NEMO on HECToR

Dr Fiona J L Reid
Applications Consultant, EPCC
f.reid@epcc.ed.ac.uk
+44 131 651 3394

NAG dCSE Technical Workshop, 23rd September 2009

Acknowledgements

- Cray Centre of Excellence team for their help throughout the project
- Chris Armstrong, NAG for help with netCDF on the X2

Talk outline

- Overview of the NEMO dCSE Project
- What is NEMO?
- System introductions
- XT results
  - Baseline performance and optimisations
  - netCDF 4.0 performance
  - Optimising NEMO I/O
  - Nested model performance and troubleshooting
- Achievements

Overview of NEMO dCSE project

- The NEMO Distributed Computational Science and Engineering (dCSE) Project is a collaboration between EPCC and the Ocean Modelling and Forecasting (OMF) group based at the National Oceonography Centre, Southampton (NOCS).
- The project was funded by a HECToR dCSE grant administered by NAG Ltd on behalf EPSRC
- The NEMO dCSE Project concentrated on the following areas:-
  - I/O performance on intermediate and large numbers of processors
  - Nested model performance
- In addition, a separate project investigated porting NEMO to the HECToR vector system, the X2

What is NEMO?

- NEMO (Nucleus for European Modelling of the Ocean) is a modelling framework for oceanographic research
- Allows ocean related components, e.g. sea-ice, biochemistry, ocean dynamics, tracers, etc to work either together or separately
- European code with the main developers based in France
- Major partners include: CNRS, Mercator-Ocean, UKMO and NERC
- Fortran 90, parallelised using MPI – versions 2.3 and 3.0
- Code has previously run on both scalar and vector machines
- This project uses the official releases (OPA9) with some NOCS specific enhancements

System introductions

- HECToR (Phase 1): Cray XT4
  - MPP, 5664 nodes, 2 AMD Opteron 2.8 GHz cores per node
  - 6 GB of RAM per node (3 GB per core)
  - Cray Seastar2 torus network

- HECToR (Vector): Cray X2
  - Vector machine, 28 nodes, with 4 Cray X2 processors per node
  - 32 GB of RAM per node (8 GB per Cray X2 processor)
  - Cray YARC network

XT results

NEMO 3.0 performance – compiler flags

- Various compiler flags were tested for PGI version 7.1.4 (7.2.3 also tested)

Compiler flags	Time for 60 time steps (seconds)
-O0 -r8	163.520
-O1 -r8	157.123
-O2 -r8	138.382
-O3 -r8	139.466
-O4 -r8	137.642
-fast -r8	Fails with segmentation violation
-O2 -Munroll=c:1 -Mnoframe -Mautoinline -Mscalarsse -Mcache_align -Mflushz	133.761 with 138.965 for **-O4**

- **-O4** best, but minimal difference from **-O2** to **-O4**
- **-fast** invokes a number of options; independent testing of each flag shows the problem flags to be:
  - **-Mlre** Loop redundancy elimination – this shouldn't cause a crash!
  - **-Mvect=sse** Allows vector pipelining to be used with SSE instructions
- PathScale compiler was also tested, v3.1 gave similar performance with **-O3**

NEMO performance – SN versus VN

- HECToR can be run in single core (SN) or virtual node (VN) mode
- SN mode uses one core per node, VN mode uses both cores
- If your application suffers from memory bandwidth problems SN mode may help

Number of processors	Time for 60 steps (seconds)	
	SN mode	VN mode
256	119.353	146.607
221	112.542	136.180

- Runtime reduces when running NEMO in SN mode
- NEMO doesn't benefit sufficiently to justify the increased AU usage

