ADAPTIVE MESH REFINEMENT

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PA Research Task 2
Scientific Notebook #077

Gordon Wittmeyer

PA - Research Task #2

Numerical experiments with the code ADAVAR,† a test-bed for adaptive mesh refinement strategies.

Test case used here is the COVE-2A exercise (SAND89-2558) for 1D unsaturated flow in fractured porous media similar to Yucca Mtn.

GW

Table 1: Material Properties ★

≈ van Genuchten n

	TCw	PTn	TSw1	TSw2-3	CHnv	CHnz
n_m ≈ θ_s	0.08	0.40	0.11	0.11	0.46	0.28
K_m (m/s)	9.7×10^{-12}	3.9×10^{-7}	1.9×10^{-11}	1.9×10^{-11}	2.7×10^{-7}	2.0×10^{-11}
$S_{r,m}$	0.002	0.100	0.080	0.080	0.041	0.110
α_m (1/m)	0.821×10^{-2}	1.5×10^{-2}	0.567×10^{-2}	0.567×10^{-2}	1.600×10^{-2}	0.308×10^{-2}
β_m	1.558	6.872	1.798	1.798	3.872	1.602
n_f	1.4×10^{-4}	2.7×10^{-5}	4.1×10^{-5}	1.8×10^{-4}	4.6×10^{-5}	4.6×10^{-5}
K_f (m/s)	5.3×10^{-9}	1.6×10^{-8}	0.9×10^{-9}	3.1×10^{-9}	9.2×10^{-9}	9.2×10^{-9}
$S_{r,f}$	0.0395	0.0395	0.0395	0.0395	0.0395	0.0395
α_f (1/m)	1.285	1.285	1.285	1.285	1.285	1.285
β_f	4.23	4.23	4.23	4.23	4.23	4.23
α'_{bulk} (1/m)	6.2×10^{-7}	8.2×10^{-6}	1.2×10^{-6}	5.8×10^{-7}	3.9×10^{-6}	2.6×10^{-6}
$\frac{\partial n_f}{\partial \sigma'}$ (1/m)	1.32×10^{-6}	1.9×10^{-7}	5.6×10^{-8}	1.2×10^{-7}	2.8×10^{-8}	2.8×10^{-8}

★ from (SAND88-0942), † Not controlled, this is a development platform

The test case used here considers flow in matrix only.

Input data file for ADAVAR:

```
  2    0    0    2    1    1    1
1.000d+00 1.000d+00 1.440d-02 1.100d+00 1.001d+13
5.000d-06   20   40    1    1 1.000d+12    0    1
1.001d+13
0.000d+00 1.000d+13
1.001d+13
 530.4d+0    5    1.5d+1
    α        θs       θr        n         Ss        Ks
8.210d-03 8.000d-02 1.600d-04 1.558d+00 1.000d-07 9.700d-12
1.500d-02 4.000d-01 4.000d-02 6.872d+00 1.000d-07 3.900d-07
5.670d-03 1.100d-01 8.800d-03 1.798d+00 1.000d-07 1.900d-11
5.670d-03 1.100d-01 8.800d-03 1.798d+00 1.000d-07 1.900d-11
1.600d-02 4.600d-01 1.886d-02 3.872d+00 1.000d-07 2.700d-07
     zt        zb
 530.4d+0  503.6d+0   25
 503.6d+0  465.5d+0   25
 465.5d+0  335.4d+0   25
 335.4d+0  130.3d+0   25
 130.3d+0    0.0d+0   25
-1.000d+02
  2    1
-3.170d-12-3.170d-12
0.000d+00 0.000d+00
```

Material Proper. for layer 1-5

Top & Bottom Elev. of layer 1-5

1 ⇒ SS
0 ⇒ Transient

0 ⇒ Redist for SS
0 ⇒ Non-adapt. for TR
1 ⇒ refine for TR
2 ⇒ redist. for TR

These are S_r not θ_r !!

infiltration rate at top = .1 mm/yr

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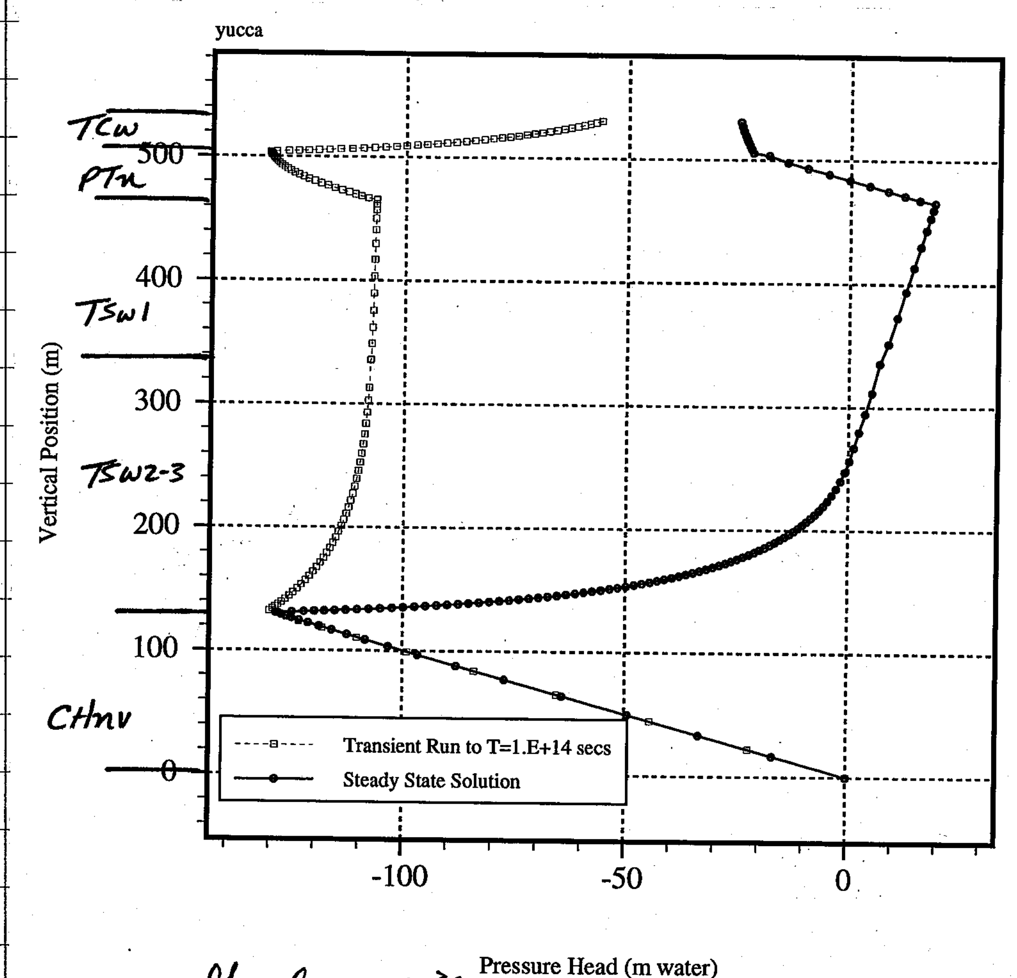
Results for steady-state run and transient run to steady state



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Steady solver uses SOR with overrelaxation $\omega = 1.5$ and a residual tolerance of 1.e-6. Allow up to 150 Picard iterations per grid and up to 30 grid adaptations. Transient solver uses Thomas algorithm for solver; allows up to 20 Picard iterations before time step is reduced by half. Time step is allowed to grow by factor of 1.1 if convergence is achieved in less than 10 Picard iterations for transient case.

