A monotonically damping, second-order accurate, unconditionally stable, numerical scheme for diffusion

Nigel Wood, Michail Diamantakis

&

Andrew Staniforth

Dynamics Research, Met Office, Exeter EX1 3PB

Outline

- Requirements of a new scheme
- Development of scheme - linear case
- The nonlinear case
- Results
- Conclusions

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

Preliminaries 1

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 $\beta \equiv k^2 K$.

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

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

ie:

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

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

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

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

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

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.**

Extension based on Kalnay & Kanamitsu (1988)'s generalised damping equation:

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

Result is two semi-implicit steps:

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

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

Extension to the nonlinear case 2

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

Parameter P characterises the nonlinearity of the problem

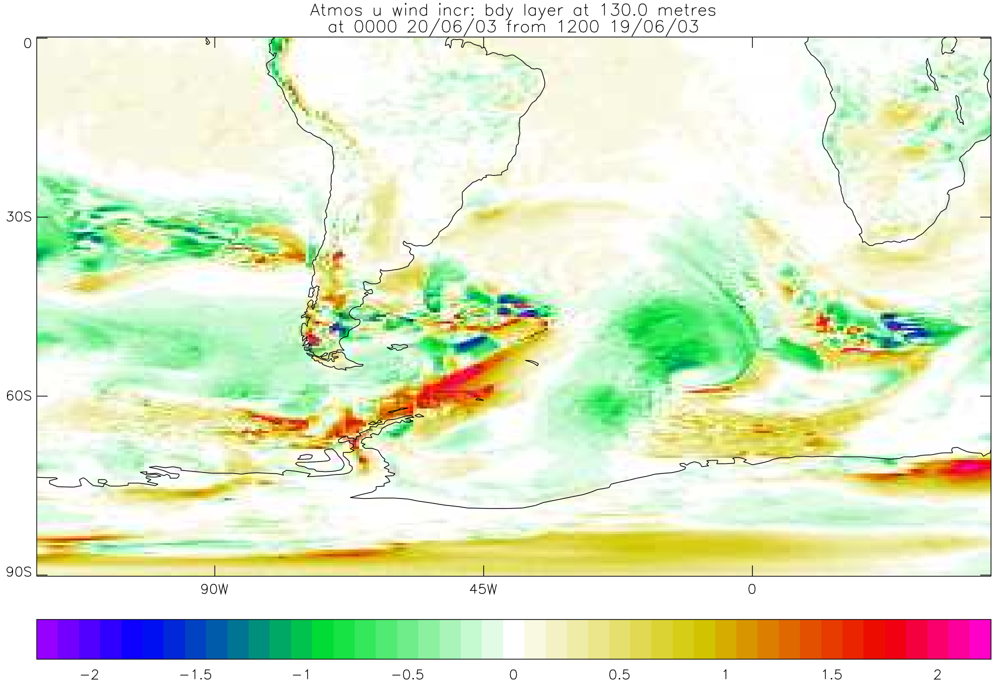
Empirically: $P \simeq 1/4$ for unstable BLs; $P \simeq 2$ for stable BLs