NEMO grid

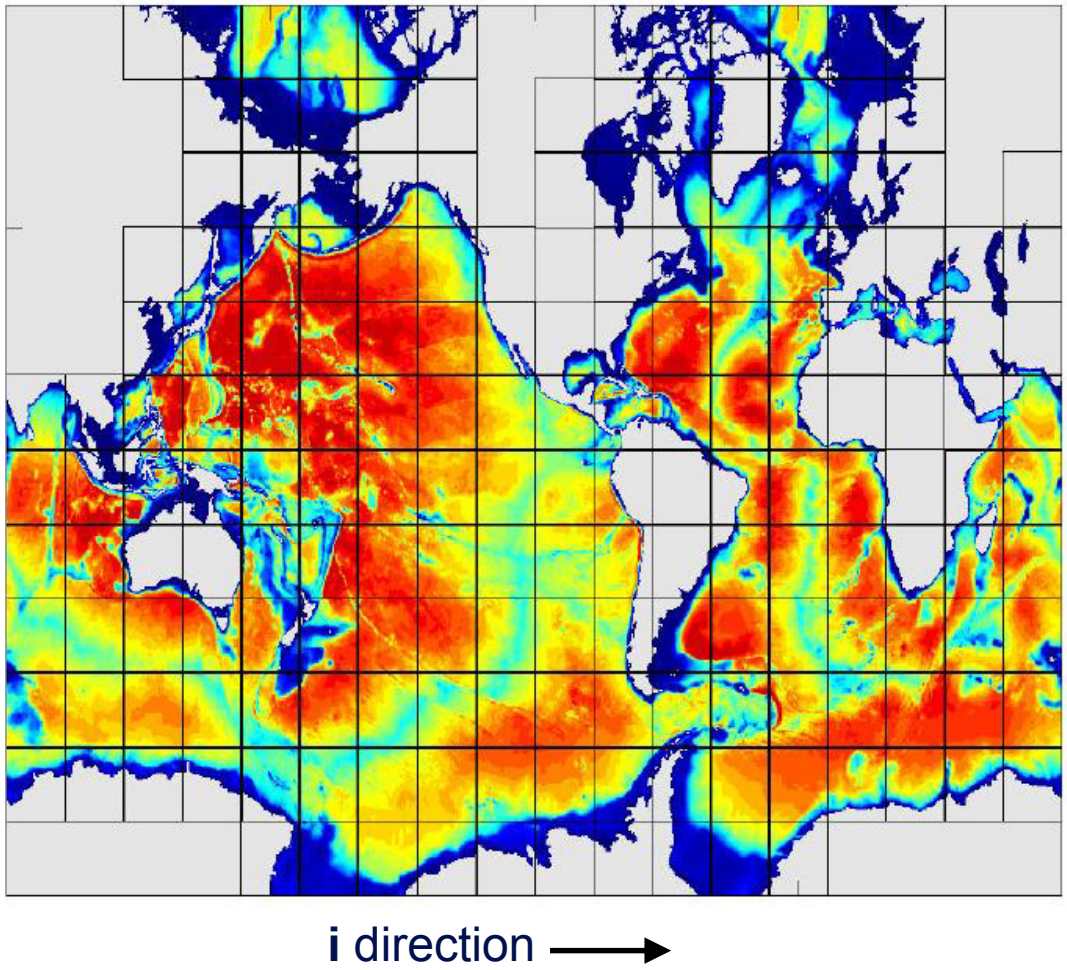


Image provided courtesy of Dr Andrew Coward, NOCS

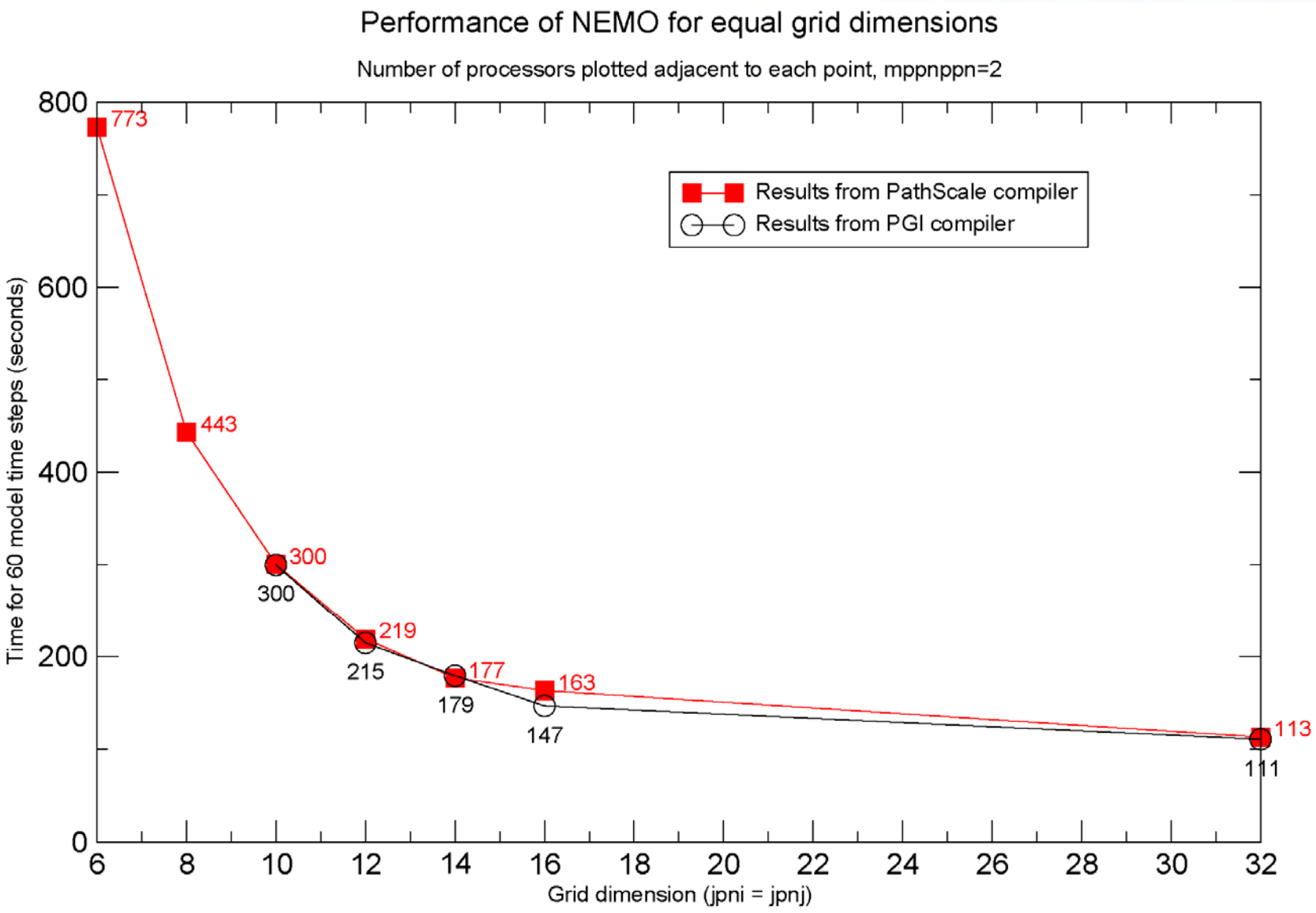
Grid used for ORCA025 model

jpn**i** = number of cells in the horizontal direction

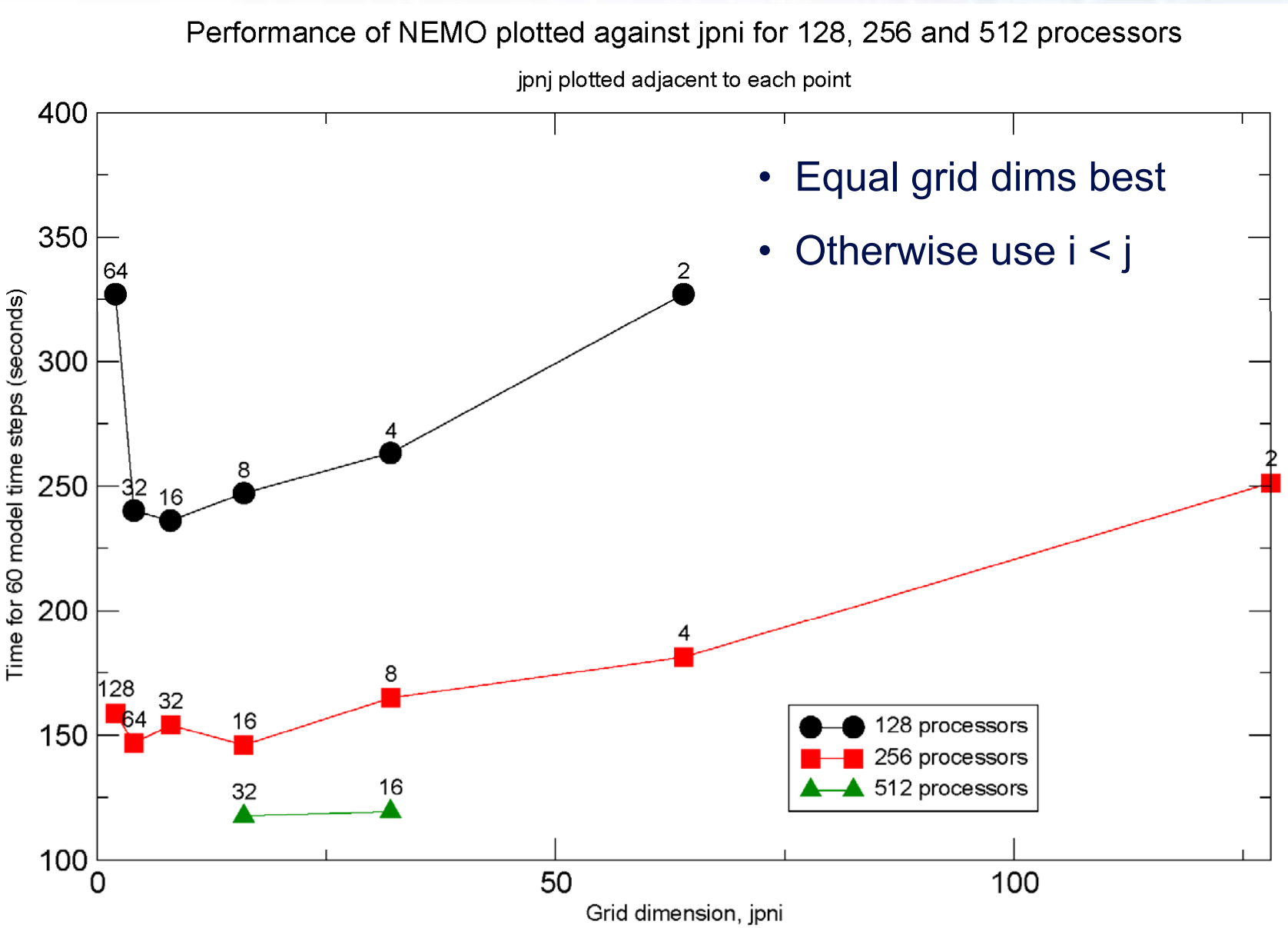
jpn**j** = number of cells in the vertical direction

Here, jpn**i** = 18, jpn**j** = 12

NEMO performance – equal grid dims



NEMO performance – different grid dims



- Equal grid dims best
- Otherwise use i < j

NEMO performance – removal of land cells

- Ocean models only model the ocean
- Depending on the grid, some cells may contain just land
  - Land only cells do not have any computation associated with them
  - However, they do have I/O
  - A zero filled netCDF file is output for each land cell
- The land only cells can be removed prior to running NEMO
  - Work out how many land only cells there are via the bathymetry file
  - Set the value of jpnij equal to the number of cells containing ocean
  - E.g. for a 16 x 16 grid there are 35 pure land cells so jpnij = 221

NEMO performance – removal of land cells

jpni	jpnj	jpnij	Reduction in AU's used	Time for 60 steps (seconds)
8	16	128		236.182
8	16	117	8.59%	240.951
16	16	256		146.607
16	16	221	13.67%	136.180
16	32	512		117.642
16	32	420	17.97%	111.282
32	32	1024		110.795
32	32	794	22.46%	100.011

