From Weather Dwarfs to Kilometre-Scale Earth System Simulations

Nils P. Wedi, Peter Bauer, ECMWF colleagues, ESCAPE project partners
European Centre for Medium-Range Weather Forecasts (ECMWF)
Outline

• Numerical weather prediction & climate, a brief (HPC) history
• Ensemble-based assimilation and forecasts of Weather & Climate
• Earth-System complexity and the notion to resolve rather than parametrise
• An intermediate goal: globally uniform weather & climate modelling at 1 km horizontal resolution
  – Defining and encapsulating the fundamental algorithmic building blocks ("Weather and Climate Dwarfs")
  – Pioneering algorithm development with hardware adaptation using DSL toolchains
  – Reviewing the need for precision
  – A HPCW benchmark and cross-disciplinary Verification, Validation, and Uncertainty Quantification (VVUQ)
ECMWF’s progress in degrees of freedom
(levels x grid columns x prognostic variables)

(Schulthess et al, 2018)
Sustained HPC performance
I/O - Impact of NVRAM on Data Access

Byte Addressable Hypercubes

- Longitude (3600)
- Latitude (1800)
- Atmospheric levels, Physical parameters (~200)
- Time steps (~100)
- Probabilistic pertubations (50)

@ double precision

- 9km 48 TiB
- 5km 192 TiB
- 1.25km 1.82 PiB

Not included: historical observations, multiple models, etc...

EUROPEAN CENTRE FOR MEDIUM-RANGE WEATHER FORECASTS

Clients want to do different analytics across multiple axis

ECMWF archives ~150TB / Day
Growing exponentially …
Ensemble of assimilations and forecasts
Ocean – Land – Atmosphere – Sea ice
Copernicus climate change monitoring service C3S

Surface air temperature anomaly for May 2018 relative to 1981-2010

°C
Observation impact on reducing the short-range forecast error

Future:
Mobile phones, cars, homes, ....
CO₂ OBSERVATIONS

GOSAT CO₂ (IUP- Uni Bremen)

CO₂ SURFACE FLUXES

Vegetation (CTESSEL)
Fires (GFAS)
Ocean (inventory)
Anthropogenic (inventory)

TRANSPORT (ECMWF)

PBL mixing
Advection
Convection

CHEMISTRY

Oxidation of CO
(not yet represented in model)

Graphic: A Agusti-Panareda, S Massart (ECMWF)
Extreme events: Hurricane IRMA

High impact disruptive events: Use of high-resolution ensembles to estimate uncertainty in large-scale (steering) flow.
Hurricane IRMA 18km vs 5km ensemble

ECMWF Strategy 2025
a 5km ensemble …
Global KE - Spectra \(\sim 500\text{hPa}\)

Resolve rather than parametrize much of the crucial vertical transport of momentum and heat.
TCo1279 9km
48h forecast ~9km

Take the “Turing test” of climate & weather modelling (T. Palmer)

http://gigapan.com/gigapans/206287

48h forecast ~1km
DCMIP16

- 1 km simulation on reduced planet
- No convection parameterization!
- Same microphysics scheme
- Different dynamical cores
- Different physics-dynamics coupling
- Different time stepping
Where do we spend the time?

Single electrical group:~47minutes wallclock time
(single electrical group==384 nodes)

1408 MPI tasks x 18 threads
306 FC/day
Ocean resolution requirements

Hallberg 2013

From the presentation of H. Hewitt, at ECMWF (2016)
Arctic Ocean circulation at ~1km

AWI FESOM2 team
Animation: Nikolay Koldunov (AWI)

4 months/day, time step 2 min, 1700 Broadwell Cores on Cray CS400
Arctic sea-ice evolution at ~1km

AWI FESOM2 team
Animation: Nikolay Koldunov (AWI)
IFS KE spectra compared to altimeter observations

Cut-off where power is 50% of $k^{-5/3}$

Resolved 1 km scales need at least $\times 6$ more resolution and $\times 10000$s in compute => intermediate goal 1 km grid

[Courtesy S. Abdalla]
Near-global climate simulation at 1 km resolution: establishing a performance baseline on 4888 GPUs with COSMO 5.0

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Weather & Climate Dwarfs

Extract model dwarfs...

