AMANZI ATS

Debugging & Getting Help

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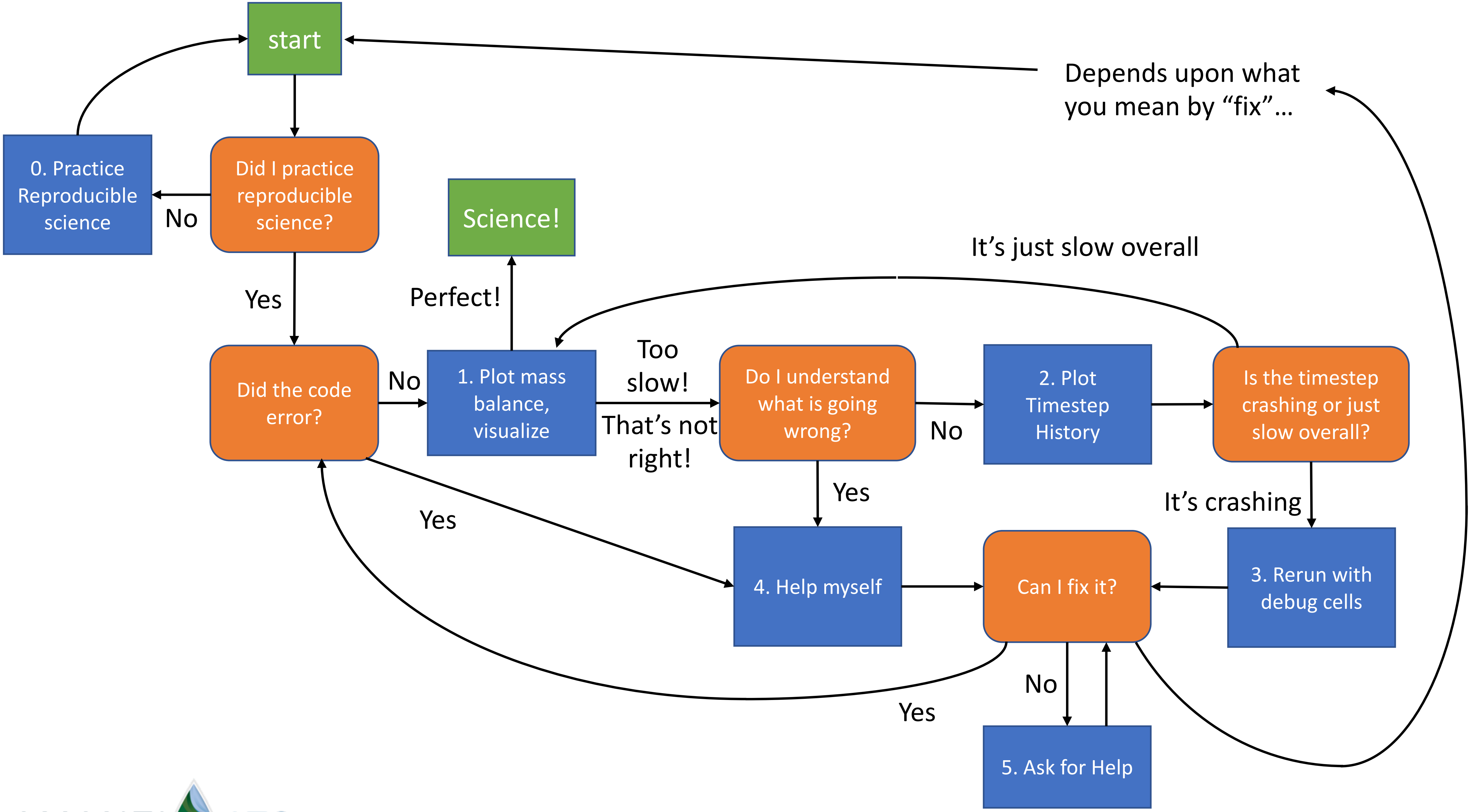
Debugging

There are a lot of ways that things can go wrong.

