A physically based, second-order accurate, unconditionally stable, numerical scheme for diffusion

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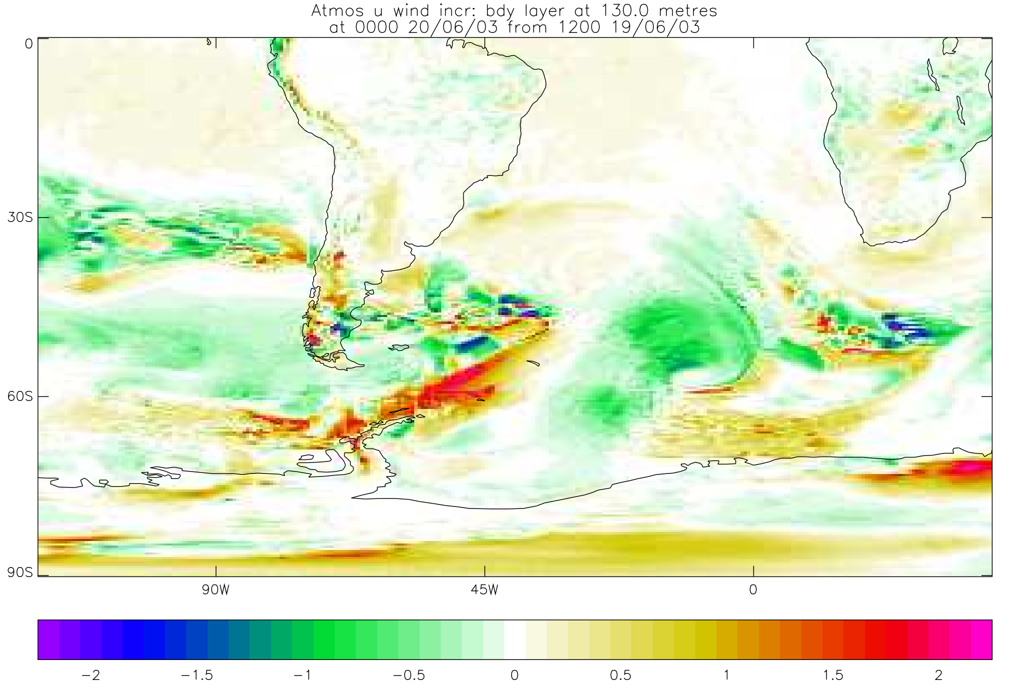
Outline

- Motivation
- Requirements of a new scheme
- Development of scheme - linear case
- Extension to the nonlinear case
- Results
- Conclusions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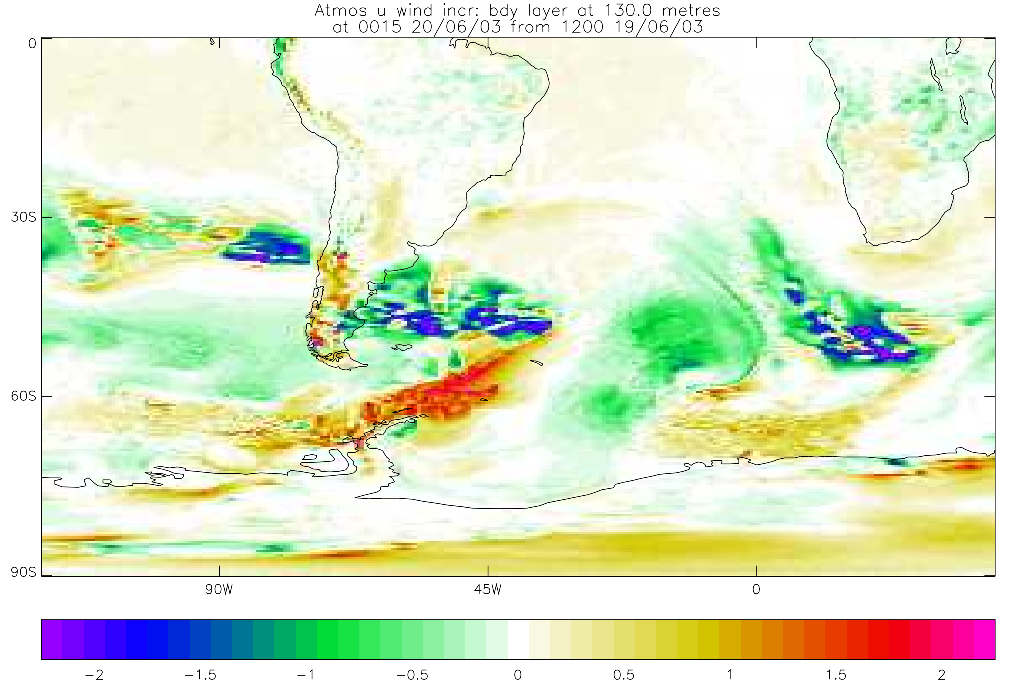
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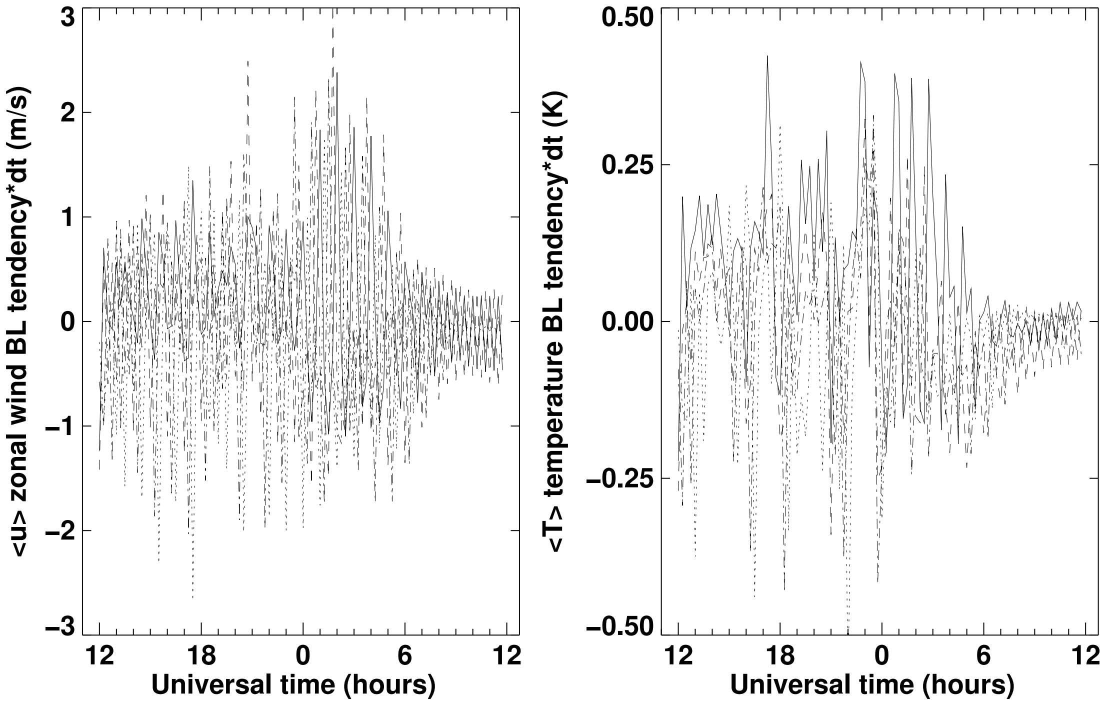

