

A PGAS implementation by co-design of the ECMWF Integrated Forecasting System

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#### Acknowledgements

Mats Hamrud Nils Wedi Jens Doleschal Harvey Richardson ECMWF ECMWF Technische Universität Dresden Cray Research UK

And my other partners in the CRESTA Project

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#### What is CRESTA - see http://cresta-project.eu/

- Collaborative Research into Exascale Systemware, Tools and Applications
- EU funded project, 3 years (year 1 just completed), ~ 50 scientists
- Six co-design vehicles (aka applications)
  - ELMFIRE (CSC, ABO, UEDIN) fusion plasma
  - GROMACS (KTH) molecular dynamics
  - HEMELB (UCL) biomedical
  - IFS (ECMWF) weather
  - NEK5000 (KTH) & OPENFOAM (USTUTT, UEDIN) comp. fluid dynamics
- Two tool suppliers
  - ALLINEA (ddt : debugger ) & TUD (vampir : performance analysis )
- Technology and system supplier CRAY UK
- Many Others (mostly universities)
  - ABO, CRSA, CSC, DLR, JYU, KTH, UCL, UEDIN-EPCC, USTUTT-HRLS



#### IFS model: current and planned model resolutions

| IFS model resolution  | Envisaged<br>Operational<br>Implementation | Grid point<br>spacing (km) | Time-step<br>(seconds) | Estimated<br>number of<br>cores <sup>1</sup> |
|-----------------------|--|----------------------------|------------------------|--|
| T1279 H <sup>2</sup>  | 2010 (L91)<br>2012 (L137)                  | 16                         | 600                    | 1100<br>1600                                 |
| T2047 H               | 2014-2015                                  | 10                         | 450                    | 6K   |
| T3999 NH <sup>3</sup> | 2020-2021                                  | 5                          | 240                    | 80K  |
| T7999 NH              | 2025-2026                                  | 2.5                        | 30-120                 | 1-4M   |

1 - a gross estimate for the number of 'Power7' equivalent cores needed to achieve a 10 day model forecast in under 1 hour (~240 FD/D), system size would normally be 10 times this number.

2 – Hydrostatic Dynamics

3 – Non-Hydrostatic Dynamics



56



Thank you to Nils Wedi for providing this figure

57

63

## % cost of Spectral Transforms on IBM Power7



20102014-152020-212025-261279 L91 (H)2047 L91 (H)2047 L1373999 L913999 L1377999 L40

#### Planned IFS optimisations for [Tera,Peta,Exa]scale



#### **Semi-Lagrangian Transport**

- Computation of a trajectory from each grid-point backwards in time, and
- Interpolation of various quantities at the departure and at the mid-point of the trajectory



#### Semi-Lagrangian Transport: T799 model, 256 tasks

Task 11 encountered the highest wind speed of 120 m/s (268 mph) during a 10 day forecast starting 15 Oct 2004



#### blue: halo area

Halo width assumes a maximum wind speed of 400 m/s x 720 s T799 time-step (288 km)

Get u,v,w wind vector variables (3) from 'neighbour' tasks to determine departure and mid-point of trajectory



#### red: halo points actually used



Get rest of the variables (26) from the red halo area and perform interpolations

Note that volume of halo data communicated is dependent on wind speed and direction in locality of each task



#### IFS Optimisations for ExaScale & Co-design

- All currently planned IFS optimisations in the CRESTA project
  - Involve use of Fortran2008 coarrays (CAF)
  - Used within context of OpenMP parallel regions
- Overlap Legendre transforms with associated transpositions
- Overlap Fourier transforms with associated transpositions
- Rework semi-Lagrangian communications
  - To substantially reduce communicated halo data
  - To overlap halo communications with SL interpolations
- CAF co-design team
  - <u>caf-co-design@cresta-project.eu</u>
  - ECMWF optimise IFS as described above
  - CRAY optimize DMAPP to be thread safe
  - TUD visualize CAF operations in IFS with vampir
  - ALLINEA debug IFS at scale with ddt (MPI/OMP/CAF)

