.B speedup, 1 to 64 cores

- EC2 fluctuations for EP.B suspected due to jitter (CPU scheduling and hyperthreading
- IS shows the poorest scaling of all benchmarks:
  - IPM profiling shows % communication at 64 cores is 98% (DCC), 85% (DCC) and 68% (vayu)

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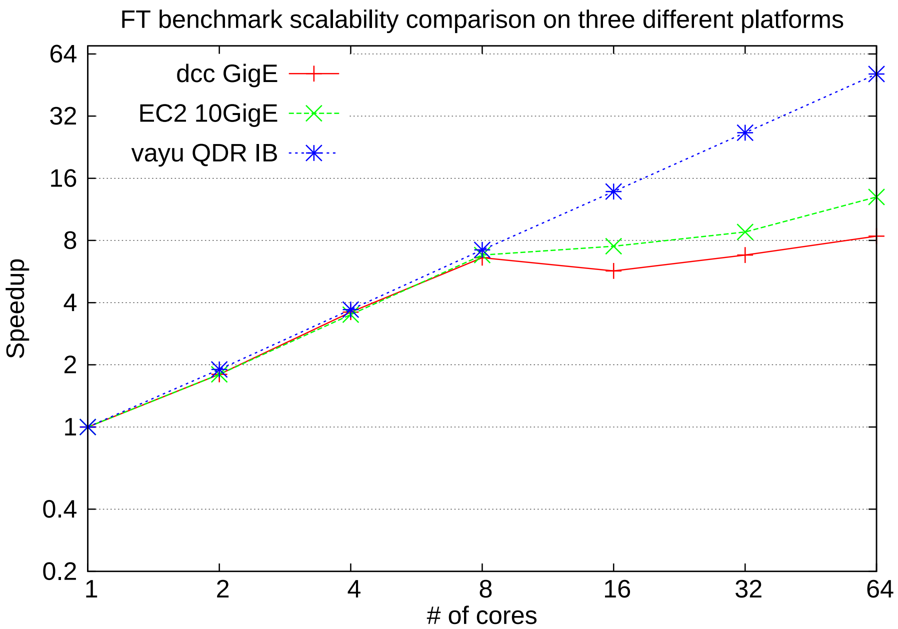
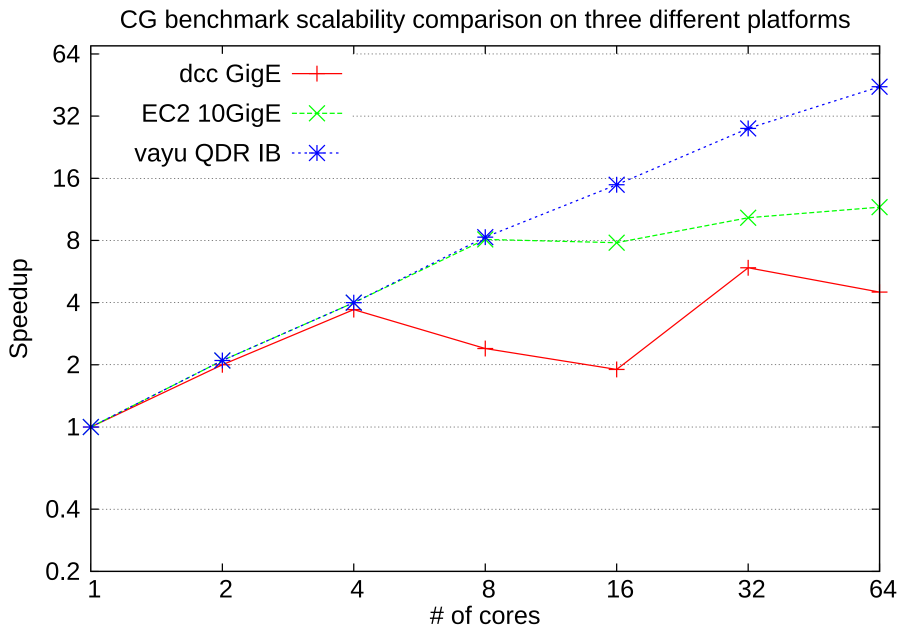
25 Cloud Results: NAS Parallel Benchmarks (II)