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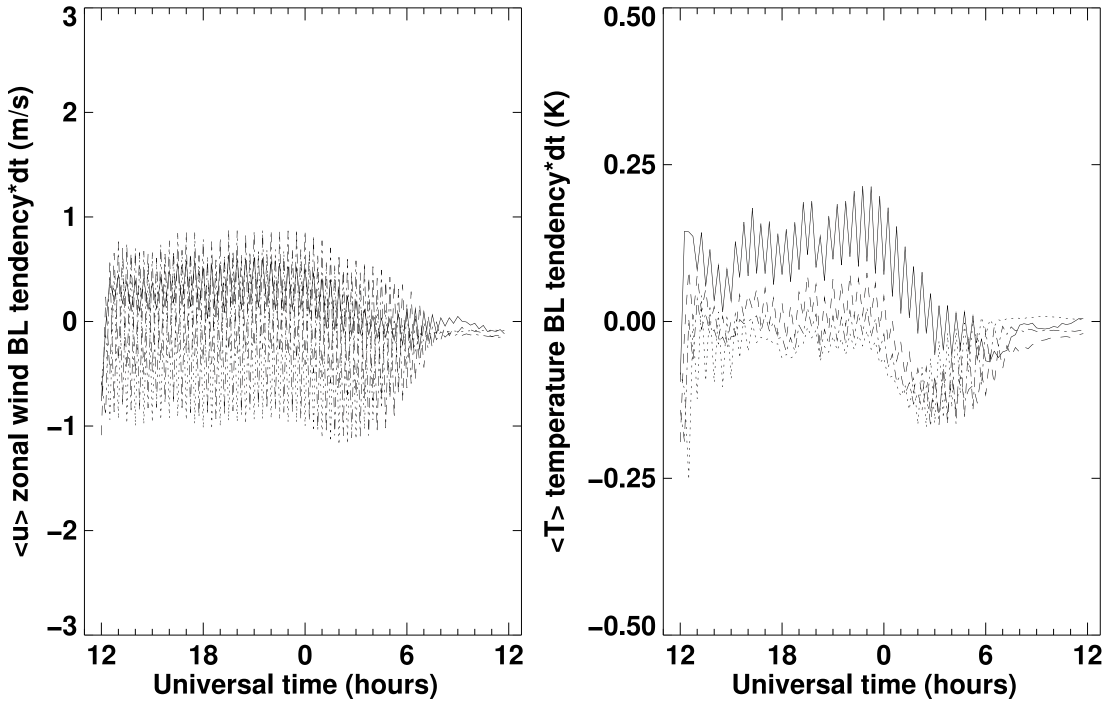


The challenge!

Requirements of a new scheme:

1. Unconditional stability

2. Second-order accuracy

3. Monotonic damping (damping rate increases as diffusion coefficient increases)

4. Maintenance of any steady state

Consider the general diffusion equation:

$$\frac{\partial F}{\partial t} = \frac{\partial}{\partial x}\left(K\frac{\partial F}{\partial x}\right)$$

Assume K constant (linear case) and make a Fourier decomposition.

Gives first-order damping equation:

$$\frac{dF}{dt} = -\beta F$$

Damping coefficient is $\beta \equiv k^2 K$.

Preliminaries 2

Consider two-time-level discrete schemes of the form:

$$\frac{F^{t+\Delta t} - F^{t}}{\Delta t} = -\frac{\beta}{2}\left[(1+\epsilon)\,F^{t+\Delta t} + (1-\epsilon)\,F^{t}\right]$$

Response function is

$$E \equiv \frac{F^{t+\Delta t}}{F^{t}} = \frac{1-(1-\epsilon)\,\beta\Delta t/2}{1+(1+\epsilon)\,\beta\Delta t/2}$$

$\epsilon = -1 \Rightarrow$ **explicit scheme;**
$\epsilon = 0 \Rightarrow$ **Crank-Nicolson scheme;**
$\epsilon = 1 \Rightarrow$**fully implicit scheme.**

Here though retain ϵ as arbitrary function (independent of time).

1. Unconditional stability

Requires $|E| \leq 1$ for all Δt.

Holds provided that both:

- $\beta \Delta t \geq 0$
  (i.e. physical system is stable)

  and

- $\epsilon \geq 0$
  (corresponds to requirement of off-centring weights $\geq 1/2$).

2. Second-order accuracy

Requires $E = E_{exact} + O\left(\Delta t^3\right)$ **where** $E_{exact} = e^{-\beta \Delta t}$**.**

Expanding E_{exact} **and** E **for small** $\beta \Delta t$ **and** $\epsilon \beta \Delta t$**, this requires**

$$1 - \beta \Delta t + (1 + \epsilon) \frac{(\beta \Delta t)^2}{2} + O\left(\Delta t^3\right) = 1 - \beta \Delta t + \frac{(\beta \Delta t)^2}{2} + O\left(\Delta t^3\right)$$

Satisfied if $\epsilon = O\left(\beta \Delta t\right)$**.**

[Trivially satisfied by $\epsilon = 0$**, consistent with the Crank-Nicolson scheme being second-order accurate.]**

3. Monotonic damping

Requires

$$\frac{\partial \left| E \right|^2}{\partial \beta} < 0$$

ie:

$$\left[1 - \frac{(\beta \Delta t)}{2} (1 - \epsilon)\right] \left[1 - \frac{(\beta \Delta t)^2}{2} \frac{\partial \epsilon}{\partial \left(\beta \Delta t\right)}\right] > 0$$

Development of the new scheme 1

Choosing

$$\epsilon = \frac{n\beta\Delta t}{1+n\beta\Delta t}$$

with $n > 1/2$ satisfies all three constraints. This gives

$$\frac{F^{t+\Delta t} - F^t}{\Delta t} = -\frac{\beta}{2}\left[\left(1+\frac{n\beta\Delta t}{1+n\beta\Delta t}\right)F^{t+\Delta t} + \left(1-\frac{n\beta\Delta t}{1+n\beta\Delta t}\right)F^t\right]$$

Works because:

- It dynamically keeps the off-centring parameter close to zero for small damping coefficients
- But, as the damping increases, it asymptotes to fully implicit off-centring.

But...

...in general β is an operator!

Can the scheme be written as a multi-step scheme?

Development of the new scheme 2

Response function is

$$E = \frac{1 + \left(n - \frac{1}{2}\right)\beta\Delta t}{1 + \left(n + \frac{1}{2}\right)\beta\Delta t + n\,(\beta\Delta t)^2}$$

Choosing $n \geq \sqrt{2} + 3/2$ guarantees that $n > 1/2$ and the denominator can be factorised in real space, and rewritten as

$$E = \frac{1 - (1 - a - b)\,\beta\Delta t}{(1 + a\beta\Delta t)\,(1 + b\beta\Delta t)}$$