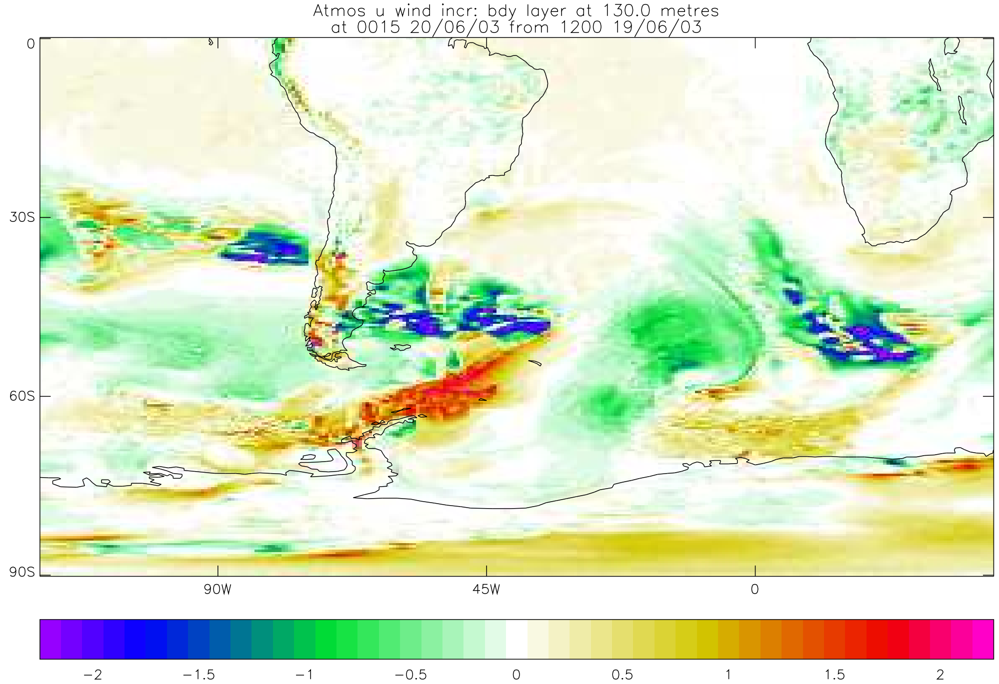
For $P = 2$: $\mathcal{I}_1 = \mathcal{I}_2 \simeq 5$; $\mathcal{E}_1 \simeq 6$; $\mathcal{E}_2 \simeq 3$

For $P = 1/4$: $\mathcal{I}_1 = \mathcal{I}_2 \simeq 2$; $\mathcal{E}_1 \simeq 3$; $\mathcal{E}_2 \simeq 0$

For details see Wood, Diamantakis & Staniforth (QJRMS 2007)