... explore alternative numerical algorithms ...

... hardware adaptation ...

... reassemble model and benchmark

(hpc-escape.eu)
Atlas: a library for NWP and climate modelling

https://github.com/ecmwf

Deconinck et al. 2017
Domain-specific language toolchain

\[ F(\Psi_L, \Psi_R, U) \equiv [U]^+\Psi_L + [U]^−\Psi_R \]

\[ U \equiv \frac{u \delta t}{\delta x}, \quad [U]^+ \equiv 0.5(U+|U|), \quad [U]^− \equiv 0.5(U−|U|) \]

Complementary skills of CLAW, GridTools (MeteoSwiss) and Atlas (ECMWF)
## Weather & Climate Dwarfs

<table>
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<tr>
<th>Dwarf</th>
<th>prototype implemented</th>
<th>documented</th>
<th>based on Atlas</th>
<th>MPI</th>
<th>Open MP</th>
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<td>P - cloud microphysics - CloudSC</td>
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<td>P - radiation scheme - ACRANEB2</td>
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<td>I - LAITRI (3d interpol. algorithm)</td>
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**planned next:**
- D - advection - discontinuousGalerkin
- D - elliptic solver - multigridPrecon

**Comparison of software optimized for GPU and Xeon processors**

Poulsen & Berg (2017)
Advection

Rossby-Haurwitz test case after 7 days

Path-based
dwarf-D-advection-SemiLagrangian

Control-volume-based
dwarf-D-advection-MPDATA

Atlas library support for both prototype implementations
Moist baroclinic instability with FVM and spectral-transform IFS (ST) using large-scale condensation and diagnostic precipitation!

Choice of dynamical core on the same grid with the same physics!
Bespoke Krylov solvers

Parallel restriction, prolongation and Atlas mesh generation
Fast Legendre Transform

Reduces number of floating point operations

Number of floating point operations for direct or inverse spectral transforms of a single field, scaled by $N^2 \log^3 N$

(Wedi et al, 2013)
Schematic description of the spectral transform method in the ECMWF IFS model

Alan Gray, Peter Messmer, NVIDIA
Hardware co-design

Spectral transforms

peak bandwidth

goal

peak performance

10x speedup

Advection

GPU speed-up

figure: courtesy of Alan Gray, Peter Messmer (NVIDIA)
The cost profile of a 1.25km IFS atmosphere simulation on Piz Daint (CPU only)

Example: TCo7999 L62 (~1.25km)

4880 MPI tasks x 12 threads
69 FC/day ~ 0.19 SYPD
single precision / FLT
~85.21 MWh / SY

Based on the Piz Daint, Swiss Cray XC50 Haswell, Aries interconnect, ~5000 nodes total

75% comms; 25% compute
Simulating performance and scalability of MPI communications

Communication time as a function of halo size, topology & routing algorithm, compared to spectral transpositions

Zheng and Marginaud (GMD, 2018)

MPI collectives at least across a subset of nodes are required in NWP & climate!
Communication is bad – small time steps are worse

**Total data communication volumes [TB] for 48-hour forecast**

- **Spectral element model**
  - Time step = 4s
  - Data movement: 34 TB

- **Spectral transform model**
  - Time step = 240s
  - Data movement: 427 TB

- **Spectral element model**
  - Time step = 4s
  - Data movement: 689 TB

Same time to solution! Energy efficiency?

Data movement x100 (x1000) more expensive than computations in time (energy)!

[Shalf et al. 2011]
Will Deep Learning influence algorithmic choices for weather & climate?

NVSwitch Delivers a >2X Speedup for Deep Learning and HPC*

System Configs: Each of the two DGX-1 servers have dual-socket Xeon E5 2690v4 Processor, 8 x V100 GPUs; servers connected via a 4 EDR (100Gb) InfiniBand connections. DGX-2 server has dual-socket Xeon Scalable Processor Platinum 8168 Processors, 16 x Tesla V100 GPUs.