where a and b are the two roots of

$$y^2 - \left(n + \frac{1}{2}\right) y + n = 0.$$

Proposed scheme

Original scheme can then be written as

$$\frac{F^* - F^t}{\Delta t} = -a\beta F^*$$

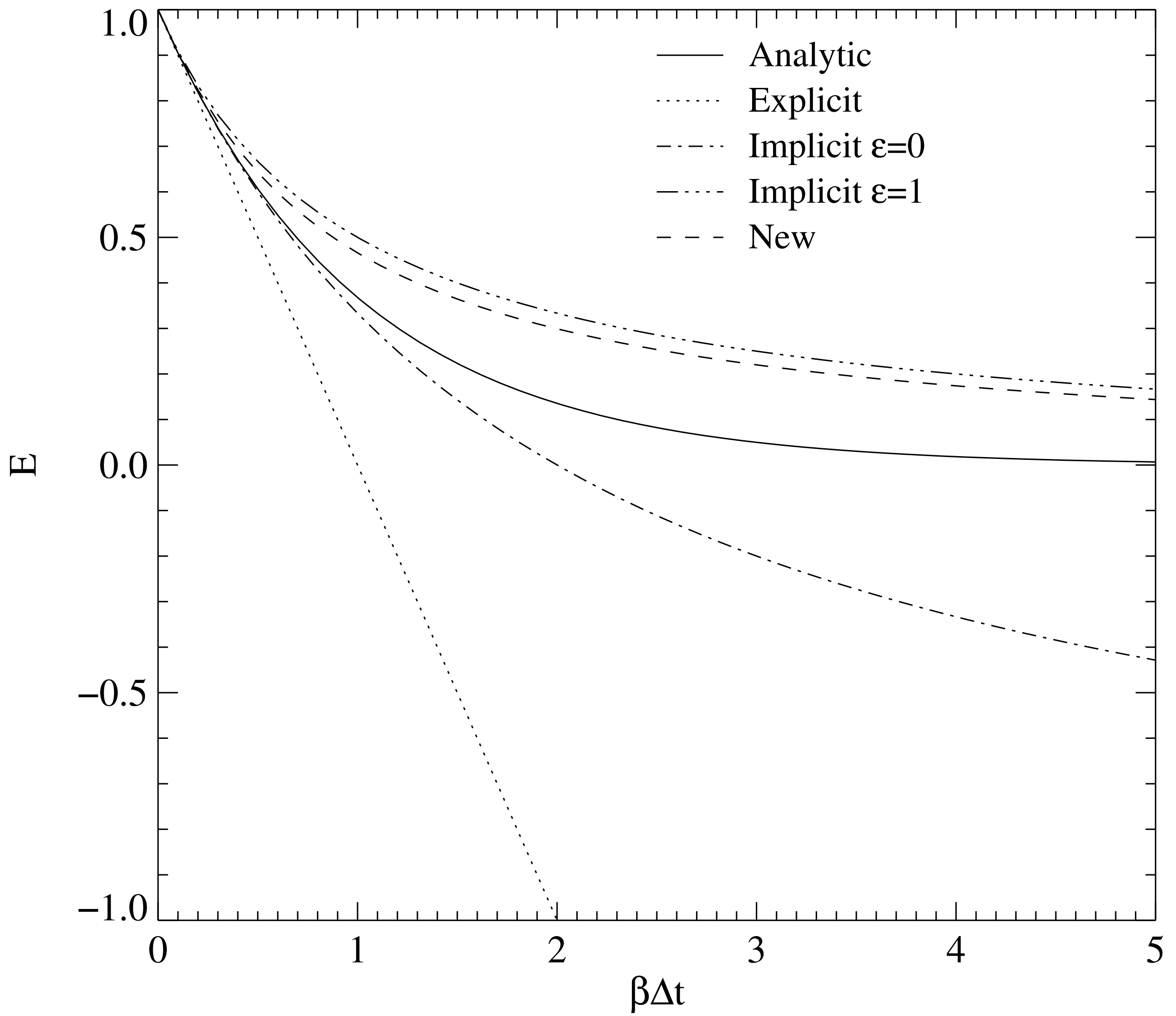
$$\frac{F^{**} - F^*}{\Delta t} = -\left(1 - a - b\right)\beta F^*$$

$$\frac{F^{t+\Delta t} - F^{**}}{\Delta t} = -b\beta F^{t+\Delta t}$$

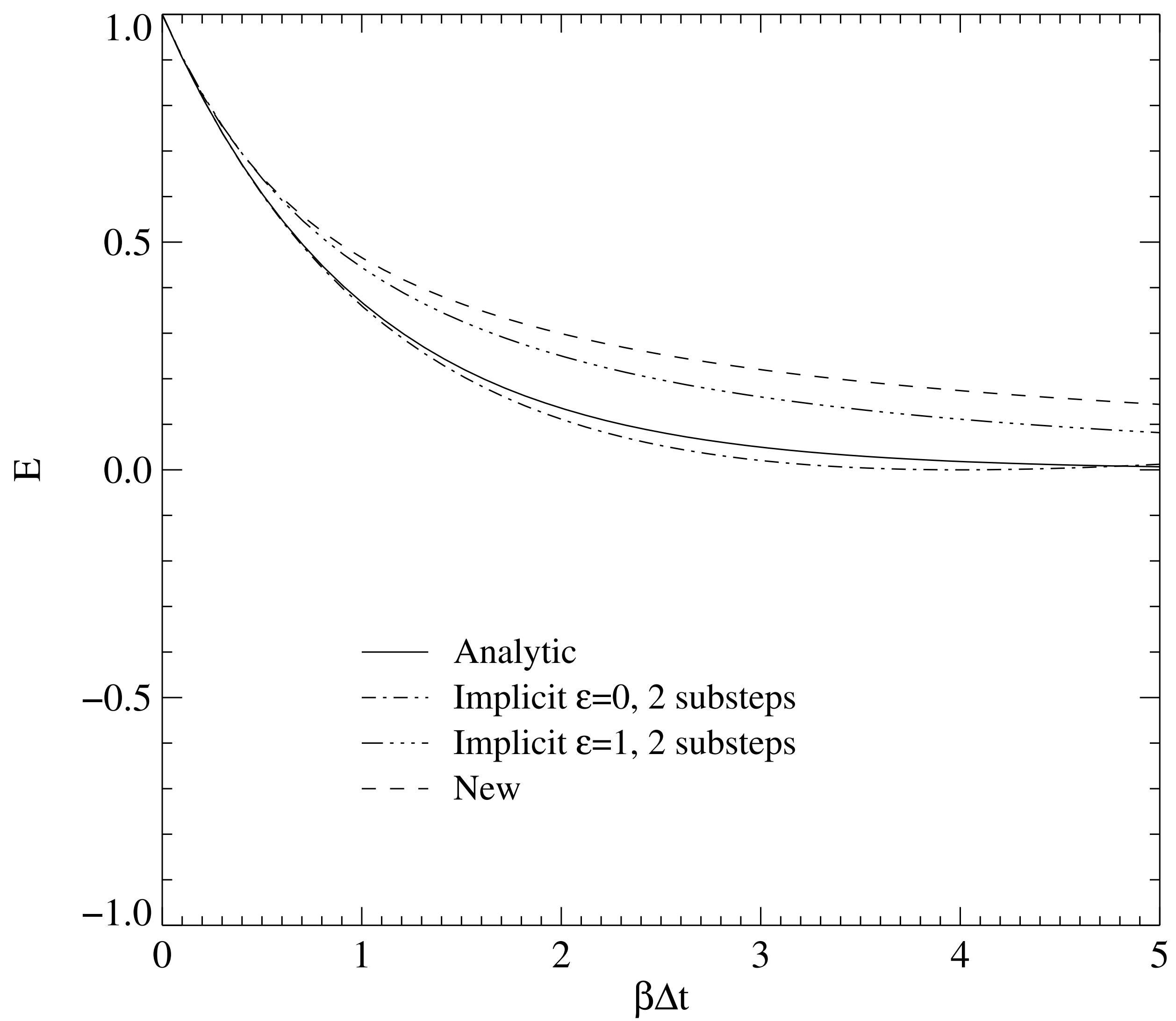
i.e. as an implicit-explicit-implicit multi-step scheme.

As n increases for fixed $\beta\Delta t$, off-centring increases. Therefore choose n as small as permitted, i.e. $n = \sqrt{2} + 3/2$.