- incorrect input spec (should error)
- bad input data (could run but give the "wrong" answer)
- bad parameters (could run but very slowly)
- bad physics (could do anything)
- incorrect code (could do anything)



start

Did I practice reproducible science?

No

0. Practice Reproducible science

Yes

Did the code error?

No

1. Plot mass balance, visualize

Perfect!

Science!

Too slow!

That's not right!

Do I understand what is going wrong?

No

2. Plot Timestep History

Is the timestep crashing or just slow overall?

It's just slow overall

It's crashing

3. Rerun with debug cells

Yes

4. Help myself

Yes

Can I fix it?

No

5. Ask for Help

Yes

Depends upon what you mean by "fix"…

Debugging

0. Practice reproducible simulation science.
1. Understand the processes and what is happening
2. Plot a timestep history
3. Rerun with “debug cells” and “verbosity level”=“high”
4. How to help yourself
5. How to ask for help

Practice reproducible simulation science

- Version control your input files, data, mesh, and scripts/notebooks.
- Document them with a README. Document code versions and scripts to visualize the results.
- Checkpoint runs regularly (Annually? Monthly?)
- If you ask for help, we will ask you to send a link to your repo (and so will journals).

Practice reproducible simulation science

- `README.md`
- `data_raw/`
- `data_processed/`
- `scripts/`
- `01_spinup/`
- `02_transient/`
- `figures/`

Practice reproducible simulation science

- `README`
- `data_raw/`
  - `README.md`
  - `DayMet_raw.nc`
  - `DEM.tif`

Raw data, as downloaded from the original source, with sources in the README. Note these can be omitted from the final submission for size constraints if DOIs are in order.

- `data_processed/`
  - `mesh.exo`
  - `DayMet_ATS.h5`

Data reformatted, smoothed, gap-filled, or otherwise processed for ATS.

- `scripts/`
  - `create_mesh.ipynb`
  - `process_DayMet.ipynb`

All scripts needed to go from raw to processed.
Follow good Jupyter notebook practices.
(Rule et al 2019; 10.1371/journal.pcbi.1007007)

- `01_spinup/`
- `02_transient/`
- `figures/`

Practice reproducible simulation science

- `data_raw/`
- `data_processed/`
- `scripts/`
- `01_spinup/`
  - `spinup.xml`
  - `spinup/{run-directory}`
- `02_transient/`
  - `transient.xml`
  - `transient/{run-directory}`
- `figures/`

Runs grouped by concept. May include multiple runs per directory (e.g. ensembles, scenarios, test cases), each run in their own subdirectory. Save input file, observations from all runs; downsample checkpoints & visualization as needed to re-generate figures.

Note, scripts provided in `$ATS_SRC_DIR/tools/utils` to downsample visualization files.

Practice reproducible simulation science

- `data_raw/`
- `data_processed/`
- `scripts/`
- `01_spinup/`
- `02_transient/`
- `figures/`
  - `figure1.py`
  - `figure1.pdf`
  - `...`

Jupyter Notebook

See the Jupyter notebook at:

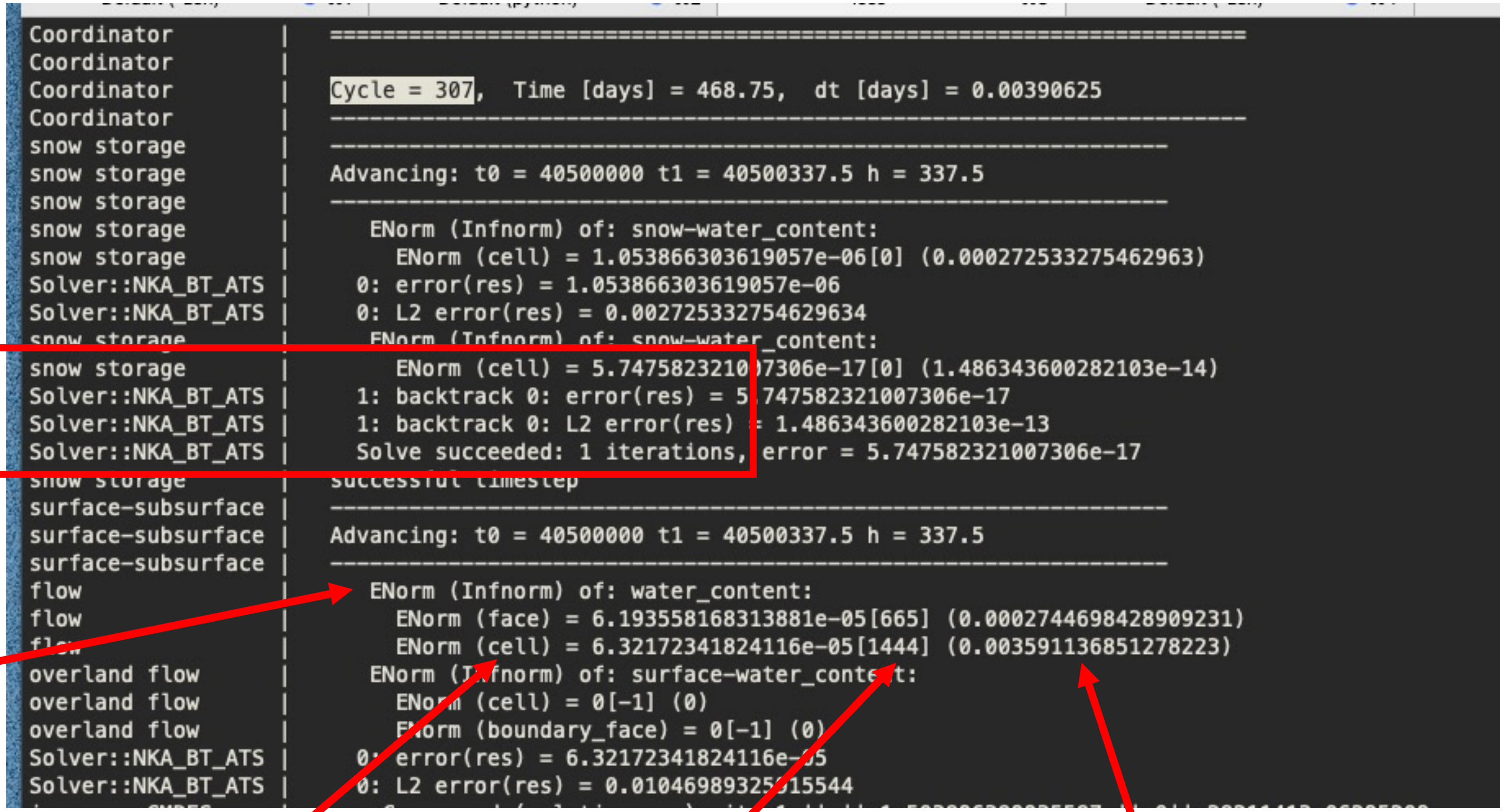
ats-short-course/05_debugging/debugging.ipynb

--verbosity=medium

“snow storage” solve succeeded

Starting the integrated “surface-subsurface” water solve

ErrorNorm is a custom norm based on the conserved quantity. It includes both absolute and relative terms and is always relative to the cell volume.