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5/7/93

Verification of ADAVAR by code benchmarking

The fixed grid option for ADAVAR has been compared to several other unsaturated flow codes to ensure that the basic physics are correctly modelled. I have chosen a simple 1D vertical infiltration problem described by Celia et al. WRR 26(7), July 1990.

Problem domain: 1D Vertical column 100 cm in length. Soil properties given by van Genuchten model with

$\theta_s = .368$ $\theta_r = .102$ $\alpha = .00335$ 1/cm

$n = 2.0$ $K_s = 9.22 \times 10^{-3}$ cm/s $S_s = 1.0 \times 10^{-7}$

$\psi(z,0) = -1000$ cm

$\psi(z_{top},t) = -75$ cm

$\psi(z_{bot},t) = -1000$ cm

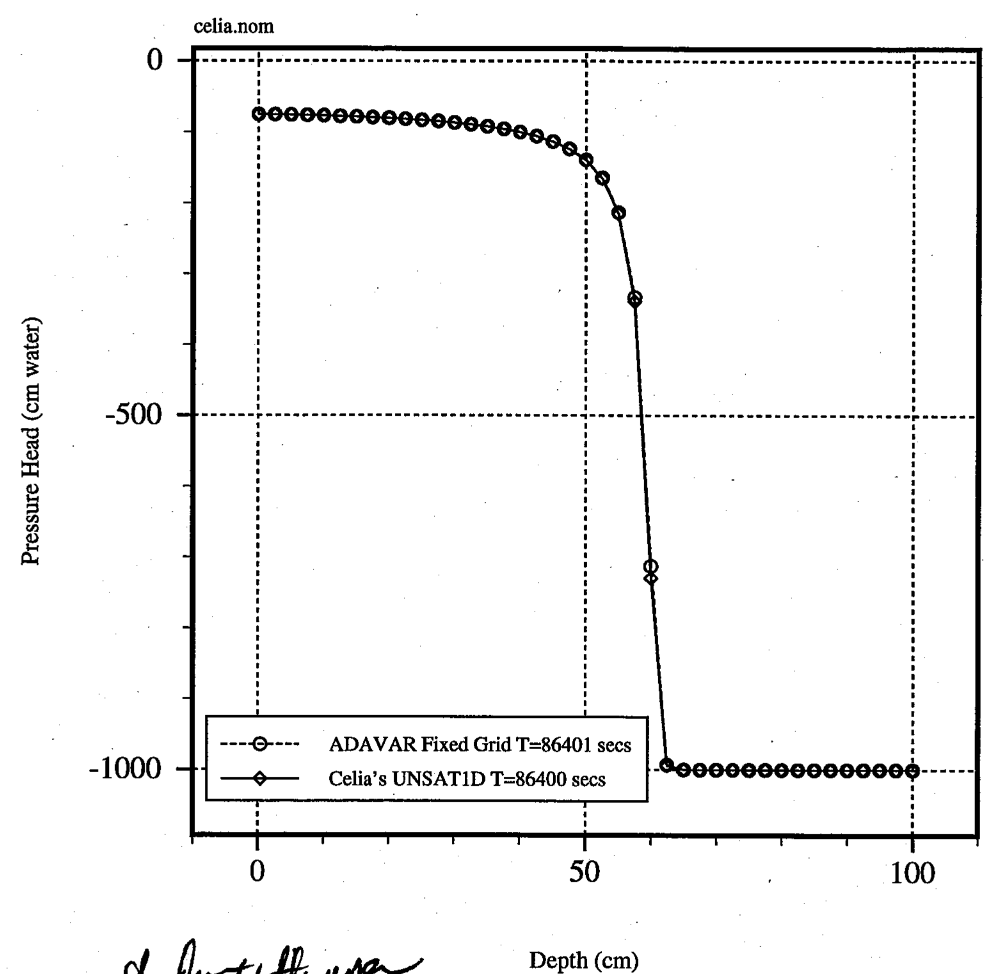
Nominal Problem

$\Delta z = 2.5$ cm $\Delta t = 144$ sec

$T_{final} = 86401$ seconds $\approx$ 1 Day (+1 sec)