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

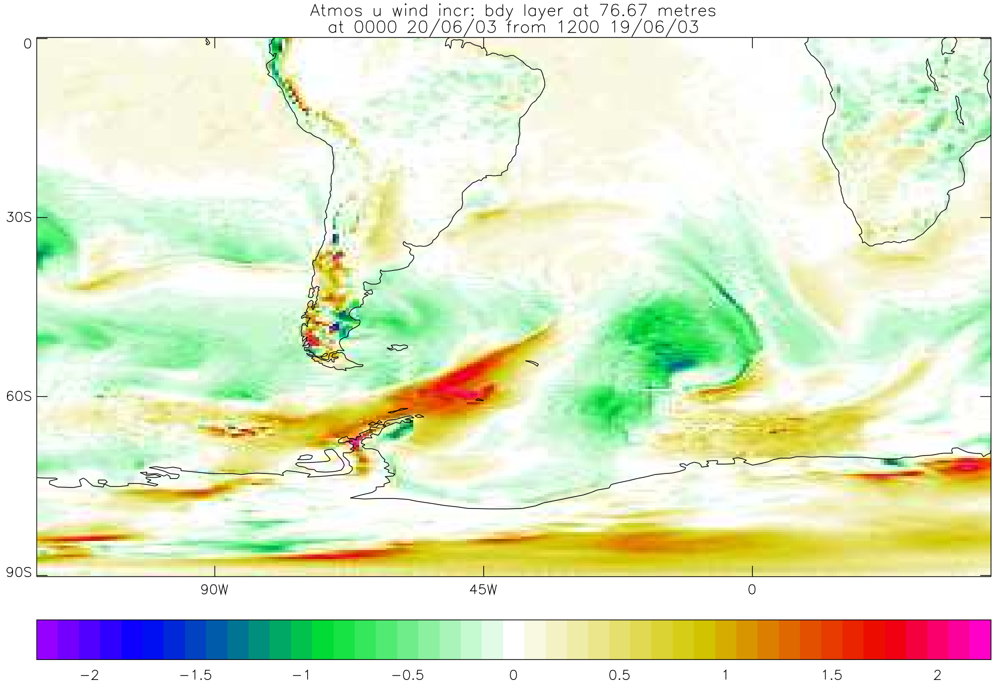


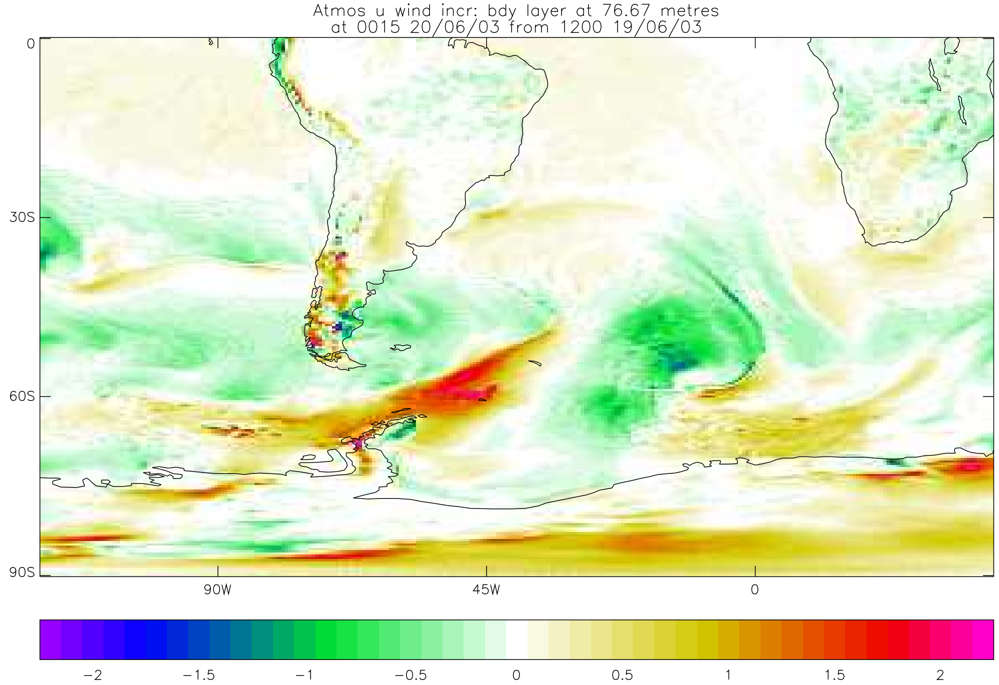


Boundary-layer zonal wind increments at two successive timesteps

Standard over-weighted scheme ($\epsilon = 2$)