- Removal of land cells reduces the runtime and the amount of file I/O
  - –No unnecessary output for land regions
- In addition the number of AU's required is greatly reduced
  - –Up to 25% reduction for a 1600 processor run

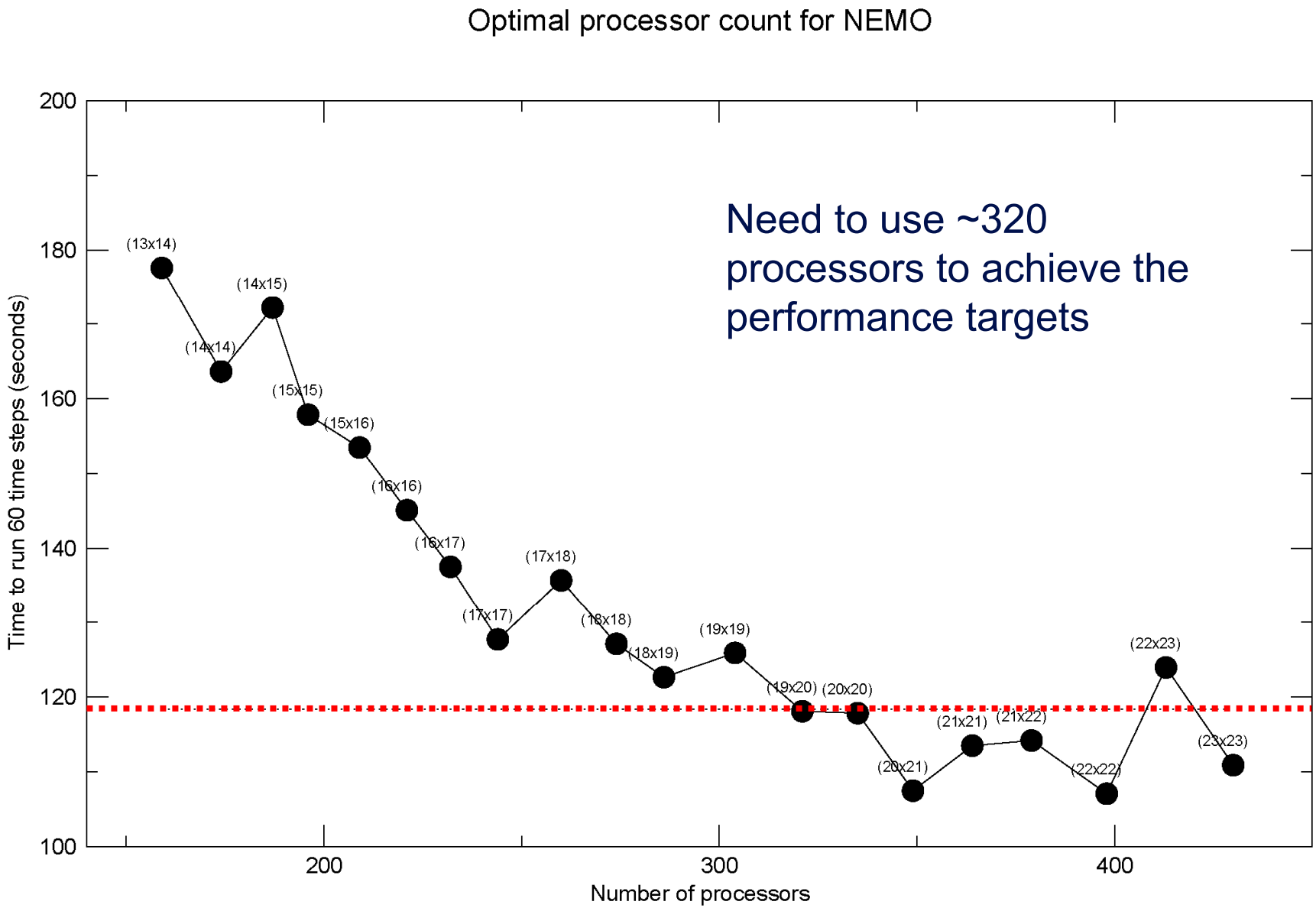
NEMO performance – optimal proc count

- NOCS researchers want to be able to run a single model year (i.e. 365 days) during a 12 hour run
  - Aids the collation and post-processing of results
  - Current runs on 221 processors provide around 300 model days
- Investigated the "optimal" processor count as follows
  - Remove land cells
  - Keep grid dimensions as close to square as possible
  - Compute the number of model days computed in 12 hours from:

$$ndays = 43000/t_{60}$$

  - Ideally want t_{60} to be ≤ 118 seconds
  - Investigated processor counts from 159 - 430

