Implicit time-integration of an atmospheric model on massively-parallel computing systems

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- ICOsashedral Models for Exascale earth system simulation (ICOMEX)
  - advantages over lat-long grid: **Scales well on MPP architectures**, No polar problems, Monotonic/PD conservative transport, Flexible local refinement (variable resolution grids)
  - involves: **Exeter University & NCAR (MPAS)**, DWD and Max-Planck (ICON), JAMSTEC (NICAM) and LMD (DYNAMICO).
- models currently explicit:
  - solution is restrictive as we move towards smaller scales
  - implicit version results in **elliptic problem** of the form:

$$\nabla^2_H p' + \frac{\partial}{\partial \zeta}\left(A\frac{\partial (Bp')}{\partial \zeta}\right) - Cp' = R$$

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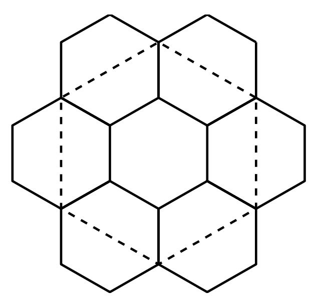
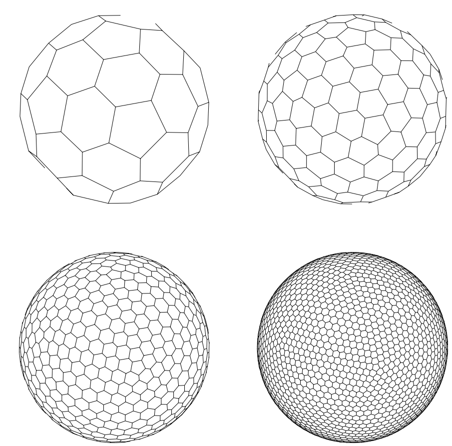
$$\nabla_H^2 p' + \frac{\partial}{\partial \zeta}\left(A \frac{\partial (B p')}{\partial \zeta}\right) - C p' = R$$

- inherent length scale *cdt* included in *C*
- multi-grid can be efficient and scale well for MPP
- only need to coarsen until CFL ~ 1 (4-5 times)
- currently being implemented in MPAS-atmosphere
- natural hierarchy to reduce data-io





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Implicit time-integration of an atmospheric model on massively-parallel computing systems

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1. Introduction

Icosahedral grids are quasi-uniform, giving the potential to overcome the scaling bottlenecks of models based on latitude-longitude grids on massively parallel computer systems. For this reason, a number of groups developing atmospheric models on icosahedral grids joined together to identify and address issues affecting parallel performance and scalability under the ICOsahedral-grid Models for EXascale earth system simulations (ICOMEX) project. Here we present some of the work from that project that addresses scalability of the model solver.

In order to increase the resolution, and hence the accuracy and realism, of weather and climate models, they must be able to exploit the massively parallel computing architectures that are becoming available. A significant bottleneck is node-to-node message-passing. For this reason, many models employ explicit time-integration which minimises the required message passing effort at each time-step.

However, implicit time integration allows significantly longer time steps, and confers advantages in stability and accuracy, but requires the solution of elliptic problems and this increases the amount of message passing. Recent research has shown that multi-grid elliptic solvers can be efficient and scale well for massively parallel problems. Here we outline the work we are doing to implement an implicit time-integration scheme within the MPAS-atmosphere model.

2. MPAS - atmosphere

The Model for Prediction Across Scales (MPAS) is a collaborative project for developing atmosphere, ocean and other earth-system simulation components for use in climate, regional climate and weather studies. MPAS-atmosphere is a fully three-dimensional, compressible, non-hydrostatic atmospheric model:

$$\frac{\partial \mathbf{V}_H}{\partial t} = -\frac{\rho_d}{\rho_m}\left[\nabla_\zeta\left(\frac{p}{\zeta_z}\right) - \frac{\partial \mathbf{z}_H p}{\partial \zeta}\right] - \eta \mathbf{k}\times\mathbf{V}_H - \boldsymbol{v}_H \nabla_\zeta \cdot \mathbf{V} - \frac{\partial \Omega \boldsymbol{v}_H}{\partial \zeta} - \rho_d \nabla_\zeta K - eW\cos\alpha_r - \frac{\boldsymbol{v}_H W}{r_e} + \mathbf{F}_{\mathbf{V}_H},$$

$$\frac{\partial W}{\partial t} = -\frac{\rho_d}{\rho_m}\left[\frac{\partial p}{\partial \zeta} + g\tilde{\rho}_m\right] - (\nabla\cdot\boldsymbol{v}W)_\zeta + \frac{uU + vV}{r_e} + e(U\cos\alpha_r - V\sin\alpha_r) + F_W,$$

$$\frac{\partial \Theta_m}{\partial t} = -(\nabla\cdot\mathbf{V}\theta_m)_\zeta + F_{\Theta_m},$$

$$\frac{\partial \tilde{\rho}_d}{\partial t} = -(\nabla\cdot\mathbf{V})_\zeta, \quad \text{and}$$