$\Rightarrow a = b = 1 + 1/\sqrt{2}$ **therefore optimising the symmetry.**



Analytic
Explicit
Implicit ε=0
Implicit ε=1
New
1.0
0.5
0.0
−0.5
−1.0
E
0
1
2
3
4
5
βΔt



1.0
0.5
0.0
−0.5
−1.0
E
0
1
2
3
4
5
βΔt
Analytic
Implicit ε=0, 2 substeps
Implicit ε=1, 2 substeps
New

Extension to the nonlinear case

Kalnay & Kanamitsu (1988) generalised damping equation:

$$\frac{dF}{dt} = -\left(KF^P\right)F + S$$

Steady state is

$$F_0 = \left(\frac{S}{K}\right)^{1/(P+1)}$$

Linearise about F_0:

$$\frac{dF'}{dt} = -\left(KF_0^P\right)\left(F' + PF'\right)$$

with solution

$$F' \propto e^{-\beta(1+P)t}$$

where $\beta \equiv KF_0^P$.

Nonlinear aspects

Consider schemes with diffusion coefficient, KF^P, evaluated explicitly.

Discrete generalised equation is

$$\frac{F^{t+\Delta t} - F^t}{\Delta t} = -\frac{\beta}{2}\left[(1+\epsilon)\, F^{t+\Delta t} + (1-\epsilon)\, F^t + 2PF^t\right]$$

with response function

$$E = \frac{1 - \frac{\beta \Delta t}{2}\,(1 - \epsilon + 2P)}{1 + \frac{\beta \Delta t}{2}\,(1+\epsilon)}$$

Satisfying the requirements

1. **Unconditional stability: requires** $\epsilon \geq P$

2. **Second-order accuracy: requires** $\epsilon = P + O\left(\beta\Delta t\right)$

3. **Monotonic damping: requires**

$$\left[1 - \frac{\beta\Delta t}{2}\left(1 - \epsilon + 2P\right)\right] \times \left[1 + P + \beta\Delta t P\left(1 + \epsilon\right) - \frac{\left(\beta\Delta t\right)^2}{2}\left(1 + P\right)\frac{\partial\epsilon}{\partial\beta\Delta t}\right] > 0$$

Choosing

$$\epsilon = P + (1+P)\left(\frac{n\beta\Delta t}{1+n\beta\Delta t}\right)$$

with $n > (1+P)/2$ **satisfies all three constraints.**

This gives the scheme as

$$\frac{F^{t+\Delta t} - F^{t}}{\Delta t} = -\frac{\beta}{2}(1+P)\left[\left(1+\frac{n\beta\Delta t}{1+n\beta\Delta t}\right)F^{t+\Delta t} + \left(1-\frac{n\beta\Delta t}{1+n\beta\Delta t}\right)F^{t}\right]$$

Note: for $P = 0$ **(linear case) this reduces to previous scheme.**

Development of the nonlinear scheme 2

No longer want to factorise E.

Operating on F by β has the discrete response

$$\beta F \to \beta \left(F^* + P F^t \right)$$

Therefore need to factorise

$$E^* \equiv \frac{F^{t+\Delta t} + P F^t}{F^t + P F^t} = \frac{E + P}{1 + P}$$

ie

$$E^* = \frac{1 + \left(n + \frac{P-1}{2} \right) \beta \Delta t + n P \left(\beta \Delta t \right)^2}{1 + \left(n + \frac{P+1}{2} \right) \beta \Delta t + n \left(P + 1 \right) \left(\beta \Delta t \right)^2}$$

Development of the nonlinear scheme 3

Viable scheme requires that E^* can be written as

$$E^* = \frac{(1 + \mathcal{E}_1 \beta \Delta t)(1 + \mathcal{E}_2 \beta \Delta t)}{(1 + \mathcal{I}_1 \beta \Delta t)(1 + \mathcal{I}_2 \beta \Delta t)}$$

with $\mathcal{E}_1$, $\mathcal{E}_2$, $\mathcal{I}_1$ and $\mathcal{I}_2$ real.

This can be achieved by requiring that

$$n \geq \left(\sqrt{2} + \frac{3}{2}\right)(P+1) > \frac{P+1}{2}$$

Development of the nonlinear scheme 3

Again choose the smallest viable value for n, i.e.

$$n = \left(\sqrt{2} + 3/2\right)(P+1)$$

to give

$$\mathcal{E}_1 = \left(1 + \frac{1}{\sqrt{2}}\right)\left[P + \frac{1}{\sqrt{2}} \pm \sqrt{P\left(\sqrt{2}-1\right) + \frac{1}{2}}\right]$$

$$\mathcal{E}_2 = \left(1 + \frac{1}{\sqrt{2}}\right)\left[P + \frac{1}{\sqrt{2}} \mp \sqrt{P\left(\sqrt{2}-1\right) + \frac{1}{2}}\right]$$

$$\mathcal{I}_1 = \mathcal{I}_2 = \left(1 + \frac{1}{\sqrt{2}}\right)(1+P)$$

Proposed nonlinear scheme

The proposed, full non-linear scheme is therefore

$$\frac{F^{*}-F^{t}}{\Delta t}=-\mathcal{I}_1\left\{\left[K\left(F^{t}\right)^{P}\right]F^{*}-S\right\}$$

$$\frac{F^{**}-F^{*}}{\Delta t}=\mathcal{E}_1\left\{\left[K\left(F^{t}\right)^{P}\right]F^{*}-S\right\}$$

$$\frac{F^{***}-F^{**}}{\Delta t}=\mathcal{E}_2\left\{\left[K\left(F^{t}\right)^{P}\right]F^{**}-S\right\}$$

$$\frac{F^{t+\Delta t}-F^{***}}{\Delta t}=-\mathcal{I}_2\left\{\left[K\left(F^{t}\right)^{P}\right]F^{t+\Delta t}-S\right\}$$

Including the source term S this way ensures the scheme retains exact steady state and satisfies fourth requirement.

An alternative form

...and finally...

Reduce scheme to two semi-implicit steps by combining each explicit step with an implicit step:

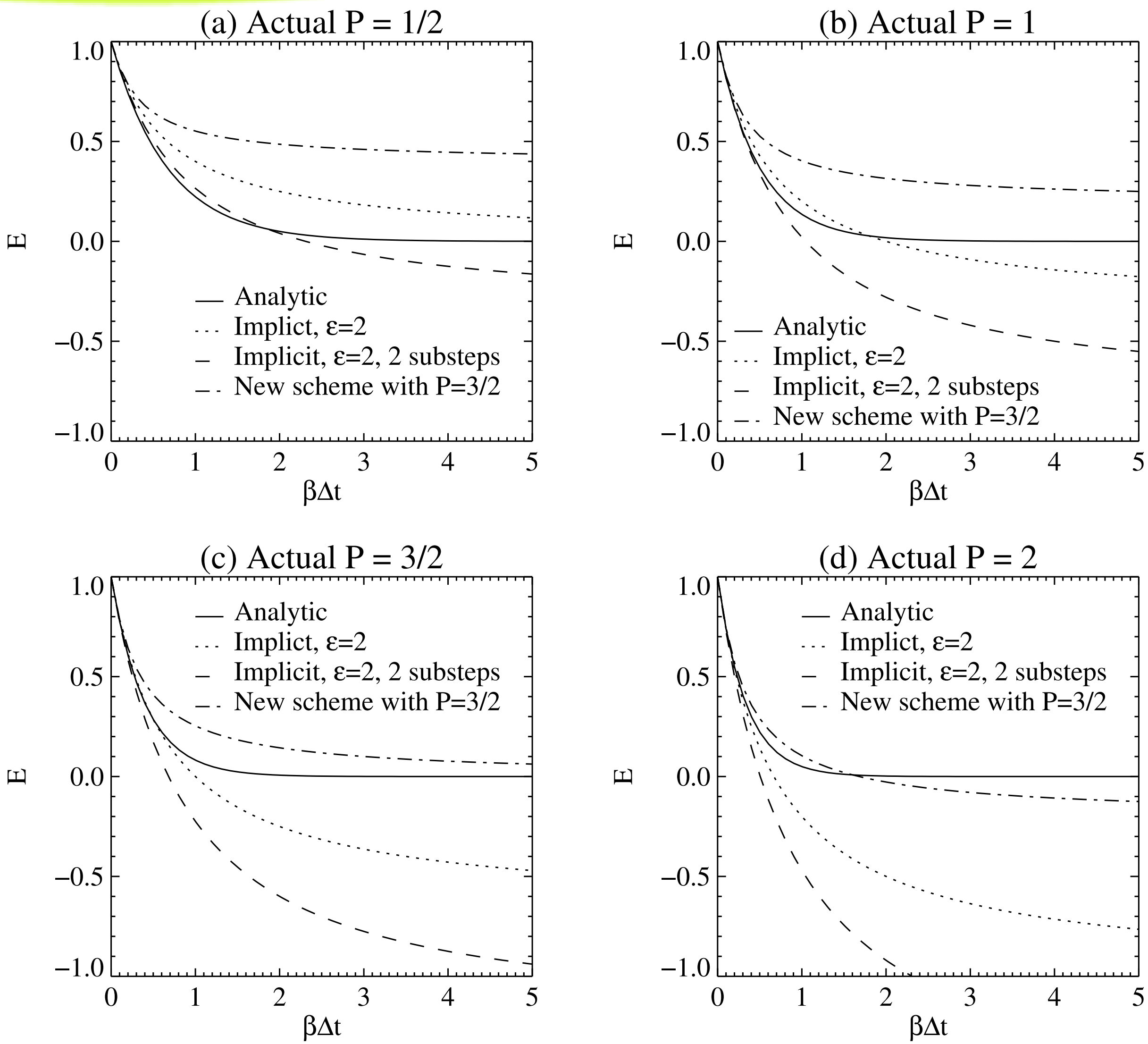
$$\frac{F^* - F^t}{\Delta t} = -\mathcal{I}_1 \left[K \left(F^t \right)^P \right] F^* + \mathcal{E}_1 \left[K \left(F^t \right)^P \right] F^t + \left(\mathcal{I}_1 - \mathcal{E}_1 \right) S$$

$$\frac{F^{t+\Delta t} - F^*}{\Delta t} = -\mathcal{I}_2 \left[K \left(F^t \right)^P \right] F^{t+\Delta t} + \mathcal{E}_2 \left[K \left(F^t \right)^P \right] F^* + \left(\mathcal{I}_2 - \mathcal{E}_2 \right) S$$

But! Need to estimate P to evaluate $\mathcal{I}_1$, $\mathcal{I}_2$, $\mathcal{E}_1$ and $\mathcal{E}_2$...

Actual nonlinearity seems to be in range $0 \le P \le 2$.

Choosing $P \approx 3/2$ seems to work well.