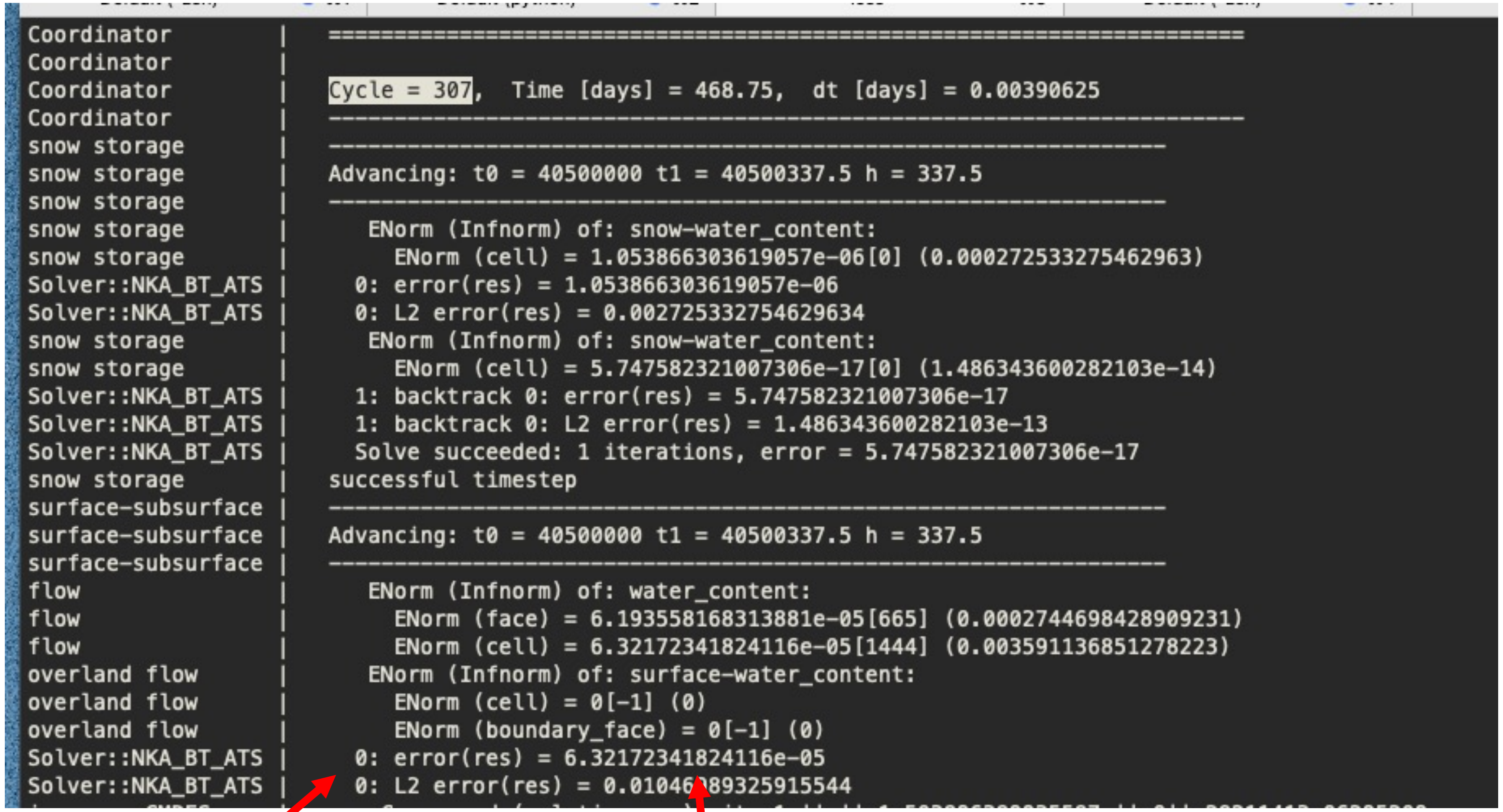
```
Coordinator          |   ==========================================================================
Coordinator          |
Coordinator          |   Cycle = 307,  Time [days] = 468.75,  dt [days] = 0.00390625
Coordinator          |   --------------------------------------------------------------------------
snow storage         |   --------------------------------------------------------------------
snow storage         |   Advancing: t0 = 40500000 t1 = 40500337.5 h = 337.5
snow storage         |   --------------------------------------------------------------------
snow storage         |      ENorm (Infnorm) of: snow-water_content:
snow storage         |        ENorm (cell) = 1.053866303619057e-06[0] (0.000272533275462963)
Solver::NKA_BT_ATS   |     0: error(res) = 1.053866303619057e-06
Solver::NKA_BT_ATS   |     0: L2 error(res) = 0.002725332754629634
snow storage         |      ENorm (Infnorm) of: snow-water_content:
snow storage         |        ENorm (cell) = 5.747582321007306e-17[0] (1.486343600282103e-14)
Solver::NKA_BT_ATS   |     1: backtrack 0: error(res) = 5.747582321007306e-17
Solver::NKA_BT_ATS   |     1: backtrack 0: L2 error(res) = 1.486343600282103e-13
Solver::NKA_BT_ATS   |     Solve succeeded: 1 iterations, error = 5.747582321007306e-17
snow storage         |   successful timestep
surface-subsurface   |   --------------------------------------------------------------------
surface-subsurface   |   Advancing: t0 = 40500000 t1 = 40500337.5 h = 337.5
surface-subsurface   |   --------------------------------------------------------------------
flow                 |      ENorm (Infnorm) of: water_content:
flow                 |        ENorm (face) = 6.193558168313881e-05[665] (0.0002744698428909231)
flow                 |        ENorm (cell) = 6.32172341824116e-05[1444] (0.003591136851278223)
overland flow        |      ENorm (Infnorm) of: surface-water_content:
overland flow        |        ENorm (cell) = 0[-1] (0)
overland flow        |        ENorm (boundary_face) = 0[-1] (0)
Solver::NKA_BT_ATS   |     0: error(res) = 6.32172341824116e-05
Solver::NKA_BT_ATS   |     0: L2 error(res) = 0.01046989325915544
```