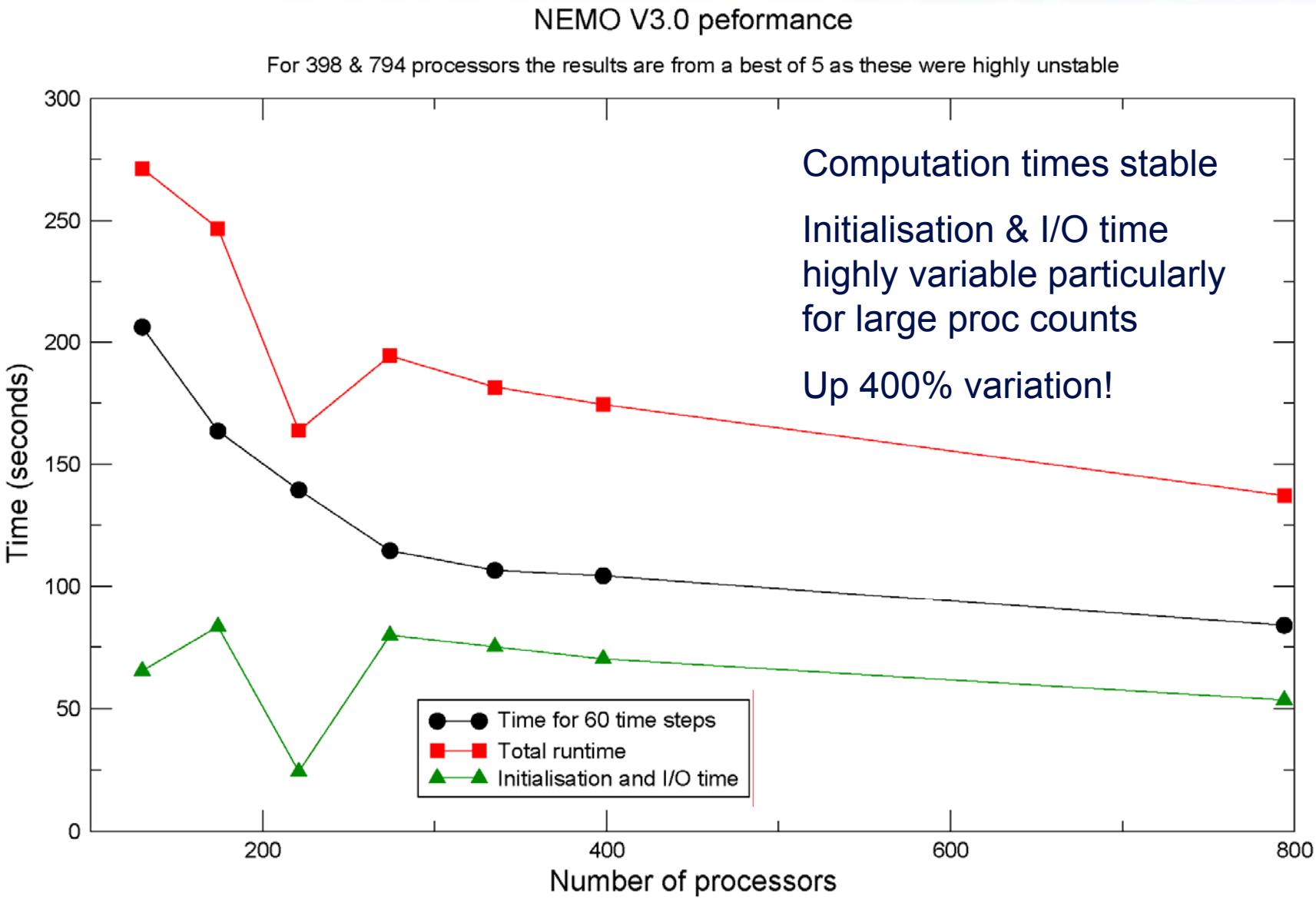
NEMO performance – optimal proc count



NEMO I/O

- NEMO input & output files are a mixture of binary and ASCII data
  - Several small **input** ASCII files which set key parameters for the run
  - Several small **output** ASCII files; time step, solver data, run progress
  - Binary **input** files for atmospheric data, ice data, restart files etc
  - Binary **output** file for model results, restart files etc
- All binary data files are in netCDF format
  - netCDF = network Common Data Format
  - Portable data format for storing/sharing scientific data
- NEMO uses parallel I/O
  - each processor writes out its own data files depending on which part of the model grid it holds
  - Should be efficient but may suffer at larger processor counts…