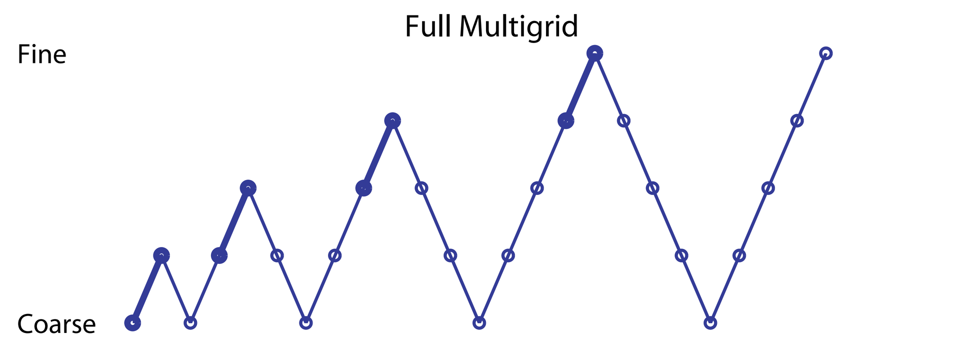
$$\frac{\partial Q_j}{\partial t} = -(\nabla\cdot\mathbf{V}q_j)_\zeta + F_{Q_j}.$$

We propose to compare the existing horizontally (split-)explicit, vertically implicit time integration scheme with a semi-implicit Strang carryover scheme.

3. Multi-grid solver

Iterative methods provide rapid convergence in the short-wavelength solution but slow convergence to the long-wavelength solution. Convergence of the longer-wavelengths may therefore be obtained by recasting the problem on a coarser mesh. This premise forms the basis of multi-grid methods. Restriction onto successively coarser grids provides convergence across-scales. Subsequent prolongation of the solution onto finer-grids coupled with smoothing using rapid iterative methods then provides the final 'fine-scale' solution. A number of multi-grid strategies exists including V-cycle and Full Multi-Grid (FMG, Fig 1).

Fig 1: Schematic representation of the Full multi grid method



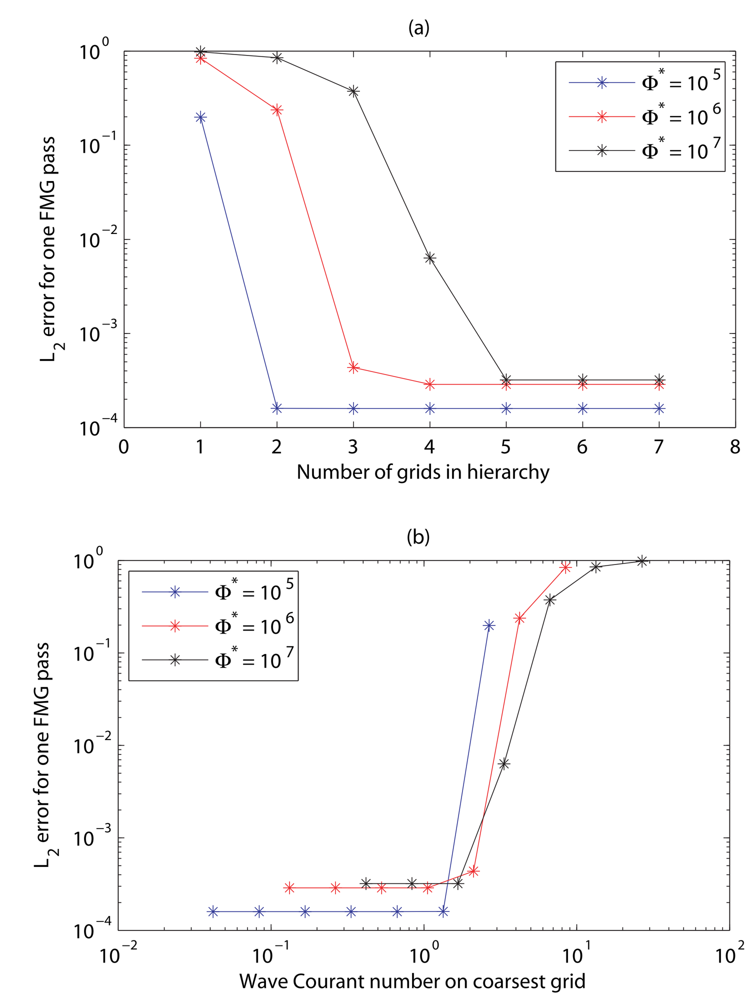
At each time step the semi-implicit scheme requires the solution of a Helmholtz problem:

$$\nabla_H^2 p' + \frac{\partial}{\partial \zeta}\left(A\frac{\partial (Bp')}{\partial \zeta}\right) - Cp' = R$$

where A, B and C are spatially variable coefficients and R represents the known right hand side. Because the equation-set has been reduced significantly, there is a reduction in the message passing and required storage space at the coarser levels. Implementation of multi-grid is well suited to MPAS. The icosahedral grid structure provides a natural hierarchy to build the grids required for the solution (Fig 2).

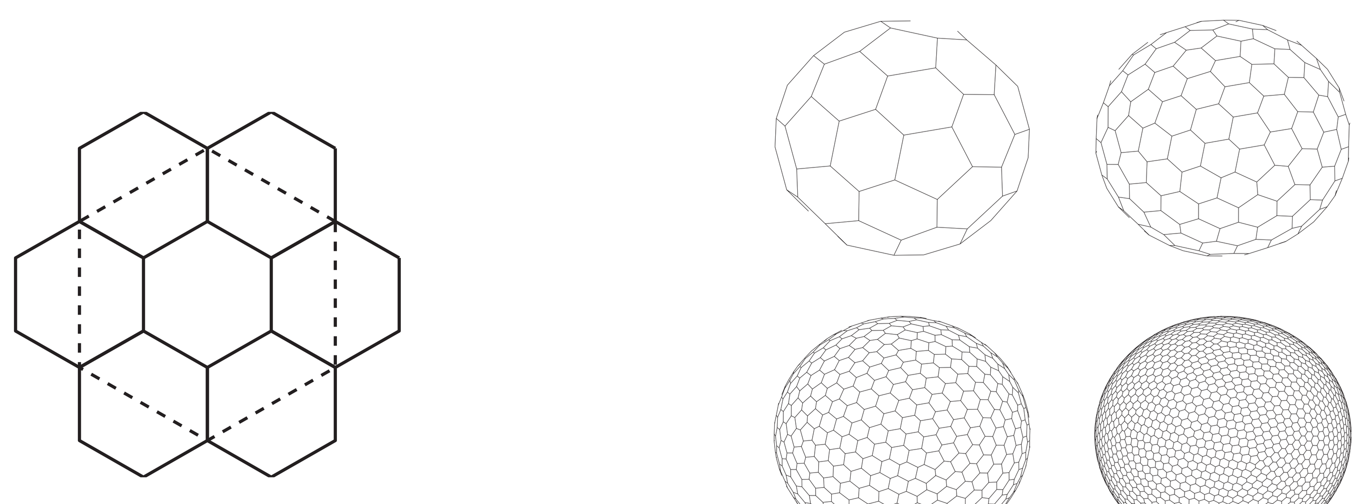
Initial tests using a shallow water model have shown that only a modest number (2-5) of grid-levels are required (Fig 3a). The Helmholtz problem has a characteristic length scale ($c_s\Delta t$, where c_s is the sound speed), and we only need to coarsen until the Courant number ($c_s\Delta t/\Delta x$) is about 1 to achieve rapid convergence (Fig 3b). This is beneficial because there is no need to redistribute data to prevent processors running out of work.

Fig 3: Convergence of FMG implemented in a shallow water code



Work is currently under-way to include a 3D version of this multi-grid solver within MPAS. The grid generating scheme has been developed to save multiple grids and MPAS has been adopted to store the additional grid information (section 4) and to read the new grid files.