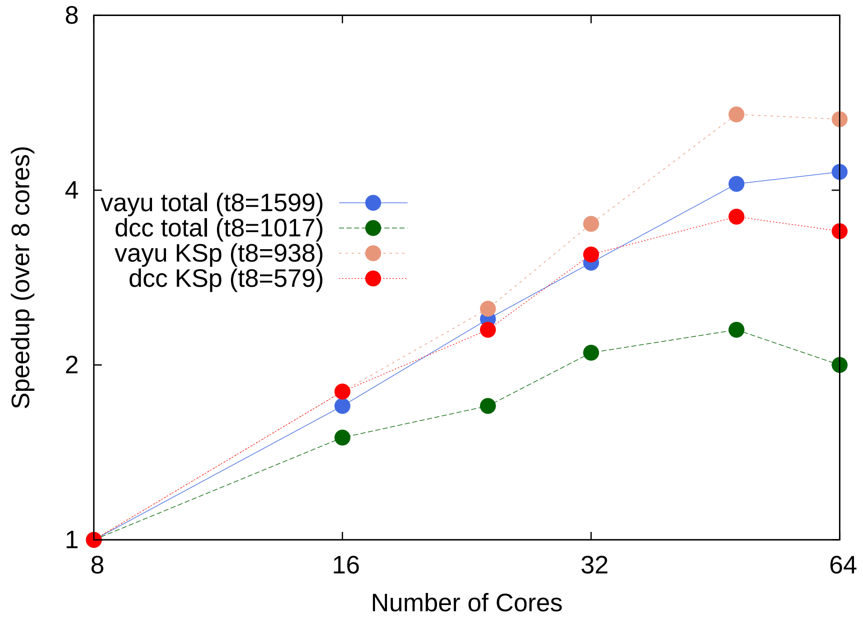


FT.B speedup, 1 to 64 cores CG.B speedup, 1 to 64 cores

- CG.B: IPM profiling shows % communication at 64 cores is 90% (DCC), 58% (DCC) and 22% (vayu)
- drop-offs on clouds occur when intra-node communication is required
- BT.B, MG.B, SP.B and LU.B showed similar scaling to FT.B
- single core performance consistently 20% (30%) faster on EC2 (vayu)

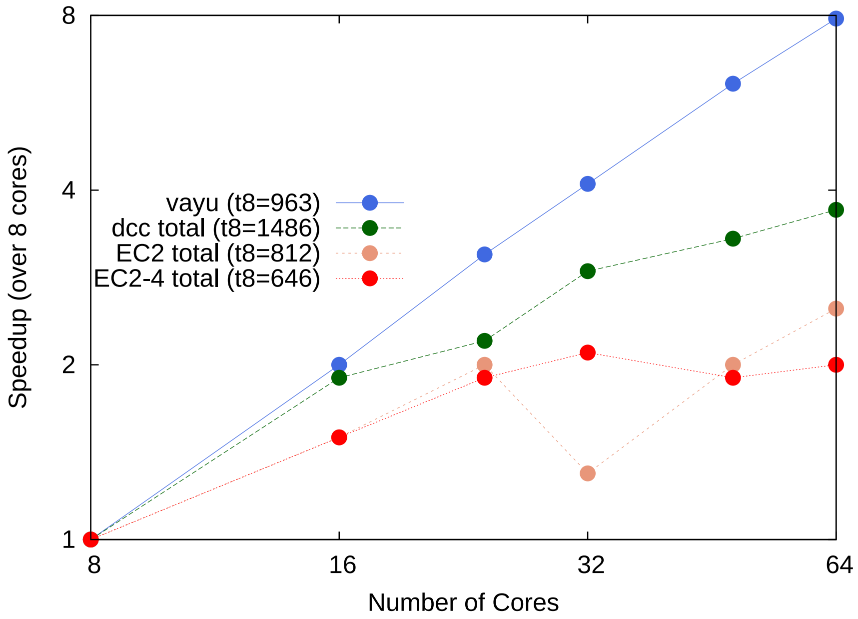
26 Cloud Results: Chaste Cardiac Simulation

- (results not available on EC2 due to complex dependencies)
- scaling of the KSp linear solver determines overall trends
  - note: benchmark scales to 1024 cores on vayu
- input mesh: 1.4× faster on vayu (8 cores), scaled the same on both
- output: 2.6× faster on vayu (8 cores) but scaled better on dcc



- @ 32 cores, 48% vs 11% of time spent in communication on dcc vs vayu
  - 13× more spent in KSp solver on dcc (large numbers of collectives)
- IPM profiles also indicated a greater degree and a higher irregularity of load imbalance on DCC
- ⇒ dcc performance hurt by high message latencies & jitter

27 Cloud Results: MetUM Global Atmosphere Simulation



	Vayu	DCC	EC2	EC2-4
time(s)	303	624	770	380
r_{comp}	1.0	1.37	2.39	1.17
r_{comm}	1.0	6.71	3.53	1.61
%comm	13	42	18	18
%imbal	13	4	18	19
I/O (s)	4.5	37.8	9.1	7.6

Details at 32 cores (EC2-4: 4 nodes used, uniformly 2$\times$ faster)

- overall load imbalance least on dcc, but generally higher & more irregular across individual sections (NUMA effects)
- EC-2 shows similar imbalance and communication profiles to vayu
- dcc spent most time in communication, particularly in sections where there were large numbers of collectives
- read-only I/O section: dcc much slower to vayu, EC2 similar, to vayu

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28 Conclusions

- performance of large-scale memory-intensive simulations
  - working with such codes and systems is hard!
  - many techniques and suitably lightweight tools needs to be applied in order to understand it
    - need to understand *what* (is the issue), then *where*, and then *why*
    - it is however possible to get useful insights, even for complex applications
- efficient methodologies need to be developed – non-trivial unless computational profile is time-invariant!
- largely successful in creating x86-64 binaries on HPC system & replicating all software dependencies into the VMs on clouds
- communication bound applications were disadvantaged on the virtualized platforms
  - large numbers of short messages were especially problematic
- over-subscription & hidden effects (e.g. NUMA) also also affected clouds

Future Work

- extend performance analysis to other large-scale applications (e.g. ANUGA, GENE)
  - methods to reduce reductions and other global operations become more attractive as we scale to larger numbers of cores
- use metrics from the ARRIVE-F framework to assess candidate workloads for private/public science clouds
- using StarCluster, cloud burst onto OpenStack based resources locally & externally

Acknowledgements

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- NCI NF for time on vayu cluster

Questions???