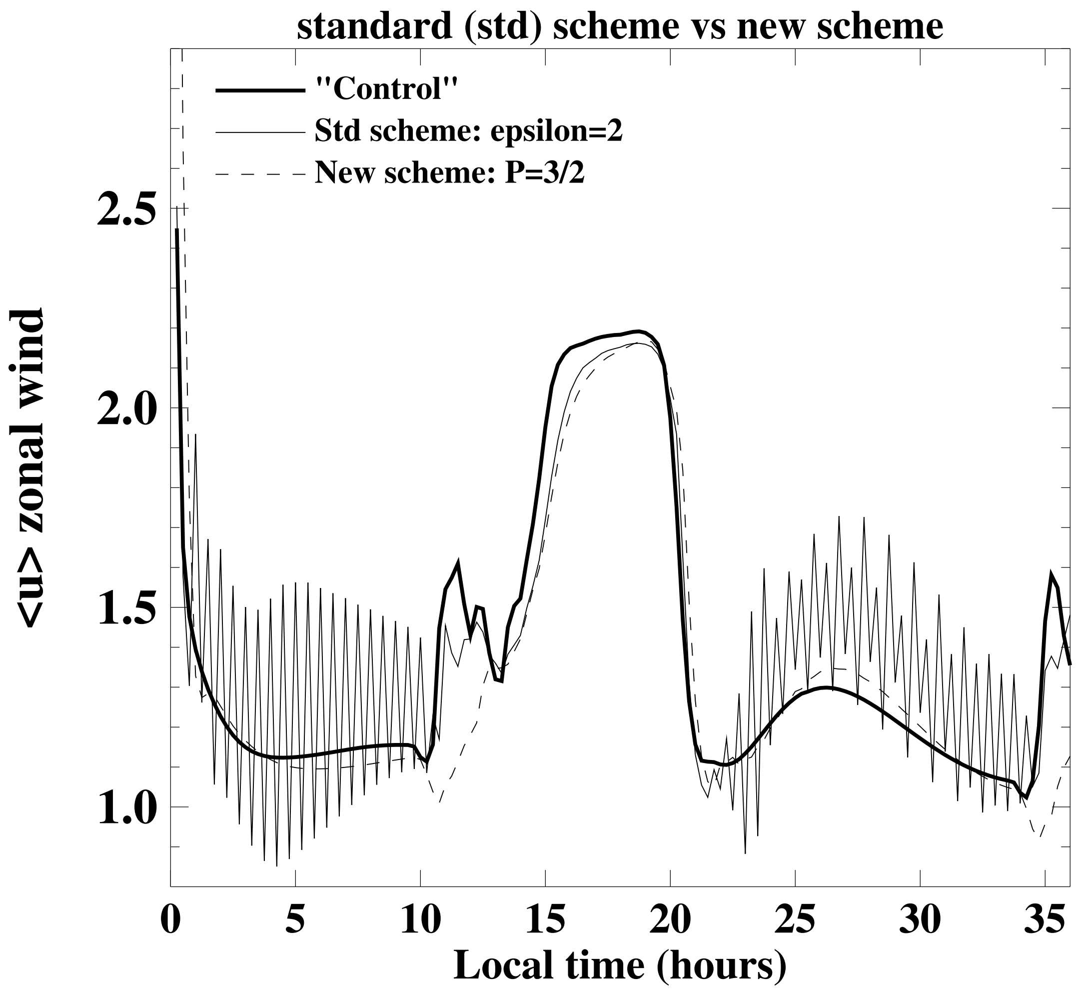


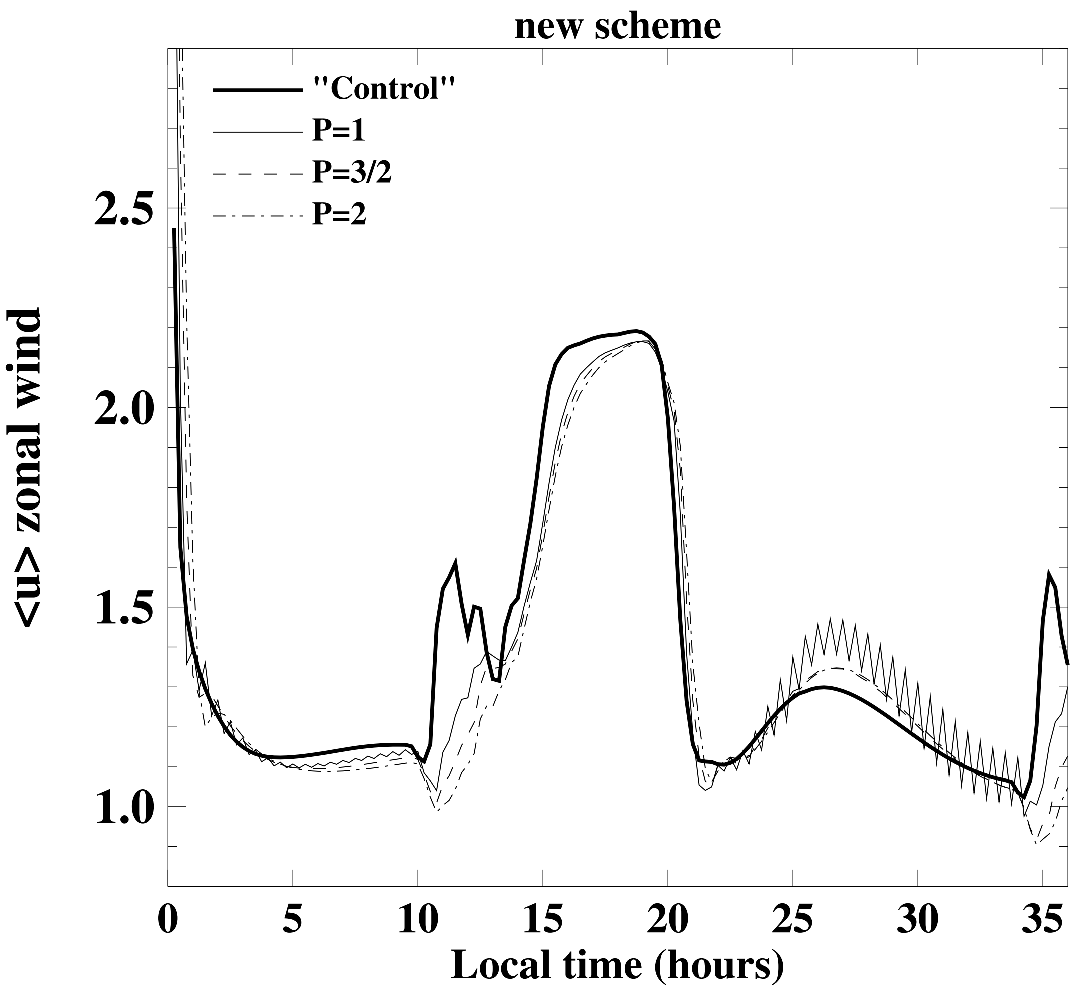
(a) Actual P = 1/2
(b) Actual P = 1
(c) Actual P = 3/2
(d) Actual P = 2
E
βΔt
1.0
0.5
0.0
−0.5
−1.0
0
1
2
3
4
5
Analytic
Implict, ε=2
Implicit, ε=2, 2 substeps
New scheme with P=3/2

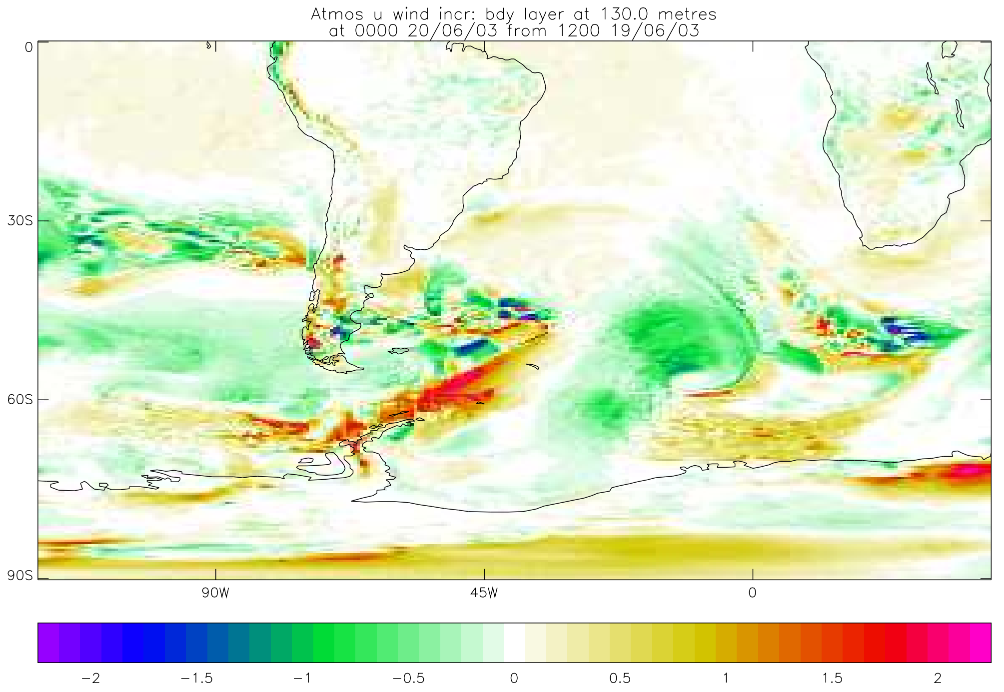
Results

1. Single Column Unified Model results:
   test with realistic diffusion scheme

2. Global Unified Model results:
   40km at midlatitudes; 70 levels; $\Delta t = 15$ mins.


standard (std) scheme vs new scheme
"Control"
Std scheme: epsilon=2
New scheme: P=3/2
<u> zonal wind
Local time (hours)


new scheme
"Control"
P=1
P=3/2
P=2
<u> zonal wind
Local time (hours)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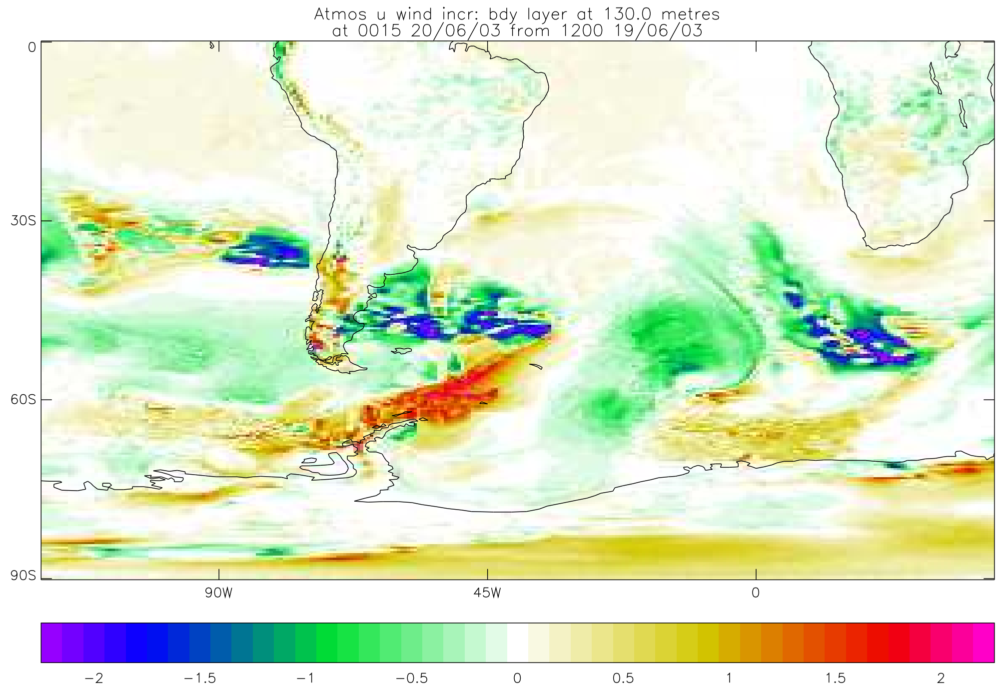
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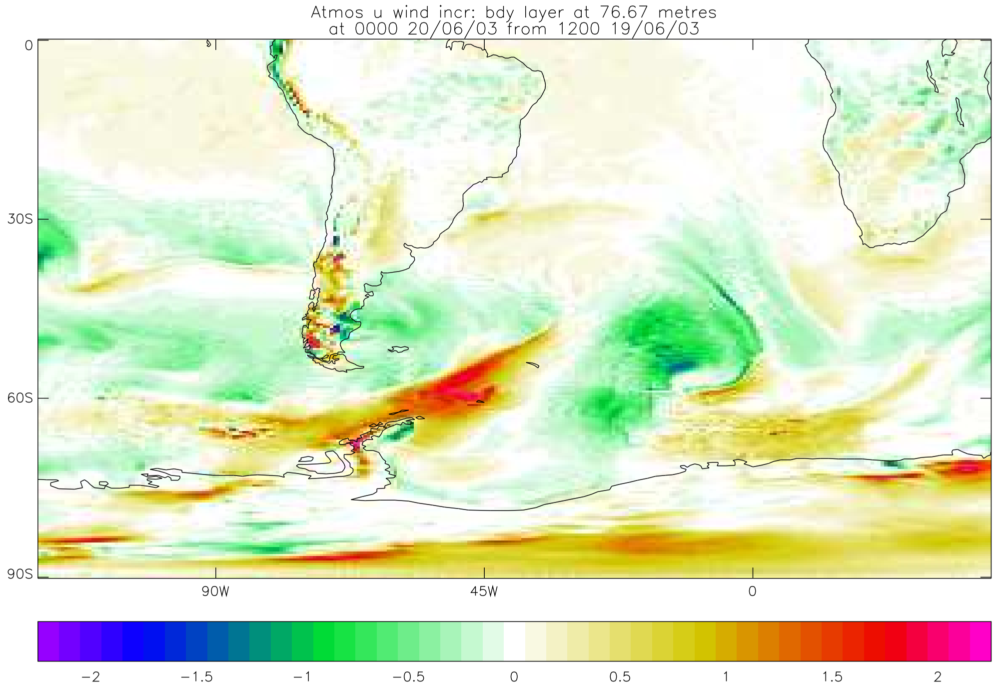