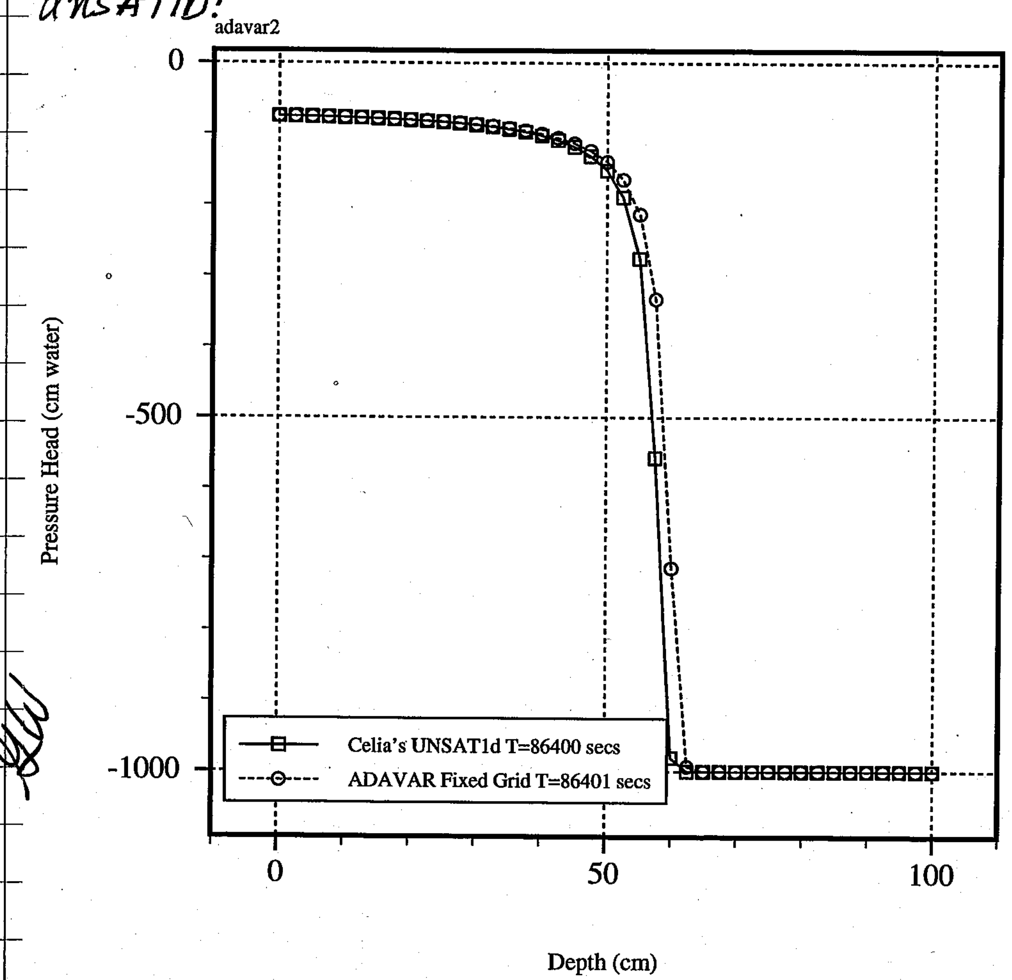
Results compared at 1 Day

The solutions here are nearly indistinguishable.



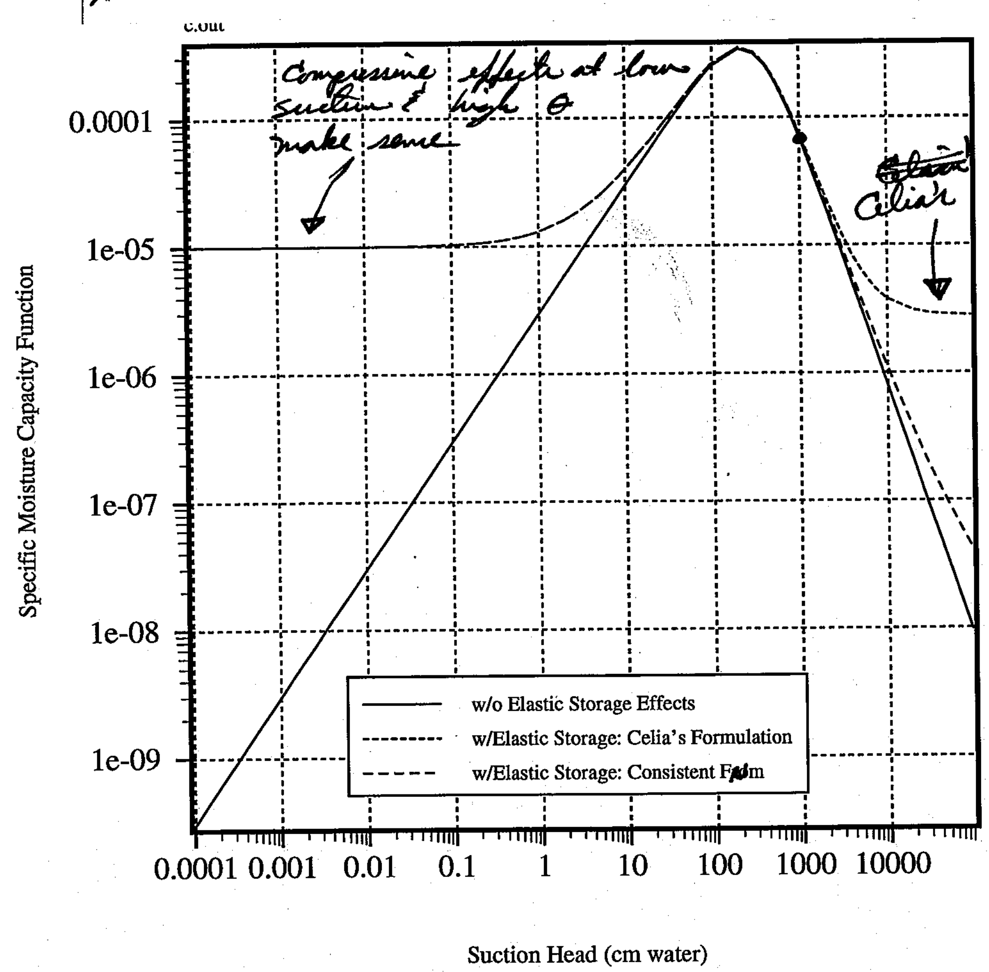
Increasing storage decreases diffusivity which decreases the rate at which the front advances

For the case where the elastic storage is increased from 1.0×10^{-7} to 1.0×10^{-5} differences in the solution for ADAVAR and Celia's UNSAT1D code become apparent. In the following plot the ~~decrease~~ increase in S_s causes the front ~~#~~ predicted by UNSAT1D to be retarded relative to ADAVAR. I believe that this is the result of inconsistent implementation of the storage term in UNSAT1D!



Celia's formulation: $S(\psi) = \left(S_s \frac{\theta}{\theta_s} + \frac{\partial \theta}{\partial \psi}\right)$
Note that at $\theta_{min} = \theta_r$, $S_s \frac{\theta}{\theta_s}$ can make a very large contribution to $S(\psi)$ at very high suctions.

My formulation $S(\psi) = \left(S_s \frac{\theta - \theta_r}{\theta_s - \theta_r} + \frac{\partial \theta}{\partial \psi}\right)$, residual or unextractable moisture should not be included in compressive media effects. This is consistent or at least moreso.



This does not really appear to explain the difference between ADAVAR and UNSAT1D afterall. Note that at $\psi = -1000$ cm, the storage term is not affected by the method used to account for compressive effects. Note again that $\psi = -1000$ is the lowest pressure (highest suction) attained in the Celia test problem.

(Lumped Mass too!)