Fig 2: Hexagonal grid volumes used in MPAS, the duel of the icosahedral grid; the figures show grid coarsening that will be implemented



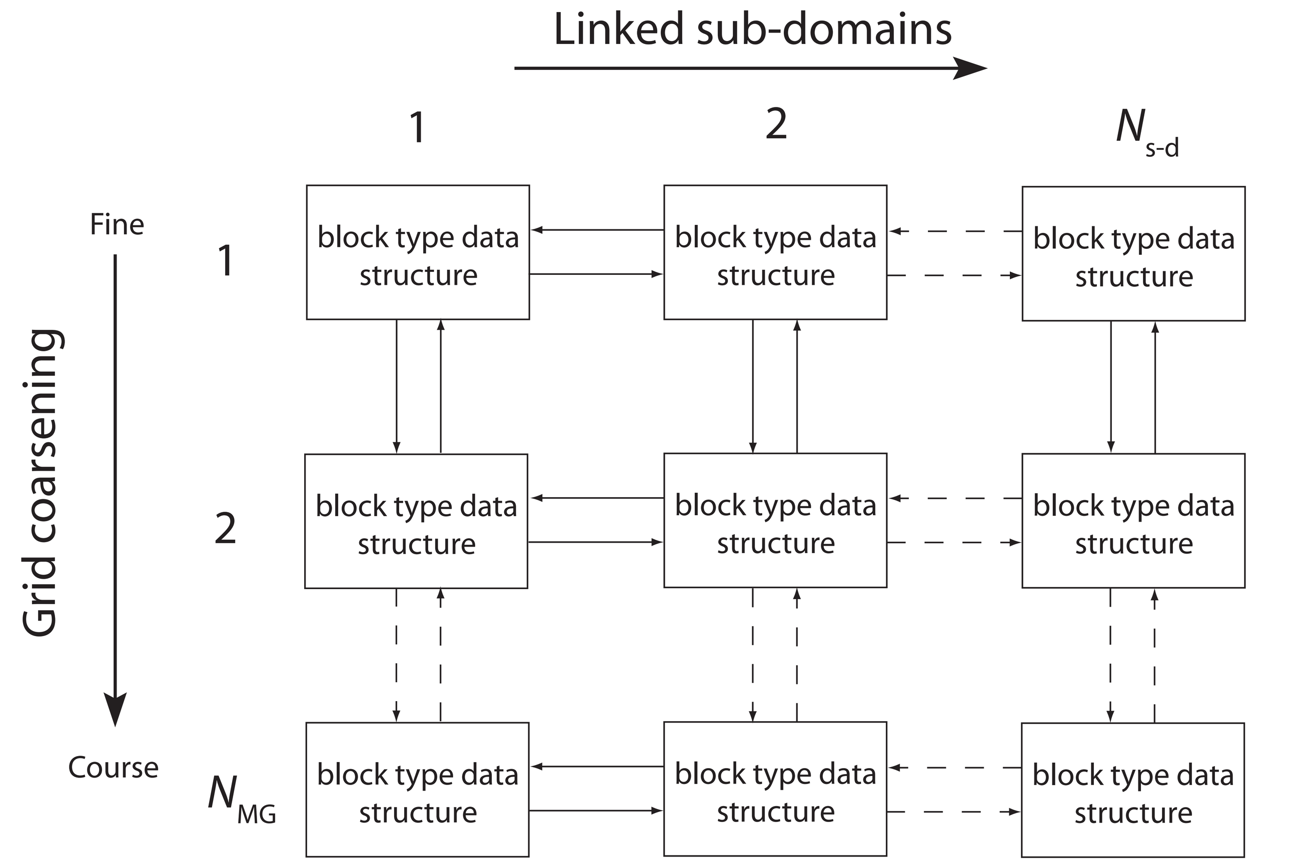
Coarse grid volume overlain on fine grid volumes

Global grid refinement

4. Data structure

MPAS has a derived data type called 'block' that provides storage for data in each sub-domain. This data type includes all the variables and parameters required for the solver on each sub-domain. Blocks assigned to each core are linked together using a pointer. For the multi-grid solver, we have extended this data type so multiple grids, variables and parameter sets can be stored in individual blocks. Additional pointers then link coarser and finer grid-blocks providing rapid and efficient storage of data (Fig 4).

Fig 4: Existing and extended linked-list derived data types for MPAS



As model resolution increases, the data IO and storage demands increase significantly. These are significant challenges in extreme-scale computing. A convenient side-effect of building multiple data structures is the ease with which data volumes can be restricted during model execution to permit reduced resolution output.

5. Future-work

- Final model coding to implement full multi-grid solver
- Testing to benchmark and evaluate solver
- Optimization
- Evaluation of performance and scalability

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