Co-models (model + radiation)

- Overlapping of compute and communication
- Co-execution on different threads

(G. Mozdzynski)
IFS single precision performance – Atmosphere only (no I/O)

Singe vs double precision

137 levels

10 days in 1 hour

62 levels

(Vana, Dueben et al 2017)
A scale-selective approach: Track of Hurricane Irma

Chantry, Düben and Palmer in preparation

- Spectral models allow to treat different scales at different precision.
- We can reduce precision when calculating the small scales.
- This is intuitive due to the high inherent uncertainty in small scale dynamics (parametrisation, viscosity, data-assimilation,...).
- The smallest scales are the most expensive.
IFS 1km: strong scaling on PizDaint

Goal ~1 year / Day

Many thanks to Thomas Schulthess & Maria Grazia Giuffreda!
Mathematical methods and algorithms:
• Semi-implicit, semi-Lagrangian CG/DG
• Hierarchical multigrid tools
• Fault resilient solver
• Artificial neural networks and:
  • DSL toolchain
  • Ensemble based URANIE
  • State-of-the-art

Benefit beyond the state-of-the-art
starting October 2018
Roadmap for weather & climate computing

- EuroEXA
- EPIGRAM HS
- ESCAPE 2
- ESCAPE
- nextgenio
- MAESTRO
- Data Orchestration
- ESIWACE
- ESIWACE-2?
- EuroHPC

Novel algorithms and benchmarks  Feature applications
New technologies  Cross-disciplinary Flagships

EUROPEAN CENTRE FOR MEDIUM-RANGE V

EXTREMECART

EXTREMECART

ETP 4 HPC

ETP 4 HPC
ExtremeEarth

Science:
- Climate prediction
- Weather forecasting
- Earthquake prediction

Impact:
- Hydrology and water
- Energy
- Food and agriculture
- Geo-engineering
- Disasters and risks

Ultra high-resolution, integrated Earth-system & impact modelling capability

Co-Design

Advanced mathematics & algorithms
Multi-scale/multi-physics models
Portable and performant science code
Domain specific computing framework
End-to-end demonstrators

Technology:
- Numerical modelling
- Data assimilation and fusion
- Deep learning
- Programming models
- Extreme and cloud computing
- Extreme data handling and storage
- Workflows and visualization

Integrated exascale Earth-system data analytics & management capability

Earth-system HPC technology and exascale capability

Integrated Earth-system information system capability
ECMWF’s mission strategy

• In collaboration with its member and associated states
  – **Address the challenges in sustainable computing and data handling**
  – **Move towards Earth-System complexity with rigorous quantification of forecast uncertainty**
    • High-resolution global ensemble of assimilation and forecasts coupling the ocean, sea-ice, land and atmosphere
  – **Supporting Copernicus Services**
    • Climate monitoring services for the atmosphere, **hydrological and carbon cycle**
    • European Reanalysis (currently producing ERA-5)
    • Atmospheric composition monitoring
    • Emergency alert system (Floods, Fires, …)
In 2016, the European Commission (EC) issued a call for ideas for future Flagships, to be funded by the Future and Emerging Technology (FET) programme.

FET Flagships are:
“... science- and technology-driven, large-scale, multidisciplinary research initiatives built around a visionary unifying goal ... tackle grand science and technology challenges ... strong and broad basis for future innovation and economic exploitation ... novel benefits for society of a potential high impact ... long-term and sustained effort.”

FETFLAG-01-2018: ‘Energy, Environment and Climate change’:
“Earth, Climate Change and Natural Resources: New technologies and ambitious approaches for high-precision modelling and simulation, including the necessary data integration, that enable an in-depth understanding of the earth and climate change, helping in the long run to manage natural resources in a sustainable way, ensure food security and sustainable farming, and protect natural ecosystems
The cost profile of a 1.25km (non-hydrostatic) IFS atmosphere simulation Piz Daint

Example: TCo7999 L62 (~1.25km)

4880 MPI tasks x 12 threads
32 FC/day ~ 0.088 SYPD
single precision / FLT
~191.74 MWh / SY

Based on the Piz Daint, Swiss Cray XC50 Haswell, Aries interconnect, ~5000 nodes total
The IFS model grid

Integrated Forecasting System (IFS)

A further ~20% reduction in gridpoints => ~50% less points compared to full grid