Celia's Modified Picard Formulation
(δ-formulation; $\delta_i^m = h_i^{n+1,m+1} - h_i^{n+1,m}$)

For node i:

$$\left(C_i^{n+1,m} + S_s \frac{\theta_i^{n+1,m}}{\theta_s}\right)\frac{\delta_i^m}{\Delta t} - \frac{1}{(\Delta z)^2}\left[K_{i+1/2}^{n+1,m}(\delta_{i+1}^m - \delta_i^m) - K_{i-1/2}^{n+1,m}(\delta_i - \delta_{i-1})\right] = \frac{1}{(\Delta z)^2}\left[K_{i+1/2}^{n+1,m}(h_{i+1}^{n+1,m} - h_i^{n+1,m}) - K_{i-1/2}^{n+1,m}(h_i^{n+1,m} - h_{i-1}^{n+1,m})\right] + \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z}$$

$$-\left(\frac{\theta_i^{n+1,m} - \theta_i^{n}}{\Delta t}\right) - S_s \frac{\theta_i^{n+1,m}}{\theta_s}\left(\frac{h_i^{n+1,m} - h_i^{n}}{\Delta t}\right)$$

n - time level ; m - iterate level

Convert to h or ψ based form

$$\left(C_i^{n+1,m} + S_s \frac{\theta_i^{n+1,m}}{\theta_s}\right) \frac{h_i^{n+1,m+1} - h_i^{n+1,m}}{\Delta t}$$

note the sign!!

$$\ominus \frac{1}{(\Delta z)^2}\Big[K_{i+1/2}^{n+1,m}\left(h_{i+1}^{n+1,m+1} - \cancelto{1}{h_{i+1}^{n+1,m}}\right)$$

$$- \left(K_{i+1/2}^{n+1,m} + K_{i-1/2}^{n+1,m}\right)\left(h_i^{n+1,m+1} - \cancelto{2}{h_i^{n+1,m}}\right)$$

$$+ K_{i-1/2}^{n+1,m}\left(h_{i-1}^{n+1,m+1} - \cancelto{3}{h_{i-1}^{n+1,m}}\right)\Big] =$$

$$\frac{1}{(\Delta z)^2}\Big[\cancelto{1}{K_{i+1/2}^{n+1,m} h_{i+1}^{n+1,m}} - \cancelto{2}{\left(K_{i+1/2}^{n+1,m} + K_{i-1/2}^{n+1,m}\right) h_i^{n+1,m}}$$

$$+ \cancelto{3}{K_{i-1/2}^{n+1,m} h_{i-1}^{n+1,m}}\Big] + \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z}$$

$$- \left(\frac{\theta_i^{n+1,m} - \theta_i^{n}}{\Delta t}\right) + S_s \frac{\theta_i^{n+1,m}}{\theta_s} \frac{h_i^{n+1,m} - h_i^{n}}{\Delta t}$$

$$\left(C_i^{n+1,m} + S_s \frac{\theta_i^{n+1,m}}{\theta_s}\right) \frac{h_i^{n+1,m+1} - h_i^{n+1,m}}{\Delta t}$$

$$-\frac{1}{(\Delta z)^2}\Big[K_{i+1/2}^{n+1,m} h_{i+1}^{n+1,m+1} - \left(K_{i+1/2}^{n+1,m} + K_{i-1/2}^{n+1,m}\right) h_i^{n+1,m+1}$$

$$+ K_{i-1/2}^{n+1,m} h_{i-1}^{n+1,m}\Big] = \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \left(\frac{\theta_i^{n+1,m} - \theta_i^{n}}{\Delta t}\right)$$

$$\boxed{+ S_s \frac{\theta_i^{n+1,m}}{\theta_s} \frac{h_i^{n+1,m} - h_i^{n}}{\Delta t}} \Longrightarrow \text{Term } \Sigma_i$$

My formulation

$$-\frac{1}{(\Delta z)^2}\Big[K_{i+1/2}^{n+1,m} h_{i+1}^{n+1,m+1} - \left(K_{i+1/2}^{n+1,m} + K_{i-1/2}^{n+1,m}\right) h_i^{n+1,m+1}$$

$$+ K_{i-1/2}^{n+1,m} h_{i-1}^{n+1,m}\Big] = \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z} - \left(\frac{\theta_i^{n+1,m+1} - \theta_i^{n}}{\Delta t}\right)$$

$$\theta_i^{n+1,m+1} \approx \theta_i^{n+1,m} + \left.\frac{\partial \theta}{\partial h}\right|_i^{n+1,m} \left(h_i^{n+1,m+1} - h_i^{n+1,m}\right)$$

$$S_i^{n+1,m} = \frac{\theta_i^{n+1,m} - \theta_r}{\theta_s - \theta_r}$$

$$\left.\frac{\partial \theta}{\partial h}\right|_i \approx \left(C_i^{n+1,m} + S_s \cdot S_i^{n+1,m}\right)$$

add effect of elastic storage

Taylor series used to obtain the so-called modified Picard, mass-conserving form.

$$\frac{\theta_i^{n+1,m+1} - \theta_i^{n}}{\Delta t} \cong$$

$$\frac{\theta_i^{n+1,m} - \theta_i^{n}}{\Delta t} + \left(C_i^{n+1,m} + S_s S_i^{n+1,m}\right) \frac{h_i^{n+1,m+1} - h_i^{n+1,m}}{\Delta t}$$

So I get

$$\left(C_i^{n+1,m} + S_s S_i^{n+1,m}\right) \frac{h_i^{n+1,m+1} - h_i^{n+1,m}}{\Delta t}$$

$$-\frac{1}{(\Delta z)^2}\Big[K_{i+1/2}^{n+1,m}\, h_i^{n+1,m+1} - \left(K_{i+1/2}^{n+1,m} + K_{i-1/2}^{n+1,m}\right) h_i^{n+1,m+1}$$
$$+ K_{i-1/2}^{n+1,m}\, h_{i-1}^{n+1,m+1}\Big] = \frac{K_{i+1/2}^{n+1,m} - K_{i-1/2}^{n+1,m}}{\Delta z}$$
$$-\left(\frac{\theta_i^{n+1,m} - \theta_i^{n}}{\Delta t}\right)$$

I do not get the Σ_i term identified on page 11 which Celia gets in his formulation! This is the cause of our differences. Clearly as $S_s \to 0$, $\Sigma_i \to 0$ and the formulations are identical.