NEMO 3.0 performance – I/O

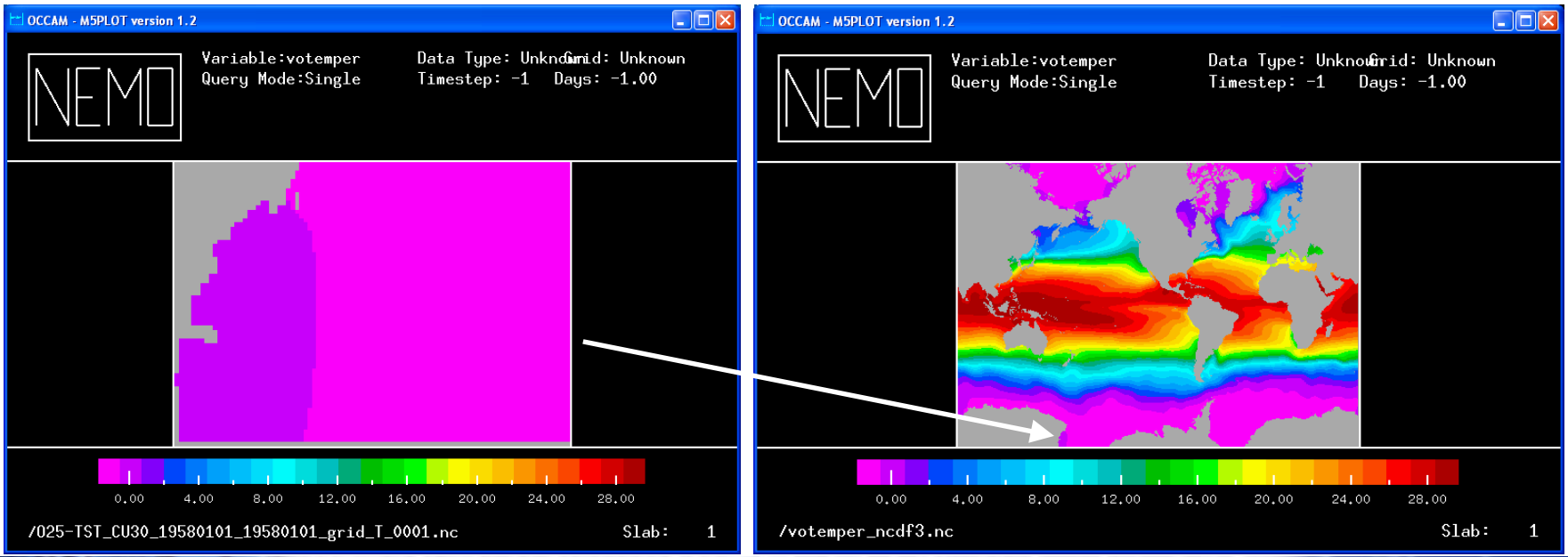


netCDF 4.0

- netCDF 4.0 was used to improve I/O performance of NEMO
- Key features
  - Lossless data compression and chunking
    - areas with the same numeric value require far less storage space
  - Backward compatibility with earlier versions
- Requires:-
  - HDF 5.0 1.8.1 or later
  - Zlib 1.2.3
  - Szip (optional)
- All codes tested with supplied test suites – all tests pass
  - Cross compiling caused a few hiccups
  - Now available centrally as Cray supported modules on HECToR

netCDF 4.0 performance

- Performance evaluated using the NOCSCOMBINE tool
- NOCSCOMBINE is a serial tool written by the NOCS researchers which reads in multiple NEMO output files and combines them into a single file
  - The entire file can be combined or
  - Single components e.g. temperature can be extracted



netCDF 4.0 performance

- NOCSCOMBINE compiled with various versions of netCDF
- A single parameter (temperature) is extracted across 221 input files
  - Minimal computation, gives a measure of netCDF & I/O performance
  - Time measured and the best (fastest) of 3 runs reported
  - netCDF 3.6.2 and 4.0 output compared using CDFTOOLS* to ensure results are accurate

*CDFTOOLS – set of tools for extracting information from NEMO netCDF files

netCDF performance

netCDF version	NOCSCOMBINE time (seconds)	File size (Mb)
3.6.2 classic	344.563	731
4.0 snapshot un-optimised	86.078	221
4.0 snapshot optimised	85.188	221
4.0 release	85.188	221
4.0 release*	78.188	221
4.0 Cray version	92.203	221
4.0 release classic	323.539	731

*system Zlib 1.2.1 used

- Compiler optimisation doesn't help
- System zlib 1.2.1 faster than version 1.2.3
  - –Use with care, netCDF 4.0 specifies zlib 1.2.3 or later
- File size is 3.31 times smaller
- Performance of netCDF 4.0 is 4.05 times faster
  - –Not just the reduced file size, may be algorithmic changes, c.f. classic
- Cray version ~ 18% slower than dCSE install (for this example)

Converting NEMO to use netCDF 4.0

- NEMO should benefit from netCDF 4.0
  - The amount of I/O and thus time spent in I/O should be significantly reduced by using netCDF 4.0
- NEMO was converted to use netCDF 4.0 as follows:-
  - Convert code to use netCDF 4.0 in Classic Mode
  - Convert to full netCDF 4.0 without chunking/compression
  - Implement chunking and compression
  - Test for correctness at each stage
  - Full details in the final report