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#### Overlap Legendre transforms with associated transpositions







time



## Overlap Legendre transforms with associated transpositions/3 (LTINV + coarray puts)



Expectation is that compute (LTINV-blue) and communication (coarray puts-yellow) overlap in time. We should be able to see this in the future with an extension to vampir being developed in CRESTA



#### Semi-Lagrangian – coarray implementation

red: only the halo points that are used are communicated



Note no more blue area (max wind halo) and associated overhead.

Also, halo coarray transfers take place in same OpenMP loop as the interpolations.



#### T2047L137 model performance on HECToR (CRAY XE6) RAPS12 IFS (CY37R3), cce=7.4.4

**APRIL 2012** 



#### T2047L137 model performance on HECToR (CRAY XE6) RAPS12 IFS (CY37R3), cce=8.0.6 -hflex\_mp=intolerant





#### T2047L137 model Efficiency on HECToR (CRAY XE6) RAPS12 IFS (CY37R3)





#### Schedule for IFS optimisations in CRESTA

| When          | Activity   |
|---------------|--|
| 4Q2011-1Q2012 | Coarray Kernel 🖌   |
| 1Q2012        | IFS CY37R3 port to HECToR ✔<br>Run T2047 model at scale and analyze performance ✔  |
| 2Q2012        | Scalability improvements arising from T2047 analyses ("low hanging fruit") ✓<br>Overlap Legendre transform computations with associated TRMTOL & TRLTOM<br>transpositions ✓  |
| 3Q2012        | Semi-Lagrangian optimisation 🖌<br>Overlap TRGTOL & TRLTOG transpositions with associated Fourier transforms 🖌  |
| 4Q2012        | RAPS13 IFS CY38R2 port to HECToR (contains Fast Legendre Transform)<br>T3999 model runs on HECToR<br>Test with IBM F2008 'coarray technology preview' compiler on Power7 at ECMWF  |
| 1Q2013        | Use coarrays to optimise TRMTOS/TRSTOM transpositions<br>Initial use of GPUs for IFS (targeting LTDIR/LTDIR dgemm's)   |
| 2013-2014     | Other IFS scalability optimisations (transpose SL data, physics load balancing, +++)<br>Development & testing of a future solver for IFS (Plan B)<br>Following closely developments in GungHO! project (MetOffice, NERC, STFC)<br>GungHO= <u>G</u> lobally <u>Uniform Next Generation Highly Optimised</u> |

# Thank you for your attention

QUESTIONS?

HINHALLI

#### IFS model coarray developments

Compile with –DCOARRAYS

for compilers that support Fortran2008 coarray syntax

Run with,

&NAMPAR1 LCOARRAYS=true,

LCOARRAYS=true, to use coarray optimizations

&NAMPAR1 LCOARRAYS=false,

to use original MPI implementation



470 FD/D

28 FD/D

#### Motivation – T2047 and T3999 costs on IBM Power7 (percentage of wall clock time)

|           |                              | T2047(%)  | T3999(%)  |
|-----------|------------------------------|-----------|-----------|
|           |                              | 2014-15   | 2020-21   |
| LTINV_CTL | - INVERSE LEGENDRE TRANSFORM | 3.30      | 8.40      |
| LTINV_CTL | - M TO L TRANSPOSITION       | 5.37      | 5.24      |
| LTDIR_CTL | - DIRECT LEGENDRE TRANSFORM  | 3.56      | 5.30      |
| LTDIR_CTL | - L TO M TRANSPOSITION       | 2.84      | 3.14      |
| FTDIR_CTL | - DIRECT FOURIER TRANSFORM   | 0.20      | 1.07      |
| FTDIR_CTL | - G TO L TRANSPOSITION       | 2.85      | 2.21      |
| FTINV_CTL | - INVERSE FOURIER TRANSFORM  | 0.72      | 3.76      |
| FTINV_CTL | - L TO G TRANSPOSITION       | 4.47      | 7.36      |
|           | SUM(%)                       | 23.4      | 36.5      |
|           |                              | L137/LT   | L91/FLT   |
|           |                              | 4224Tx8t  | 1024Tx16t |
|           |                              | 528 Nodes | 256 Nodes |