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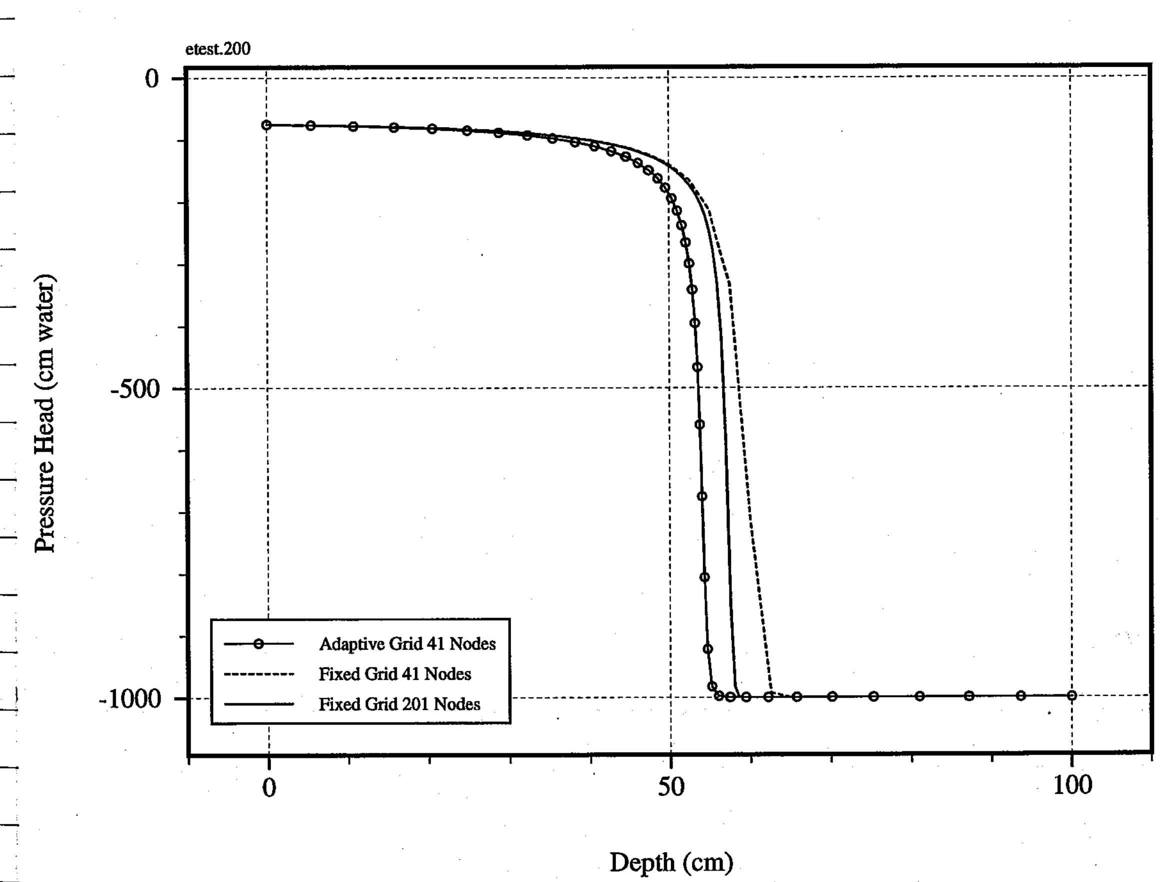
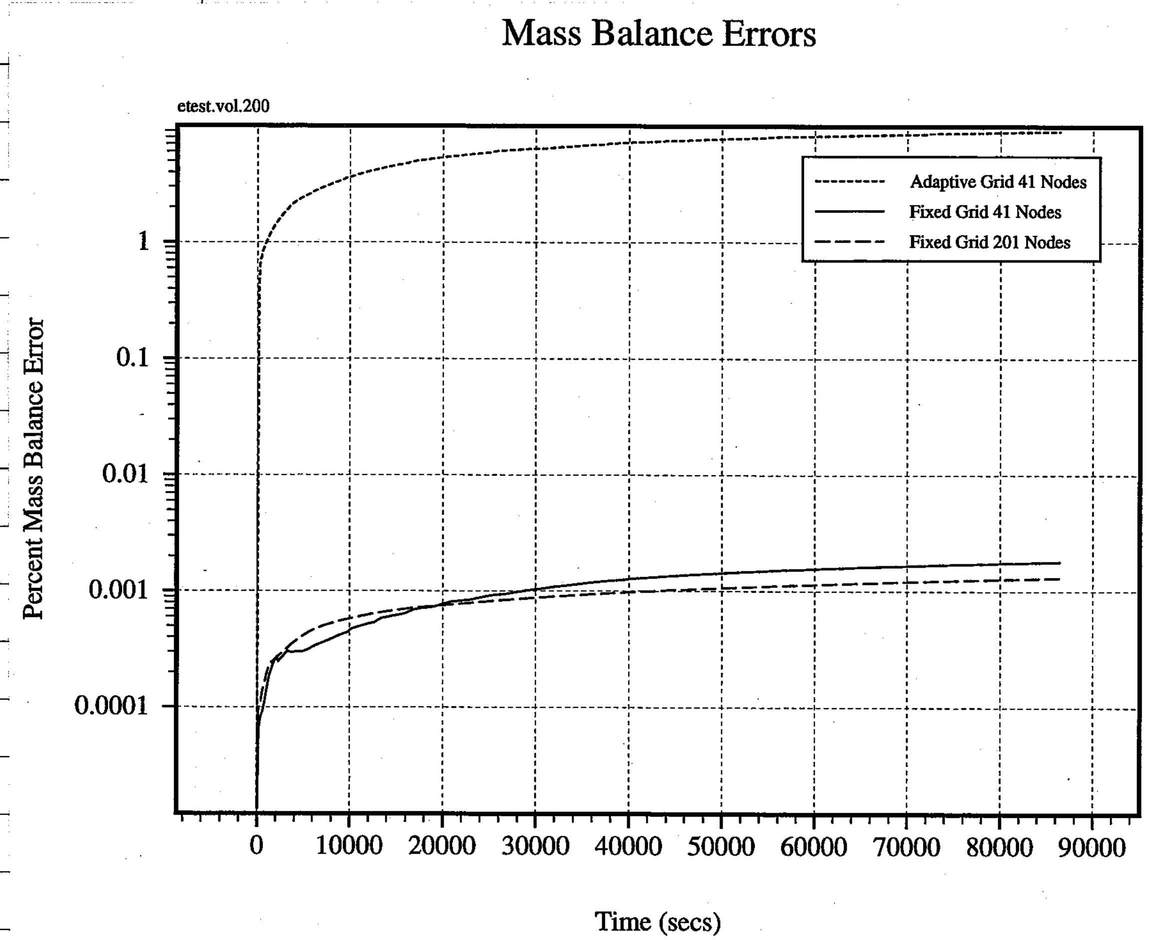
5/10/93

Documenting Mass Balance Error With Adaptive Gridding. Others (Gottardi & Venutelli, WRR 28(12), 1992 pp 3259-3267) have shown that moving grid finite element solutions to transient infiltration are not mass or volume conserving. My work shows this too. Consider the 1D test problem described on page 5.