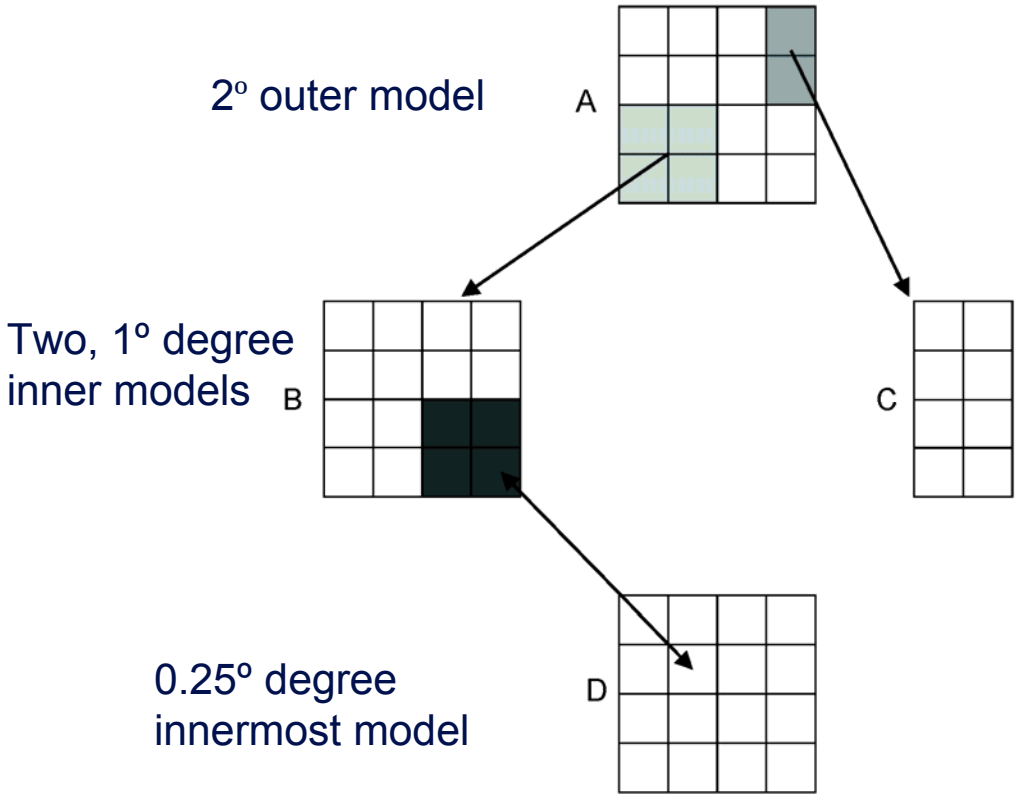
NEMO performance with netCDF 4.0

Filename	File size netCDF 3.X (MB)	File size netCDF 4.0 (MB)	Reduction factor
***grid_T*.nc**	1500	586	2.56
***grid_U*.nc**	677	335	2.02
***grid_V*.nc**	677	338	2.00
***grid_W*.nc**	3300	929	3.55
***icemod*.nc**	208	145	1.43

- Up to 3.55 times reduction in file size
- Actual performance gains will depend on output required by science

NEMO – nested models

- Nested models – enable complex parts of the ocean to be studied at a higher resolution, e.g.



Two models: BASIC, MERGED

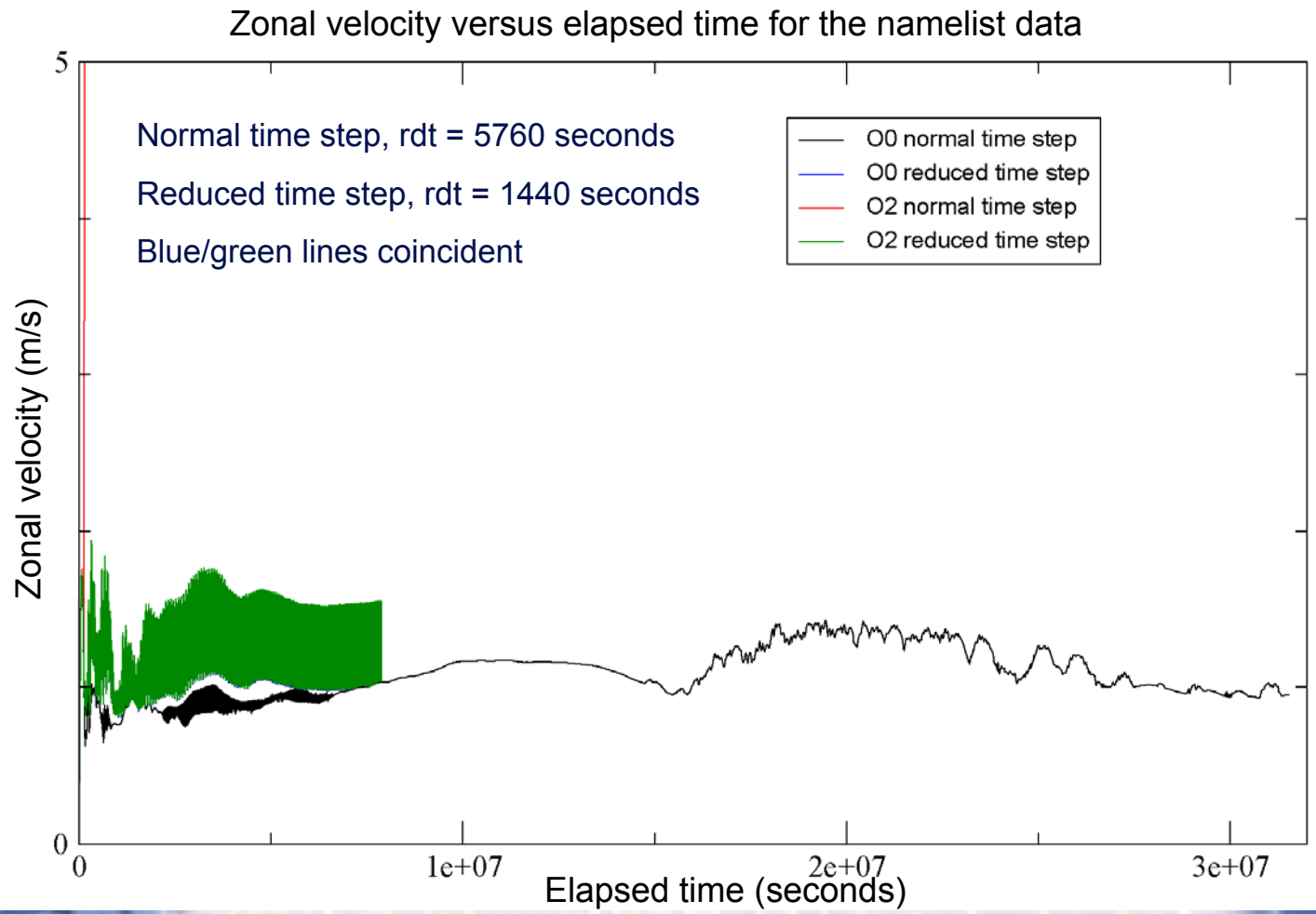
BASIC: 2º model with a 1º nested model, no NOCS features