HPC in Meteorology workshop, 1-5 October 2012



Relative *computational cost* of the spherical harmonics transforms plus the spectral computations (solving the Helmholtz equation) as a percentage of the overall model cost for various configurations. Red bars indicate the total cost *including* the global communications involved. Percentages have been derived considering all gridpoint dynamics and physics computations but without considering IO, synchronization costs (barriers), and any other ancillary costs. All runs are non-hydrostatic unless indicated with (H). All runs further show that the communications cost is less than or equal to the compute cost on the IBM Power7 and have good potential for "hiding" this overhead. However, communication cost is likely to increase with the number of cores.

#### Planned IFS optimisations for [Tera,Peta,Exa]scale







#### Similar Processes, Accumulated Exclusive Time per Function 0.00 s 0.25 s 0.50 s 0.75 s 1.00 s 1.25 s 1.50 s 1.75 s 2.00 s 2.25 s 2.50 s 2.75 s 3.00 s 3.25 s 3.50 s d**…∎**ftdir ctl\$ftdir ctl mod 5 tinv\_ctl\$ftinv\_ctl\_mod\_ MPI Wait ltinv ctl\$ltinv ctl mod Itdir mođ ttdir\_ctl\$ftdir\_ctl\_mod\_ tinv ctl\$ltinv ctl mod ctl\$ftinv\_ctl\_mod MPI\_Wait ltdir 2 cti mod ftinv ctl. ftinv\_ctl\$ftinv\_ctl\_mod MPI Wait d...r ftdir ctl\$ftdir ctl mod ltinv ctl\$ltinv ctl mod ltdir... mod

CREST







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#### Other Fortran 2008 compilers

- License finally agreed with IBM
  - ECMWF will install xlf v14 compiler on Power7
  - Only took 1 year from first inquiry (pre-CRESTA)
  - Subject to non-disclosure
  - Am sure we will be granted permission to present and publish results if they are good
  - Plan is first to test IFS RAPS12 with this compiler
- Promoting need for Fortran 2008 to vendors is important
- Intel ?
- Fujitsu ?
- gfortran ?
- PGI ?



### Using HECToR

- Moved IFS from cce=8.0.3 to cce=8.0.6
  - To pick up fix to random hangs at start of job
    - Job would run to cp time limit without executing a single application statement
    - Refunded lost KAu's
  - 8.0.6 also fixed a couple of random coarray runtime failures
  - Thanks to CRAY for providing a good compiler release
- Multiple aprun's in high core count jobs (10K to 64K cores)
  - To improve overall system resource utilization
  - Small, medium and large batched jobs
  - Some waste due to unused cores in each job
  - Promise of refund (more KAus) at some time in future



#### Hybrid runtime support - IFS

- Initial IFS MPI implementation 1994-1996
- Hybrid MPI/OpenMP implementation ~1999
  - OpenMP implementation at highest level
  - Single parallel regions for each of physics, radiation scheme, dynamics, Legendre transforms, Fourier transforms and Fourier space computations
  - Schedule dynamic used in most parallel regions
- Hybrid implementation benefits
  - About 20 percent performance improvement at scale
  - Huge memory savings, memory use reduces linearly with number of OpenMP threads
- Next evolutionary step: use of Fortran 2008 coarrays to
  - Overlap computation with communication in transpositions
    - Fourier space <-> Spectral space comms, overlapped with Legendre transforms
    - grid point space <-> Fourier space comms, overlapped with FFTs and Fourier space computations
  - Reduce total halo communication in semi-Lagrangian scheme
  - Dominant coarray communications in OpenMP parallel regions