GW

Pressure Heads from ADAVAR





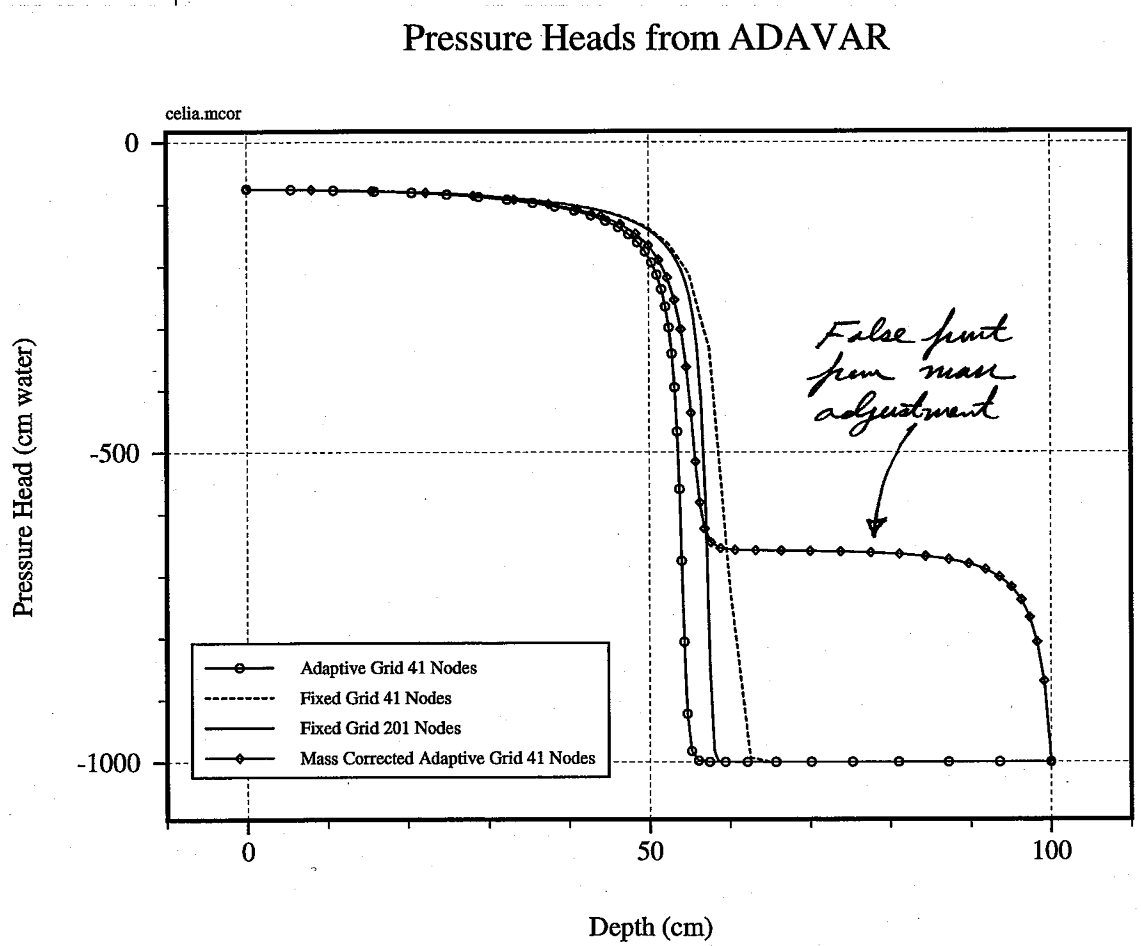
Not only does the adaptive grid solution lag behind the fixed grid solution at T = 86401 sec, it shows a much greater mass balance undershoot throughout time.

$$e(t) = \text{Percent Mass Balance Error} = \frac{\text{Net Inflow} - \text{Mass Acc.}}{\text{Net Inflow}} \times 100$$

At T = 86401 sec

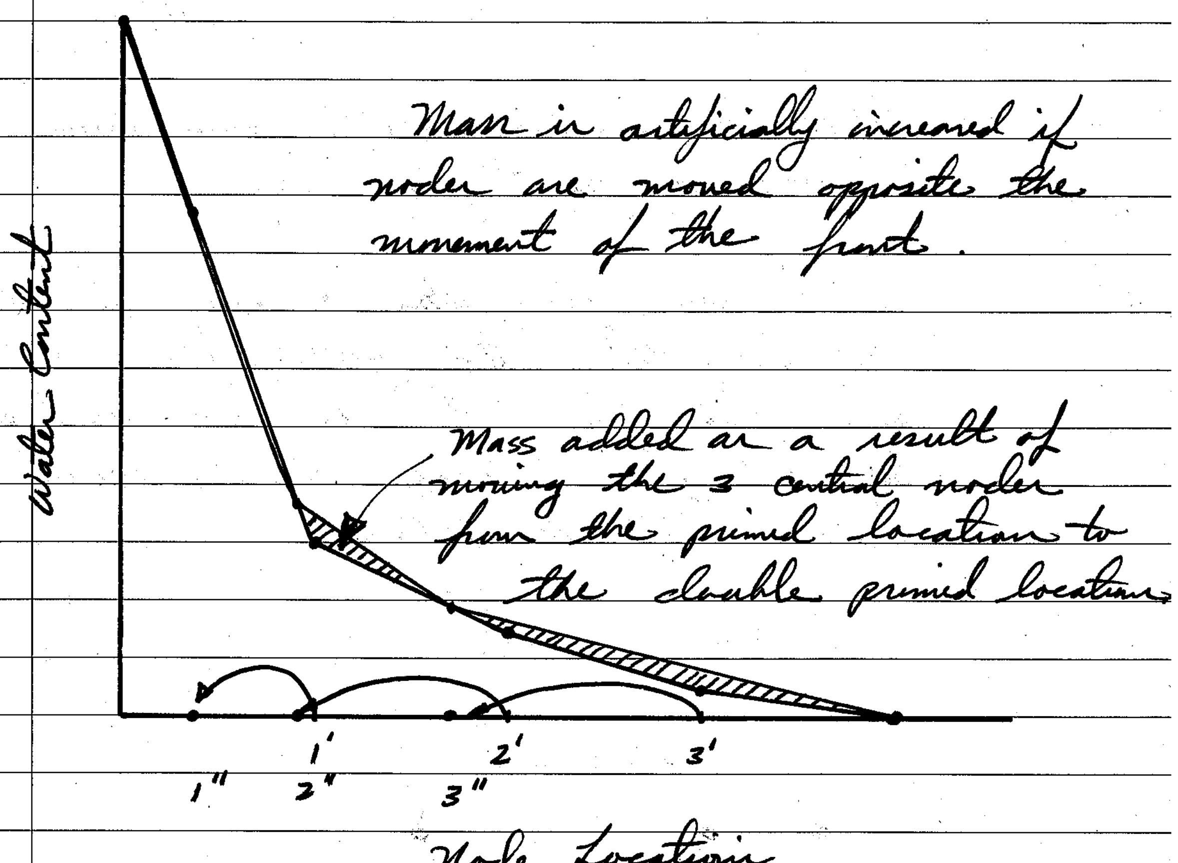
Grid	e (86401)
Fixed 41 :	−.001809 % (Undershoot)
Fixed 201 :	−.001311 % (undershoot)
Adaptive 41 :	−9.075 % (Undershoot)