Atmos u wind incr: bdy layer at 76.67 metres
at 0000 20/06/03 from 1200 19/06/03
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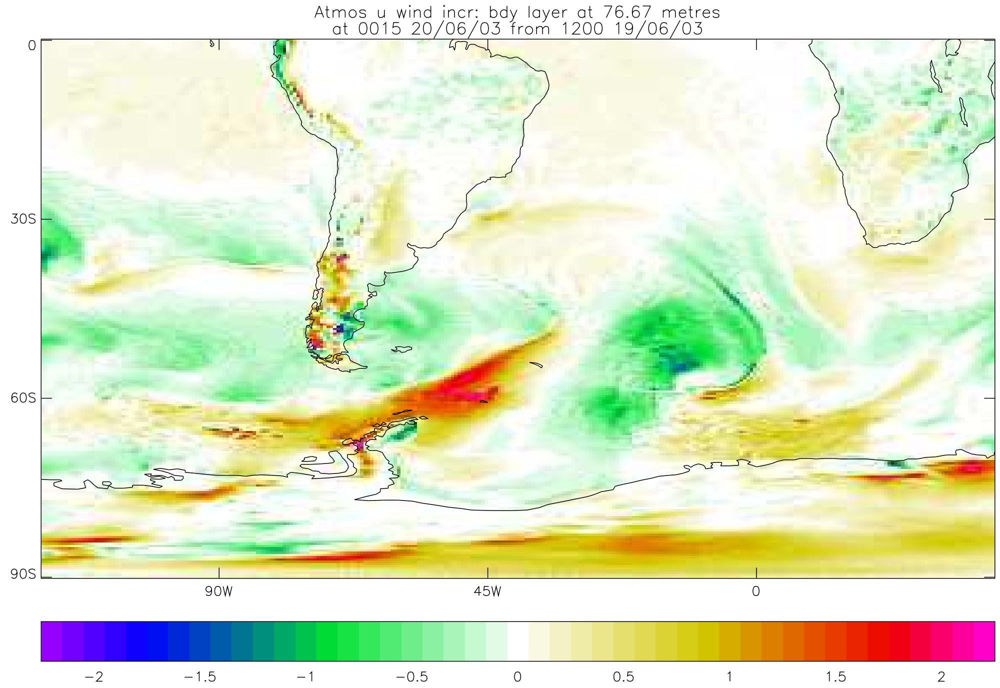

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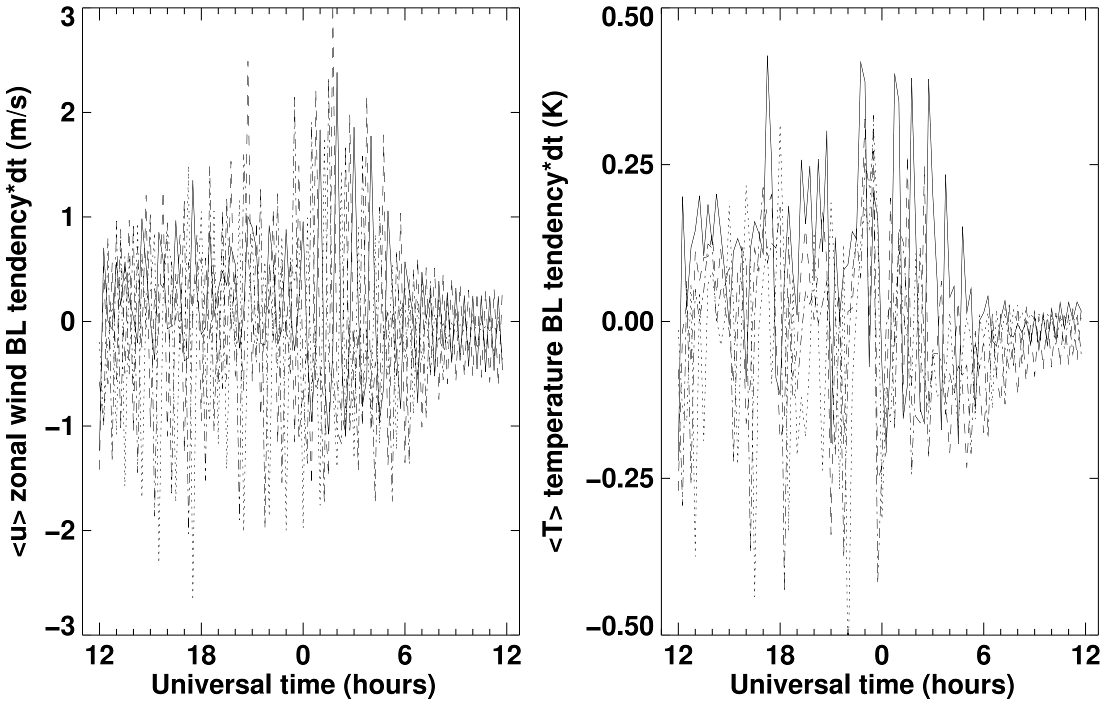
1
1.5
2