Inf-norm (max) of ErrorNorm on cells

Cell on which max error is attained

Value of absolute error [mol]

--verbosity=medium



```
Coordinator          |   ======================================================================
Coordinator          |
Coordinator          |   Cycle = 307,  Time [days] = 468.75,  dt [days] = 0.00390625
Coordinator          |   ----------------------------------------------------------------------
snow storage         |   ----------------------------------------------------------------
snow storage         |   Advancing: t0 = 40500000 t1 = 40500337.5 h = 337.5
snow storage         |   ----------------------------------------------------------------
snow storage         |      ENorm (Infnorm) of: snow-water_content:
snow storage         |        ENorm (cell) = 1.053866303619057e-06[0] (0.000272533275462963)
Solver::NKA_BT_ATS   |     0: error(res) = 1.053866303619057e-06
Solver::NKA_BT_ATS   |     0: L2 error(res) = 0.002725332754629634
snow storage         |      ENorm (Infnorm) of: snow-water_content:
snow storage         |        ENorm (cell) = 5.747582321007306e-17[0] (1.486343600282103e-14)
Solver::NKA_BT_ATS   |     1: backtrack 0: error(res) = 5.747582321007306e-17
Solver::NKA_BT_ATS   |     1: backtrack 0: L2 error(res) = 1.486343600282103e-13
Solver::NKA_BT_ATS   |     Solve succeeded: 1 iterations, error = 5.747582321007306e-17
snow storage         |   successful timestep
surface-subsurface   |   ----------------------------------------------------------------
surface-subsurface   |   Advancing: t0 = 40500000 t1 = 40500337.5 h = 337.5
surface-subsurface   |   ----------------------------------------------------------------
flow                 |      ENorm (Infnorm) of: water_content:
flow                 |        ENorm (face) = 6.193558168313881e-05[665] (0.0002744698428909231)
flow                 |        ENorm (cell) = 6.32172341824116e-05[1444] (0.003591136851278223)
overland flow        |      ENorm (Infnorm) of: surface-water_content:
overland flow        |        ENorm (cell) = 0[-1] (0)
overland flow        |        ENorm (boundary_face) = 0[-1] (0)
Solver::NKA_BT_ATS   |     0: error(res) = 6.32172341824116e-05
Solver::NKA_BT_ATS   |     0: L2 error(res) = 0.01046[illegible]89325915544
```