#### OpenMP for IFS T1279L91 model on IBM Power6 (~2009)





## OpenMP for IFS T1279L91 model on IBM Power6 (~2009)





HPC in Meteorology workshop, 1-5 October 2012





#### IFS model speedup on IBM Power6 (~2010)





#### HPC in Meteorology workshop, 1-5 October 2012





#### Overlap Legendre transforms with associated transpositions/2



#### IFS grid point space: "EQ\_REGIONS" partitioning for 1024 MPI tasks

Each MPI task has an equal number of grid points







#### LTINV recoding

#### COMPUTE COMMUNICATION

& PSPVOR, PSPDIV, PSPSCALAR, & & PSPSC3A, PSPSC3B, PSPSC2 , &

DO JM=1,D%NUMP IM = D%MYMS(JM)

ENDIF

DO JW=1,NPRTRW

IF ( ILEN > 0 ) THEN

IF ( ILENS > 0 ) THEN

!\$OMP PARALLEL DO SCHEDULE(DYNAMIC,1) PRIVATE(JM,IM) DO JM=1,D%NUMP IM = D%MYMS(JM)CALL LTINV(IM, JM, KF OUT LT, KF UV, KF SCALARS, KF SCDERS, ILEI2, IDIM1, & & PSPVOR, PSPDIV, PSPSCALAR , & & PSPSC3A, PSPSC3B, PSPSC2 , & & KFLDPTRUV, KFLDPTRSC, FSPGL PROC) ORIGINAL **ENDDO !SOMP END PARALLEL DO** code DO J=1,NPRTRW ILENS(J) = D%NLTSFTB(J)\*IFIELD IOFFS(J) = D%NSTAGT0B(J)\*IFIELD ILENR(J) = D%NLTSGTB(J)\*IFIELD IOFFR(J) = D%NSTAGT0B(D%MSTABF(J))\*IFIELD **ENDDO** CALL MPL\_ALLTOALLV(PSENDBUF=FOUBUF\_IN,KSENDCOUNTS=ILENS,& & PRECVBUF=FOUBUF, KRECVCOUNTS=ILENR, & & KSENDDISPL=IOFFS, KRECVDISPL=IOFFR, & & KCOMM=MPL ALL MS COMM, CDSTRING='TRMTOL:') !\$OMP PARALLEL DO SCHEDULE(DYNAMIC,1) PRIVATE(JM,IM,JW,IPE,ILEN,ILENS,IOFFS,IOFFR) CALL LTINV(IM, JM, KF\_OUT\_LT, KF\_UV, KF\_SCALARS, KF\_SCDERS, ILEI2, IDIM1, & & KFLDPTRUV, KFLDPTRSC, FSPGL PROC) CALL SET2PE(IPE, 0, 0, JW, MYSETV) ILEN = D%NLEN M(JW,1,JM)\*IFIELD IOFFS = (D%NSTAGT0B(JW)+D%NOFF M(JW,1,JM))\*IFIELD IOFFR = (D%NSTAGT0BW(JW,MYSETW)+D%NOFF\_M(JW,1,JM))\*IFIELD NEW FOUBUF C(IOFFR+1:IOFFR+ILEN)[IPE]=FOUBUF IN(IOFFS+1:IOFFS+ILEN) code ILENS = D%NLEN M(JW,2,JM)\*IFIELD

IOFFS = (D%NSTAGT0B(JW)+D%NOFF\_M(JW,2,JM))\*IFIELD IOFFR = (D%NSTAGT0BW(JW,MYSETW)+D%NOFF\_M(JW,2,JM))\*IFIELD FOUBUF C(IOFFR+1:IOFFR+ILENS)[IPE]=FOUBUF IN(IOFFS+1:IOFFS+ILENS) ENDIF ENDDO ENDDO **!**\$OMP END PARALLEL DO SYNC IMAGES(D%NMYSETW) FOUBUF(1:IBLEN)=FOUBUF C(1:IBLEN)[MYPROC]