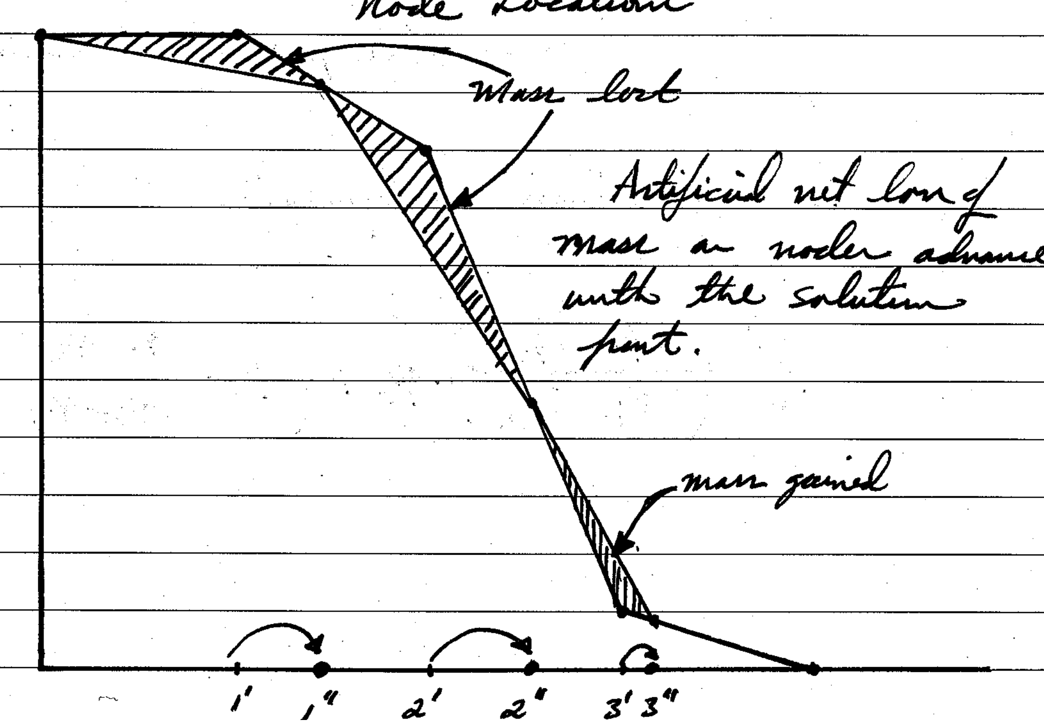
The major source of mass balance error occurs during the process of interpolating the solution from the old grid to the new grid. I simply ~~use~~ use the linear basis functions for the interpolating functions. Mass balance can be improved by explicitly adjusting the nodal values of head so that the total system mass is the same from one grid to the next. However, this procedure distorts the true head distribution and often causes a new, non-physical, wetting front to propagate. See next page for an example of this. Note that the mass balance error for the mass adjusted adaptive grid solution is −.6915 %.



. The reason for mass balance error ~~occurring~~ arising due to the process of grid mapping may be demonstrated by a simple graphing exercise. ⇒

Front Moves →





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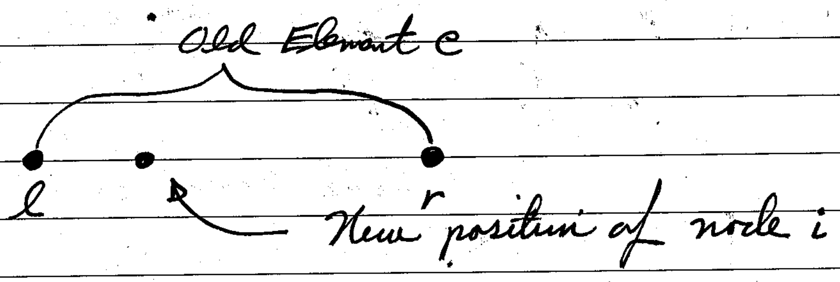
5/11/93

More on improving mass conservation in the adaptive grid method:

I have implemented a new method for interpolating the pressure head at the old grid points to the new grid points by solving a local elliptic equation with Dirichlet B.C.s.



1. Using linear interpolation

$$\psi_i' = \left(\frac{x - x_l}{x_r - x_l}\right)\cdot\psi_r + \left(1 - \frac{x - x_l}{x_r - x_l}\right)\psi_l$$

2. Local elliptic Problem on e

With ψ_r & ψ_l known solve for ψ_i:

$$* \left(\frac{K_l + K_i}{2}\right)\frac{\psi_i - \psi_l}{x_i - x_l} - \left(\frac{K_i + K_r}{2}\right)\left(\frac{\psi_r - \psi_i}{x_r - x_m}\right) = 0$$

$$\psi_i = \frac{(x_r - x_i)\left(\frac{K_l + K_i}{2}\right)\psi_l + (x_i - x_l)\left(\frac{K_i + K_r}{2}\right)\psi_r}{\left[(x_r - x_i)\left(\frac{K_l + K_m}{2}\right) + (x_i - x_l)\left(\frac{K_i + K_r}{2}\right)\right]}$$