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

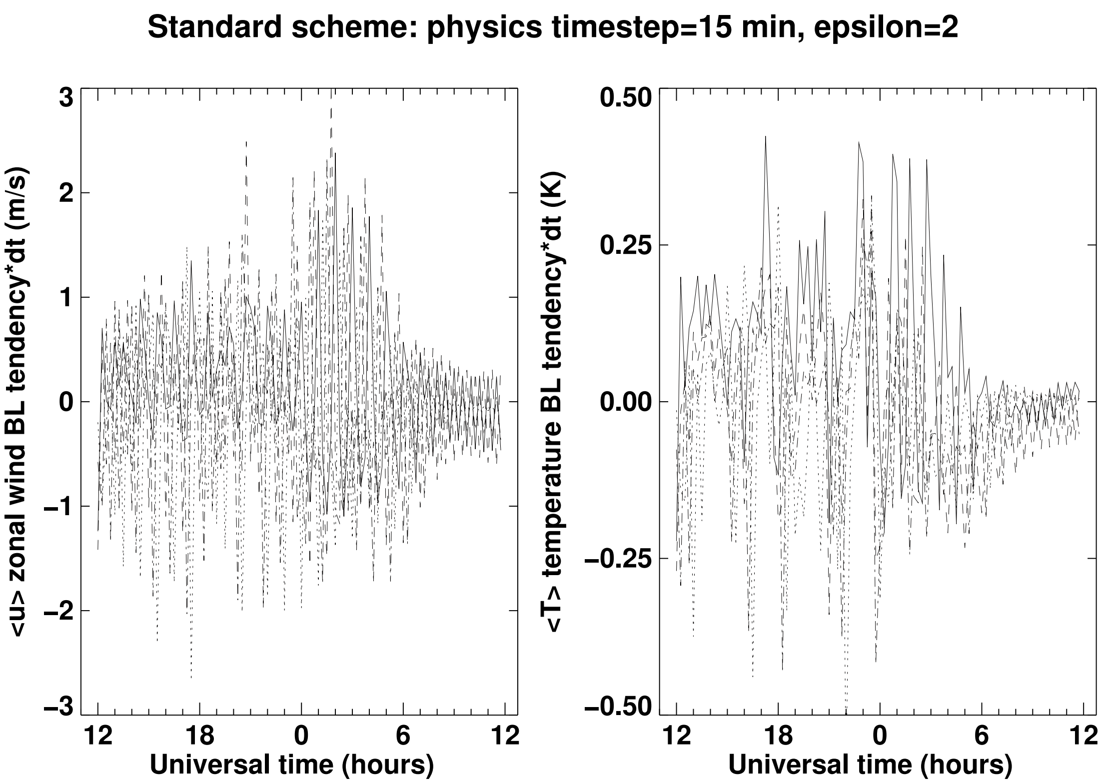




Boundary-layer zonal wind increments at two successive timesteps

New scheme ($P = 1/4$ unstable; $P = 2$ stable)

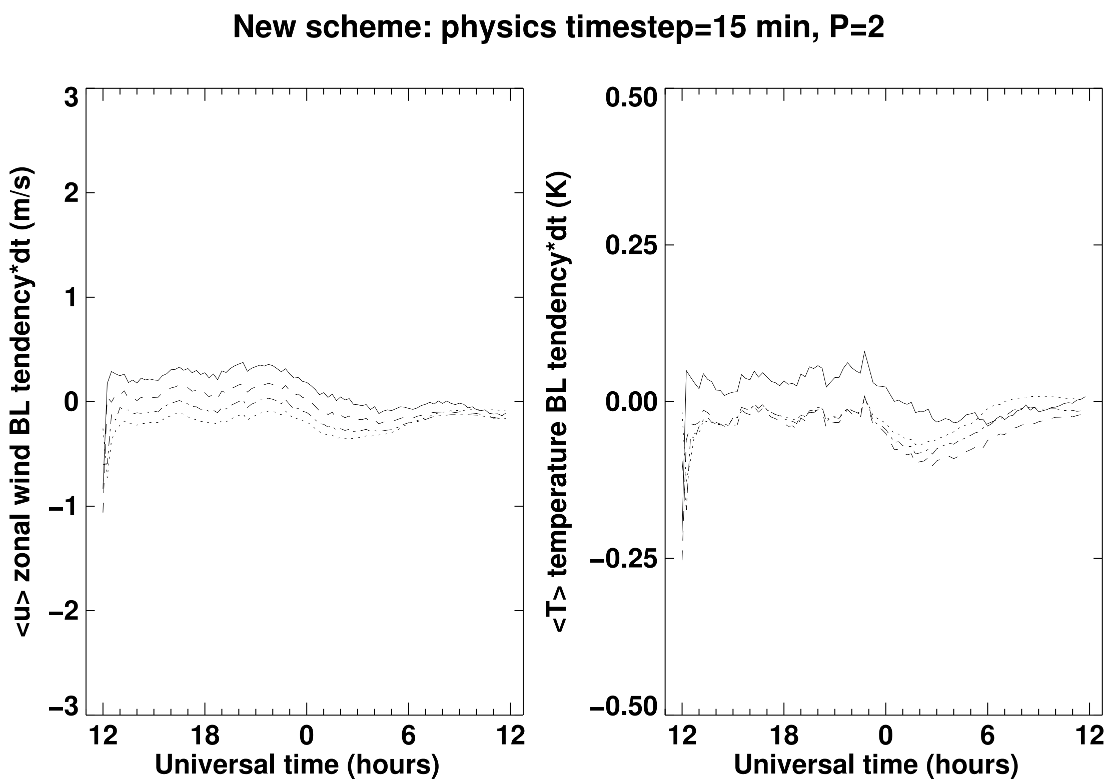
Global Unified Model: 40km at midlatitudes; 70 levels; $\Delta t = 15$ mins.