## T159 model scaling: small model with 'large' number of user threads (4 threads per task)





#### **IFS Semi-Lagrangian Comms**

#### SL comms scaling limited by

- constant width halo for u,v,w ( 400 m/s x time step)
- Halo volume communicated, which is a function of wind speed and direction in locality of each task

#### • 'Halo-lite' approach tested (2010)

- Only get (using MPI) grid columns from neighbouring tasks that your task needs, i.e. only the red points
- Requires more MPI communication steps (e.g. mid-point, departure point)
- No faster than original approach due to overheads of above

#### CRESTA optimisation using F2008 coarrays (2012)

- Only get grid columns from neighbouring tasks that your task needs, i.e. only the red points
- Do the above in the context of an OpenMP parallel region; overlapping interpolations for determining the departure point & mid-point and interpolations at these points



## wind plot





#### T159 model task 37 of 256 tasks

Task encountering the highest wind speed of 138 m/s (309 mph) during a 10 day forecast starting 17 Oct 2010



#### T159 model task 128 of 1024 tasks





#### T159 model task 462 of 4096 tasks





#### Computational Cost at T2047 and T3999



#### Hydrostatic T<sub>L</sub>2047

Tstep=450s, 5.8s/Tstep With 256x16 ibm\_power6

#### Non-Hydrostatic T<sub>L</sub>3999

Tstep=240s, 13.6s/Tstep With 512x16 ibm\_power6



#### Breakdown of TRANS cost: Computations vs. Communications



H T<sub>L</sub>2047 ~2015

Data sent/received: 117.8GB/s

NH T<sub>L</sub>3999 ~2020

Data sent/received: 289.6GB/s



### **IFS Introduction – A history**

 Resolution increases of the deterministic 10-day medium-range Integrated Forecast System (IFS) over ~25 years at ECMWF:

**ICMWE** 

- 1987: T 106 (~125km)
- 1991: T 213 (~63km)
- 1998: T<sub>L</sub>319 (~63km)
- 2000: T<sub>L</sub>511 (~39km)
- 2006: T<sub>L</sub>799 (~25km)
- 2010: T<sub>L</sub>1279 (~16km)

### **Introduction – A history**

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  - 1987: T 106 (~125km)
  - 1991: T 213 (~63km)
  - 1998: T<sub>L</sub>319 (~63km)
  - 2000: T<sub>L</sub>511 (~39km)
  - 2006: T<sub>L</sub>799 (~25km)
  - 2010: T<sub>L</sub>1279 (~16km)
  - 2015?: T<sub>L</sub>2047 (~10km)
  - 2020-???: (~1-10km) Non-hydrostatic, cloud-permitting, substantially different cloud-microphysics and turbulence parametrization, substantially different dynamics-physics interaction ?



#### The Gaussian grid

#### About 30% reduction in number of points



Reduction in the number of Fourier points at high latitudes is possible because associated Legendre functions are very small near the poles for large *m*.



## (Adaptive) Mesh Refinement

- The IFS model is inherently based on a fixed structured mesh due to the link between the spectral representation and the position of the grid-points (zero's of the ordinary Legendre polynomials), which makes selective mesh refinement (adaptive or not) difficult to achieve.
- "AMR" possibilities: coexisting global multigrids, physics/ dynamics on different grids, wavelet-collocation methods, ...: Costly investment both in RD and computational cost
- Hence it is of strategic importance to understand the added-value of adaptive or static mesh refinement for multiscale global NWP and climate prediction !



## Nonhydrostatic IFS (NH-IFS)

Bubnovă et al. (1995); Bénard et al. (2004), Bénard et al. (2005), Bénard et al. (2010), Wedi et al. (2009), Yessad and Wedi (2011)

 Arpégé/ALADIN/Arome/HIRLAM/ECMWF nonhydrostatic dynamical core, which was developed by Météo-France and their ALADIN partners and later incorporated into the ECMWF model and also adopted by HIRLAM.