Standard scheme: physics timestep=15 min, epsilon=2



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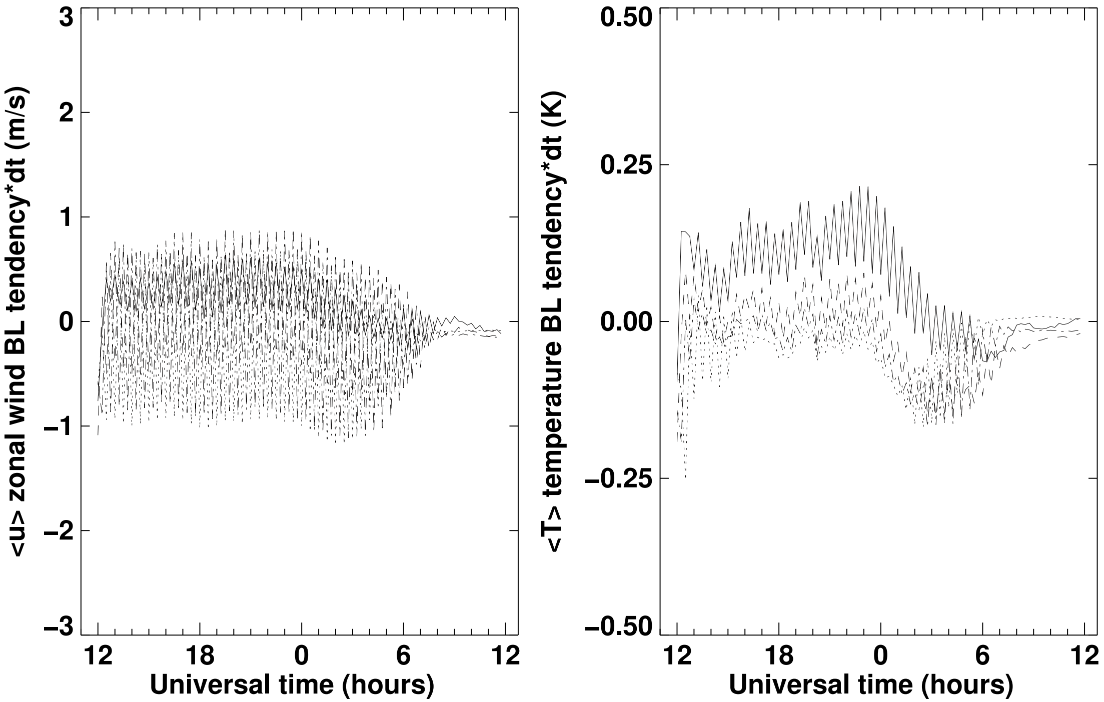
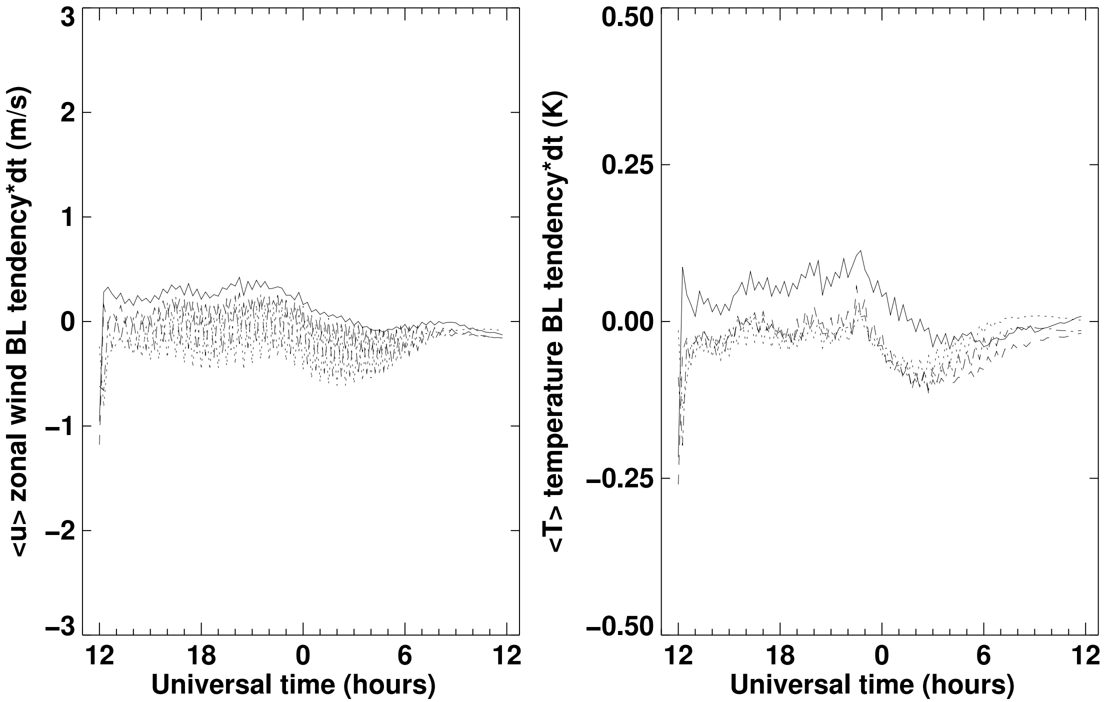
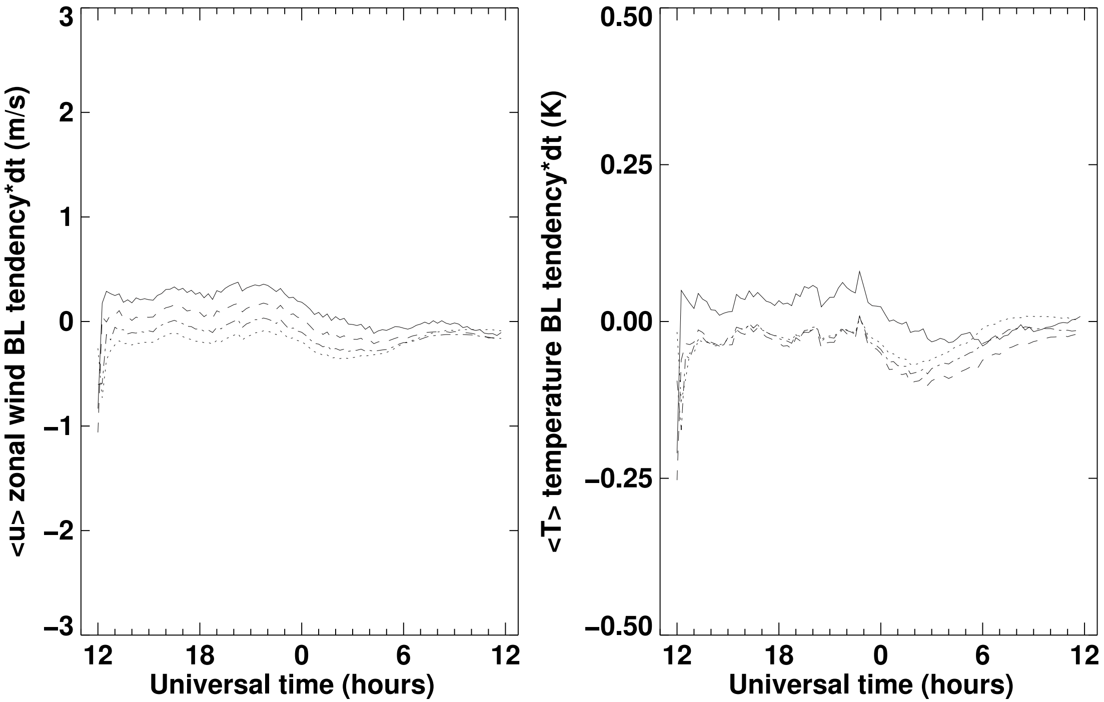


New scheme: physics timestep=15 min, P=3/2



New scheme: physics timestep=15 min, P=2



Conclusions

- New scheme developed that meets 4 identified criteria
- Extended to nonlinear case
- Diffusion coefficient frozen in time therefore cost is two 1D tri-diagonal solutions - double that of traditional schemes, but much cheaper than substepped schemes
- One free parameter - estimate of nonlinearity of diffusion coefficient
- Found that accuracy can be improved by choosing a different value depending on stability
(e.g. $P_{unstable} = 1/4$; $P_{stable} = 2$)