MERGED: 1º model with two 0.25º nested regions, NOCS code

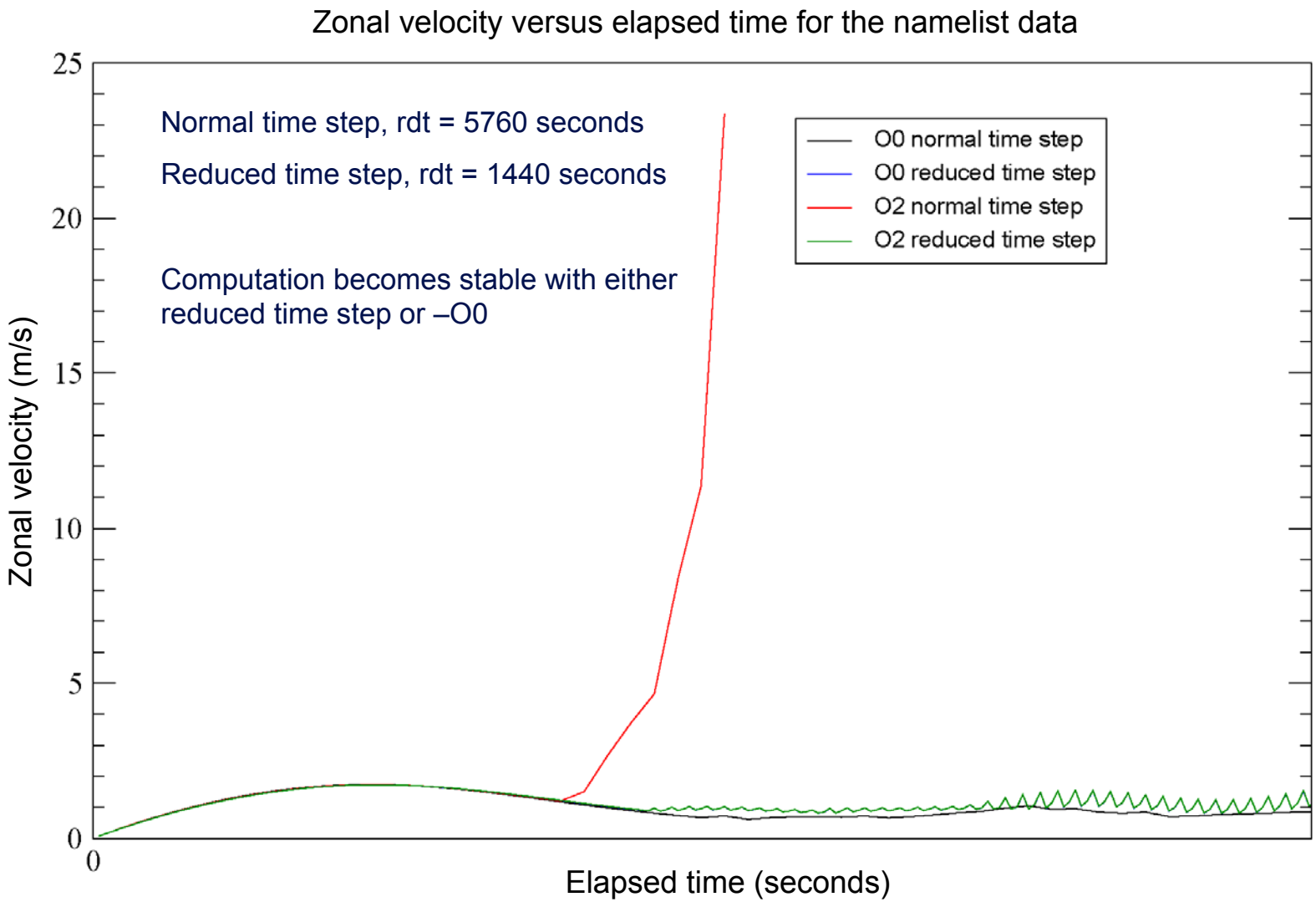
Crashes with the velocity becoming unrealistically large

NEMO – nested models

- BASIC model
  - Error occurs in outermost (i.e. un-nested) model
  - Plot of velocity against time step highlights the problem



NEMO – nested models



NEMO – nested models

- BASIC model
  - Reducing level of optimisation *or* reducing the time step resolves the problem for the BASIC model
- MERGED model still an issue
  - Velocity explodes for all levels of nesting
  - Compiler flags and reduction of timestep do not help
  - Thought to be an uninitialised value or memory problem
  - Compiler & debugger bugs discovered limiting further investigations

NEMO - achievements

- 25% reduction in AU usage by removing land-only cells from computations
- Obtained optimal processor count for a 12 hour run on HECToR
- Compiled netCDF 4.0, HDF5 1.8.1, zlib 1.2.3 and szip on HECToR
- 3 fold reduction in disk usage and 4 fold reduction in runtime with NOCSCOMBINE tool and netCDF4.0
- Adapted NEMO to use netCDF 4.0 resulting in reduction in disk usage of up to 3.55 times
- Resolved issues with nested models crashing on HECToR