Timeseries of boundary-layer zonal wind and temperature increments

Standard over-weighted scheme ($\epsilon = 2$)

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



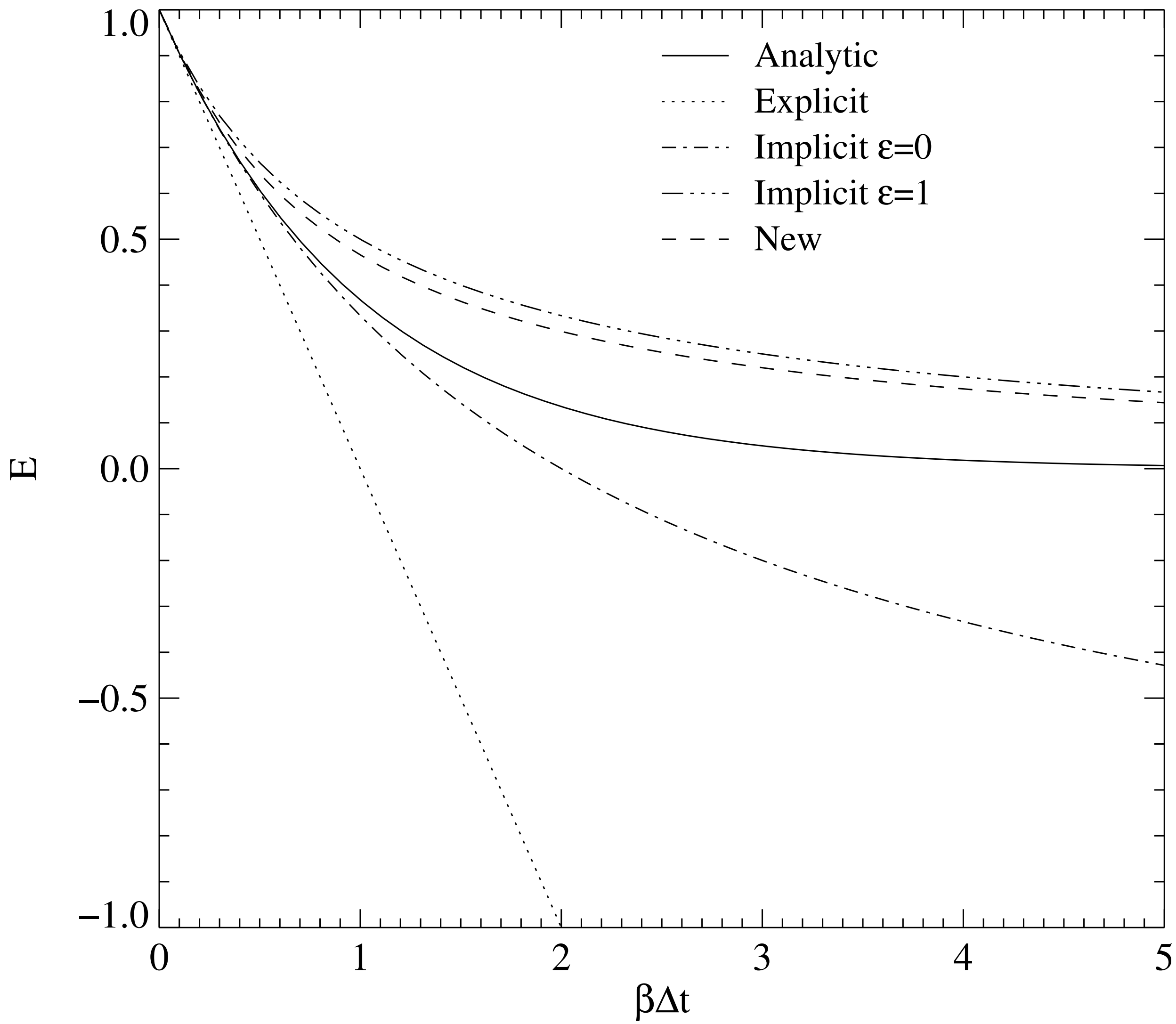
Timeseries of boundary-layer zonal wind and temperature increments

New scheme ($P = 1/4$ unstable; $P = 2$ stable)