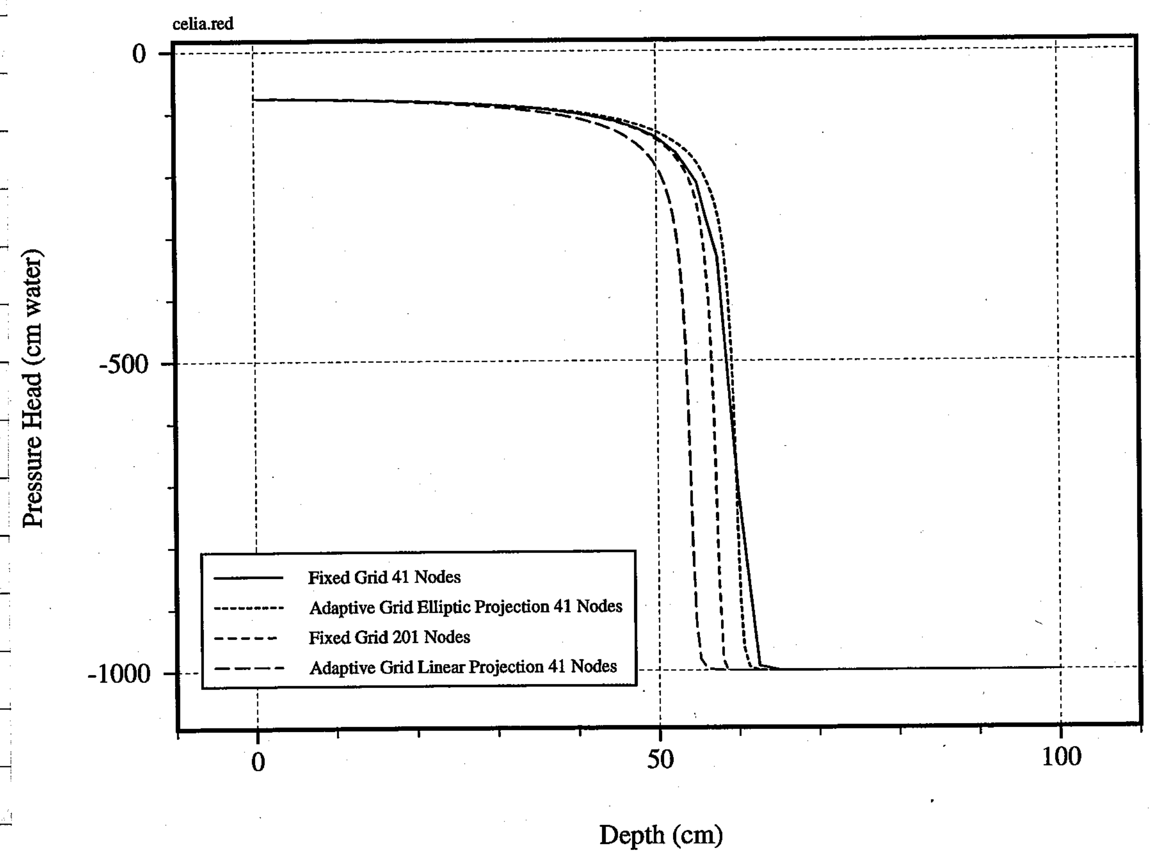
Since $K_i = K(\psi_i)$, we must iterate to find a good solution to the above equation.

A comparison of the solution to problem on page 5 is shown for both method 1 and 2 (linear & elliptic) on the following page.

* Same as:

$$-\frac{K_{i-1/2}}{\Delta x_{i-1/2}}\psi_{i-1} + \left(\frac{K_{i-1/2}}{\Delta x_{i-1/2}} + \frac{K_{i+1/2}}{\Delta x_{i+1/2}}\right)\psi_i - \frac{K_{i+1/2}}{\Delta x_{i+1/2}}\psi_{i+1} = 0$$

Pressure Heads from ADAVAR



The adaptive grid solution using elliptic projection shows a wetting front which precedes all others. However, problems with mass balance still occur.

The adaptive grid soln with linear projection recorded a mass balance error of -9.075% after 86401 sec.

The adaptive grid soln with elliptic projection recorded a mass balance error of +4.41% after 86401 seconds.

Increasing the number of nodes in the adaptive scheme from 41 to 101 results in the mass balance error decreasing from +4.41% to +.87145% at T=86401 secs. However, the time step was reduced to 36 sec from 144 to reach convergence. If, in addition to increasing the nodes from 41 to 101, we allow the time step to adapt too, the mass balance error is reduced to +.11935%.

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6/17/93

Testing the adaptive gridding algorithm for some more extreme problems.

Problem: 100 cm vertical domain
~~100~~ 50 elements

$\psi_t = \emptyset$ cm ~~-75~~

$\psi = -10{,}000$ cm

$\psi_b = -10{,}000$ cm

Run for 86401 sec ≈ 1 day

elapsed time for 50 element fixed grid is 179.4 sec.

Mass balance errors are still so severe for the adaptive procedure that something must be done. I will record here the effect of the number of elements on the final mass balance ratio. Again, this mass balance error test is for the rather extreme infil. problem above.

T = 86401 secs.

No. Elems.	Error
15	-2.0147 (+101.47%)
50	-1.0321 (+3.21%)

This problem is too time consuming for continued testing of the mass balance problem. Therefore, I will revert to the old "Celia" problem.

No. Elems	Error	Error (Fixed Gr.)
10	-1.3098 (+30.98%)	-.99999
20	-1.2015 (+20.15%)	
50	-1.0216 (+2.16%)	
100	-1.0012 (+.12%)	

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6/23/93

Some more timing marks.

1. Celia's problem; page 5 but on a 60 cm domain

a.) 40 elements adaptive.
Δt = 144 sec.
elapsed T = 142 sec.
MBE = -9.83 %

b.) 40 elements fixed grid
elapsed T = 55.4 sec
MBE = -.011 %

2. Celia's problem same as page 5
100 cm domain, $S_s = 1 \times 10^{-5}$

a) 40 fixed elements
elapsed time = 47.467 sec
MBE = .00181 %

b) 40 adaptive elements
elapsed time = 135.42 sec
MBE = 8.321 %

3. Celia's problem same as page 5
domain = 100 cm, $S_s = 1.0 \times 10^{-8}$

a) fixed grid 40 elements
elapsed time = 45.617 sec.
MBE = -.00134 %
(celia.out.fix)

b) adaptive grid 40 elements
elapsed time = 134 sec
MBE = -9.29 % (fix.plt)
(celia.out.adapt)

c) Celia's uns at 10. (my~~case~~test.out)
elapsed time = ~~33.7 sec~~ GW 6/23/93
71 sec Wallclock
(mytest.plt)

d) fixed grid 200 elements
elapsed time 313.78 sec
MBE = -.00133 %

e) fixed grid 500 elements
elapsed time 1025.74 sec
MBE = -.00133 %

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Pages 1 through 26 of this Scientific Notebook were reviewed for compliance with QAP-001 in response to Corrective Action Request 94-02. Corrections and clarifications were made as appropriate. In some cases, the date of a change will reflect the date of this review rather than the date of the original Scientific Notebook entry.

Randy Folck
SwRI - QA
12/09/94

This research project was formally closed as of January 19, 1996. This research notebook describes efforts at developing an adaptive meshing algorithm for modelling 1D unsaturated flow. The results of this effort are outlined in several CNWRA semi-annual research reports.

Gordon Wittmeyer

2/5/96

I have reviewed this scientific notebook and find that it complies with QAP-001 with one exception. There is no mention of the QA status of the code(s) used. This is not significant because the code(s) were used strictly for the purpose of testing calculational algorithms.

There is sufficient technical information so that another qualified individual could repeat the analyses.

RB Baca, PA Element
2/5/97

ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK #: 077

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Operating System: (including version number)	SUN OS; UNIX
Application Used: (including version number)	ADAVAR
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	9- 3 ½ disks
File Types: (.exe, .bat, .zip, etc.)	Various
Remarks: (computer runs, etc.)	Media contains: Bar archive data files.