Zbigniew Piotrowski*'
Jean-Francois Cossette*''

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EULAG: high-resolution computational model for research of multi-scale geophysical fluid dynamics

by:
Piotr K Smolarkiewicz*,
Joseph M Prusa#,
Andrzej A. Wyszogrodzki*

*National Center for Atmospheric Research, Boulder, Colorado, U.S.A.
#Teraflux Corporation, Boca Raton, FL, U.S.A.
'University of Warsaw, Poland
''University of Montreal, Canada

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Science Lesson - What does the application do?

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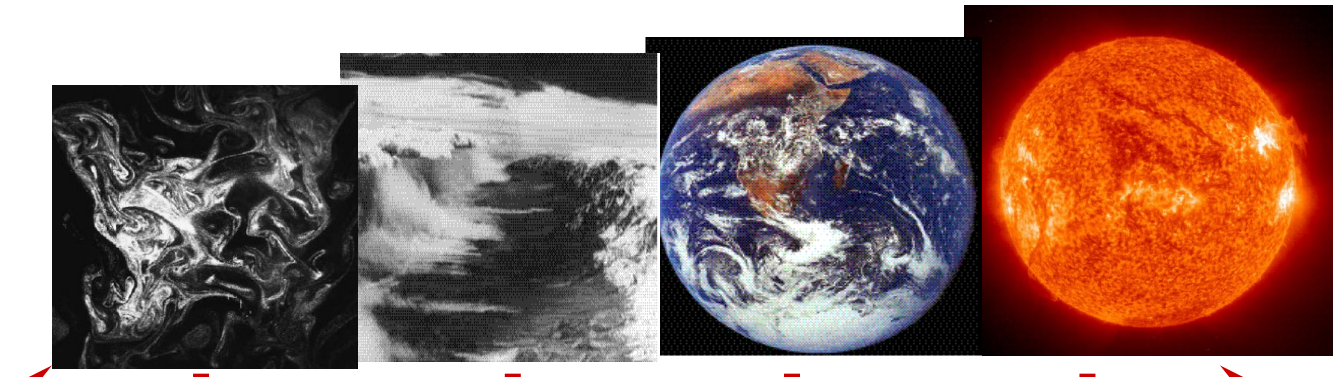
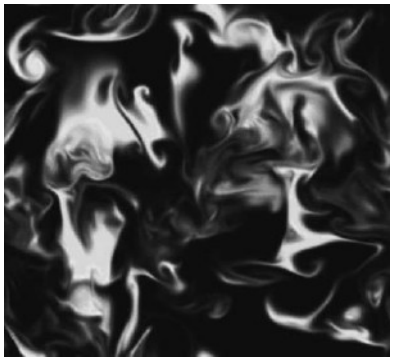
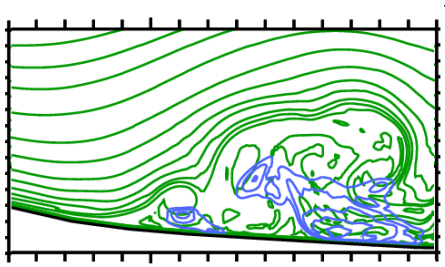
Simulating thermo-fluid flows across a range of scales and physics

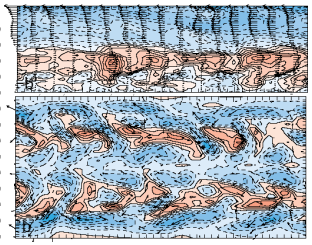




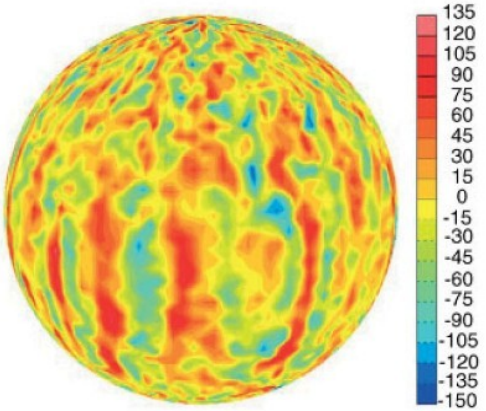
Cloud turbulence



Gravity waves



Global flows



Solar convection

Science Lesson – How?