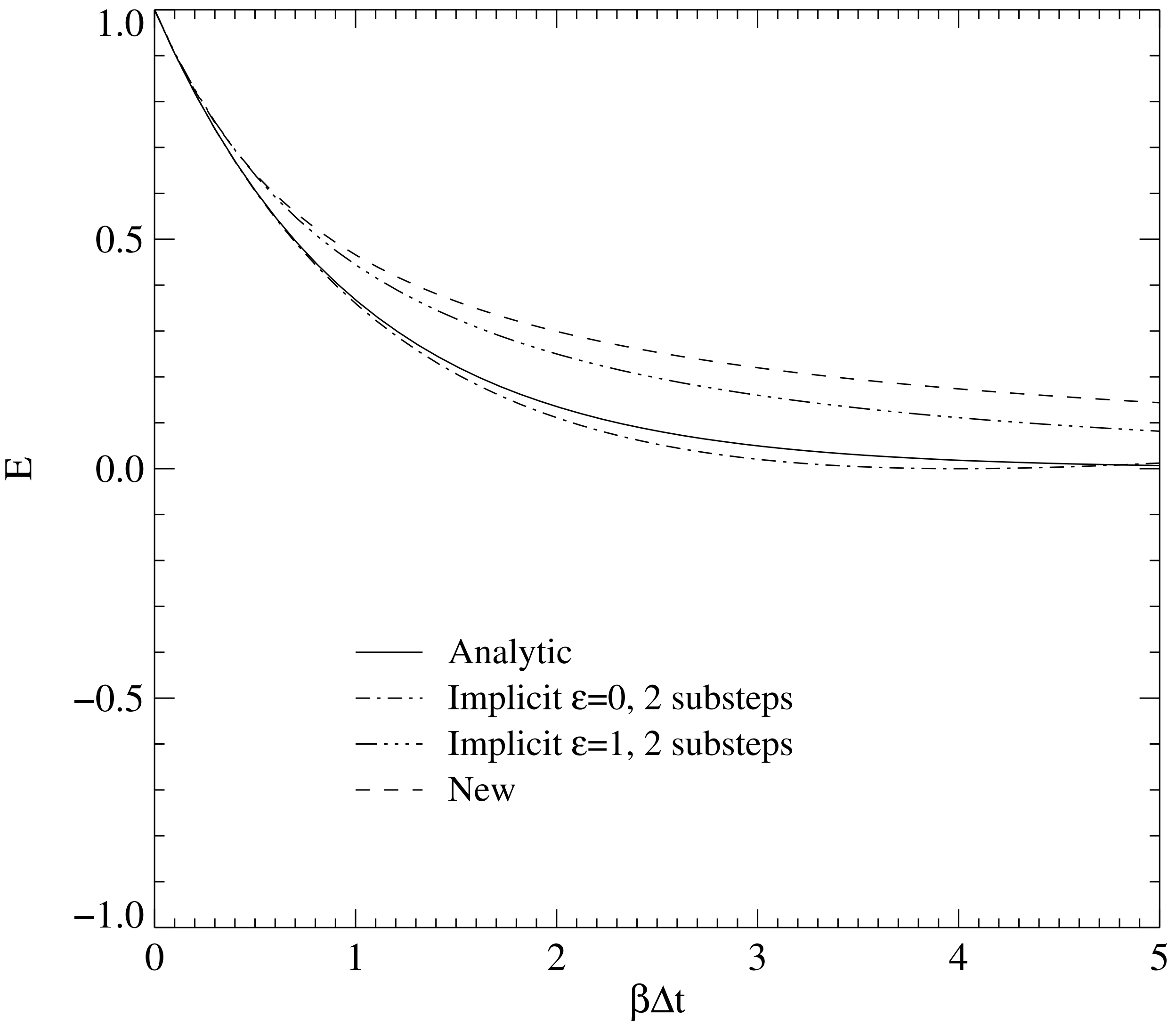
Conclusions

- 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, P = estimate of nonlinearity of diffusion coefficient, depends on stability of boundary layer
- Good accuracy achieved by choosing only one value for unstable and one value for stable boundary layers (e.g. $P_{unstable} = 1/4$; $P_{stable} = 2$)

QUESTIONS?