### **Numerical solution**

- Two-time-level, semi-implicit, semi-Lagrangian.
- Semi-implicit procedure with two reference states, with respect to gravity and acoustic waves, respectively.
- The resulting Helmholtz equation can be solved (subject to some constraints on the vertical discretization) with a direct spectral method, that is, a mathematical separation of the horizontal and vertical part of the linear problem in spectral space, with the remainder representing at most a pentadiagonal problem of dimension NLEV<sup>2</sup>. Non-linear residuals are treated explicitly (or iteratively implicitly)!

(Robert, 1972; Bénard et al 2004,2005,2010)



### The spectral transform method

Eliasen et. al (1970), Orszaag (1970)

Applied at ECMWF for the last 30 years ...

## Spectral semi-Lagrangian semi-implicit (compressible) a viable option ?

-Computational efficiency on future MPP architectures ?
-Accuracy at cloud-resolving scales ?
-Suitability for the likely mixture of medium and high resolution ensembles and ultra-high resolution forecasts ?



### The Gaussian grid





Reduction in the number of Fourier points at high latitudes is possible because associated Legendre polynomials are very small near the poles for large *m*.

Note: number of points nearly equivalent to quasi-uniform icosahedral grid cells of the ICON model.



## **Cost of the spectral transform method**

- FFT can be computed as C\*N\*log(N) where C is a small positive number and N is the cut-off wave number in the triangular truncation.
- Ordinary Legendre transform is O(N<sup>2</sup>) but can be combined with the fields/levels such that the arising matrix-matrix multiplies make use of the highly optimized BLAS routine DGEMM.
- But overall cost is O(N<sup>3</sup>) for both memory and CPU time requirements.



Desire to use a fast Legendre transform where the cost is proportional to C\*N\*log(N) with C << N

and thus overall cost N<sup>2\*</sup>log(N)



## Fast Legendre Transform (FLT)

- The algorithm proposed in (*Tygert, 2008,2010*) suitably fits into the IFS transform library by simply replacing the matrix-matrix multiply DGEMM call with a BUTTERFLY\_MATRIX\_MULT call plus slightly more expensive pre-computations.
- (1) Instead of the recursive Cuppen divide-and-conquer algorithm (Tygert, 2008) we use the so called butterfly algorithm (O'Neil et al, 2009; Tygert, 2010) based on a matrix compression technique via rank reduction with a specified accuracy to accelerate the arising matrix-vector/matrix multiplies (sub-problems still use DGEMM).
- (2) We apply the matrix compression directly on the matrix of the associated polynomials, which reduces the required precomputations and eliminates the need to apply *FMM (fast multipole method)* accelerated interpolations. Notably, the latter were an essential part of the proposed FLT in *Suda and Takami (2001)*.



## The butterfly compression (O'Neil, Woolfe, Rokhlin, 2009; Tygert 2010)

With each level I, double the columns and half the rows



I=0





l=2



I=3



Floating point operations per time-step in Gflop

Inverse transform of single field/level

Wallclock time in seconds

inverse transform of 10 fields, offline test environment



## Selected projects to prepare for exascale computing in Meteorology (NWP)

- ICOMEX ICOsahedral grid Models for EXascale Earth system simulations (2011-2014)
- Gung-Ho Development of the Next Generation Dynamical Core for the UK MetOffice (2 phases, 2011-2013, 2013-2016)
- CRESTA Collaborative Research into Exascale Systemware, Tools & Applications (2011-2014)



#### T3999 6h forecast - inverse transforms: CPU time vs. wave number



### T3999 6h forecast - inverse transforms: Floating point operations vs. wave



#### Why is Matrix Multiply (DGEMM) so efficient? VECTOR SCALAR / CACHE



FMA's >> LD's