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Two optional modes for integrating fluid PDEs:

- Eulerian --- control-volume wise integral
- Lagrangian --- trajectory wise integral

Optional fluid equations (nonhydrostatic):

- Anelastic,
- Compressible/incompressible Boussinesq,
- Incompressible Euler/Navier-Stokes'
- Fully compressible for high-speed flows

Available strategies for simulating turbulent dynamics:

- Direct numerical simulation (DNS)
- Large-eddy simulation, explicit and implicit (LES, ILES)

Parallel Programming Model

- MPI / Shmem
- Fortran 77
- Simple one-file construction
- Shell preprocessor
- Currently run on BG/L, IBM p575, Dell 1425SC and Dell PowerEdge 750 Clusters, single processor PC, etc.
- Plans: new parallel I/Os, performance improvements

Computational Methods

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Numerical algorithms:

- Nonoscillatory forward-in-time (NFT) advective/convective transport MPDATA
- Preconditioned non-symmetric Krylov-subspace elliptic solver GCR(k)

Parallelization:

- Parallel two-dimensional horizontal grid decomposition
- Non parallel in vertical direction
- Local domain contains inner processor grid and halo's (guard cells) to keep information from neighbor processors
- Global exchange of information for the purpose of elliptic solver

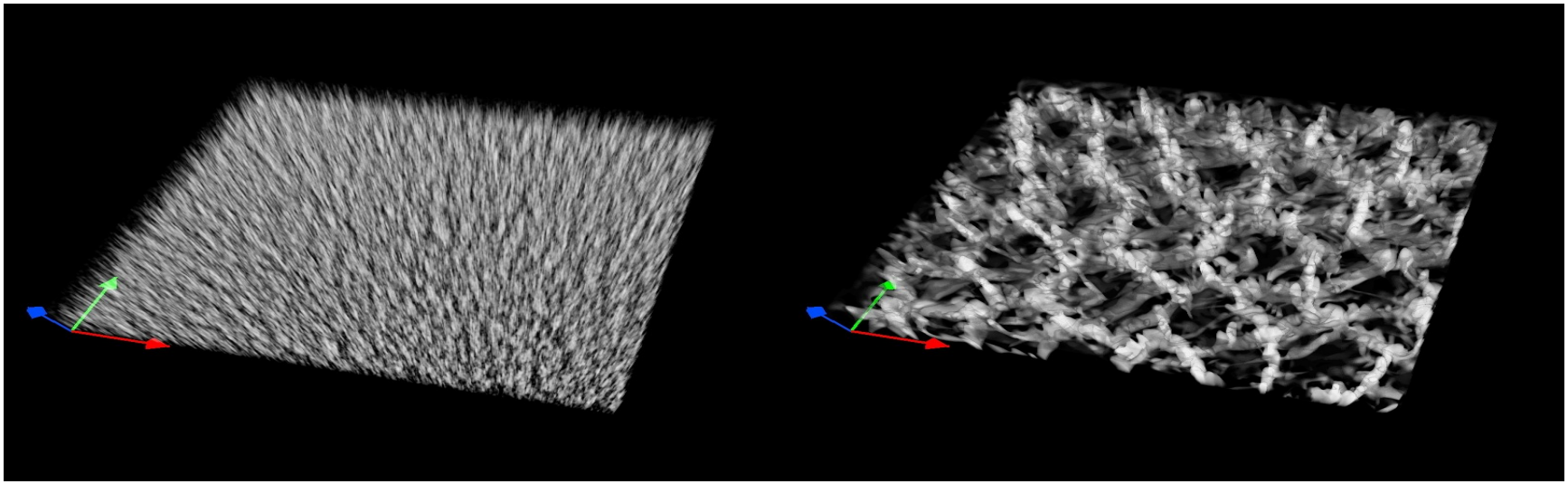
EULAG I/O

- Serial or parallel mode
- Fortran 77 tape read/write
- NetCDF ready, pNetCDF planned
- Restart from Fortran tape

Visualization

- NCAR Graphics, VIS5D, Matlab, IDL
- Hot topic and future: VAPOR

  Imagery produced by VAPOR (www.vapor.ucar.edu), a product of the National Center for Atmospheric Research



512x512x181 grid visualization –
positive vertical velocity over heated plane

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Performance

- Tools: HPM, MPI Trace, PAPI
- Bottlenecks: iterative solver, horizontal grid decomposition vs BG/L/W torus architecture
- Scaling improvement: decrease the gap between peak and sustained performance on available HPC systems
- No debugging tools used

Status and Scalability

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- Recent simulations on the Blue Gene/W supercomputer at the IBM Watson Research Center have demonstrated teraflop performance and excellent scalability up to 16 thousands of processors
- A progress with scalability up to 40.000 processors is expected
- No mayor changes in algorithms and libraries were performed
- Variable data structures for halo exchange were used to improve performance
- Algorithmic tunning, vector intrinsics, and maybe the 3D grid decomposition are planned to improve scaling

Roadmap

- Multiscale, multiphysics modeling --- from microphysics, to planetary and stellar circulations
- Demonstration that EULAG numerics' HPC scaling is capable of integrating the challenging multi-scale multi-physics flows
- More effective preconditioners for elliptic solver, and fully perturbational form of the governing equations with respect to arbitrary ambient states
- Edge-based unstructured-mesh clone of EULAG
- Improvements in parallel I/O, pNetCDF implementation
- VAPOR implementation