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

$$\beta F \rightarrow \beta \left(F^* + PF^t \right)$$

Therefore need to factorise

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

ie

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

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

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

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:

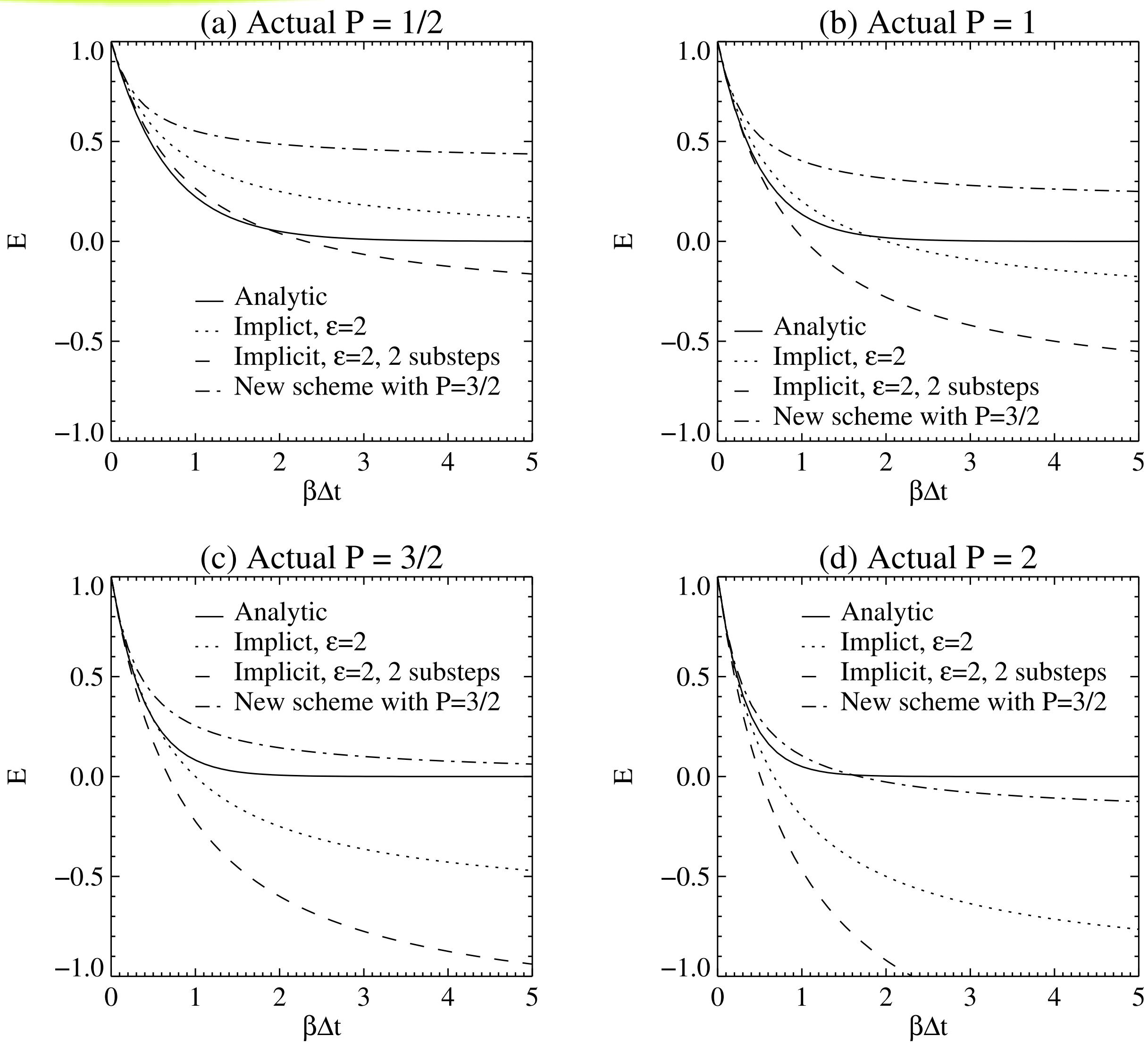
$$\frac{F^* - F^t}{\Delta t} = -\mathcal{I}_1 \left[K \left(F^t \right)^P \right] F^* + \mathcal{E}_1 \left[K \left(F^t \right)^P \right] F^t + \left(\mathcal{I}_1 - \mathcal{E}_1 \right) S$$

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

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 $0 \leq P \leq 2$.

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