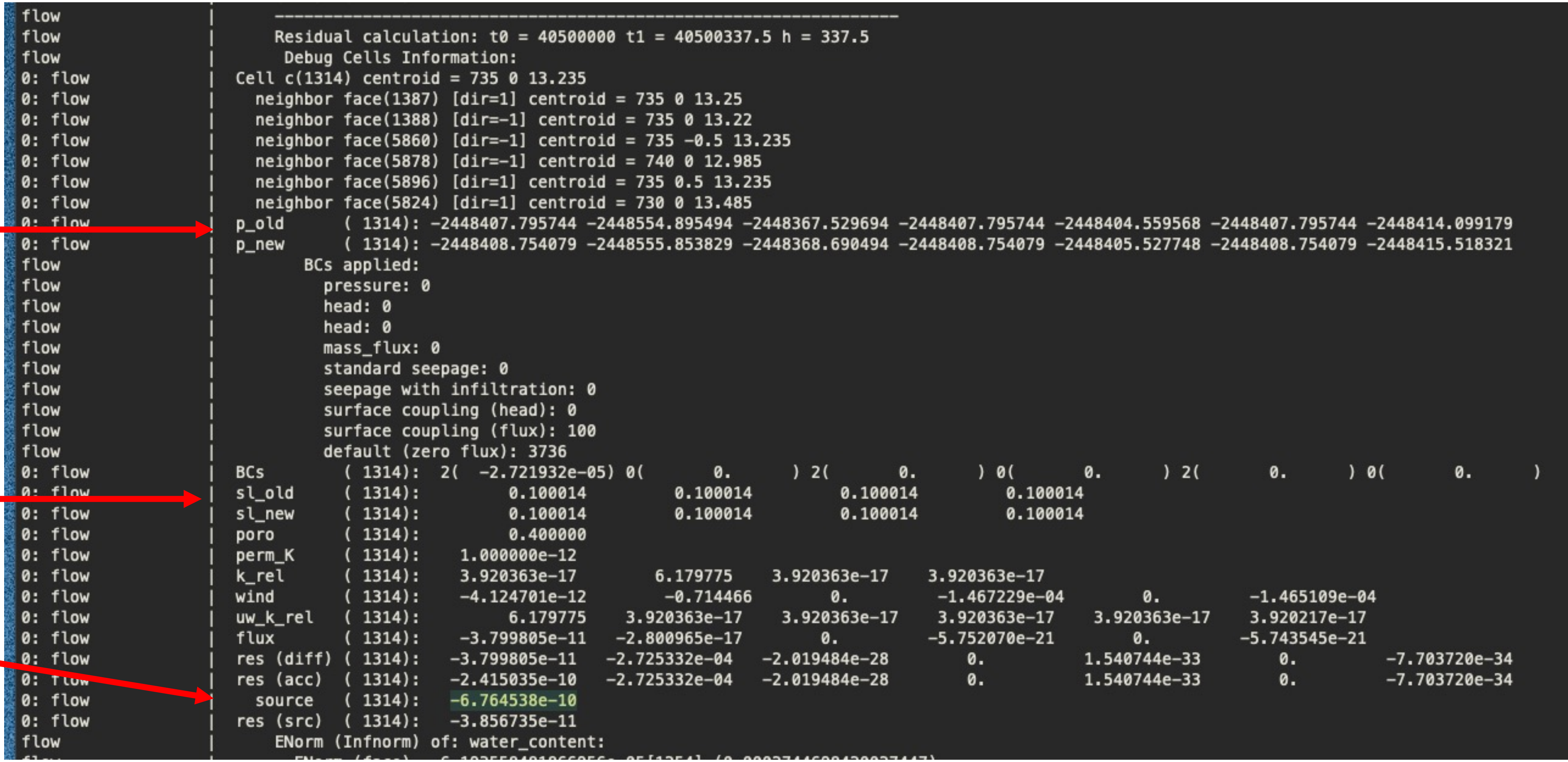
Nonlinear iteration number

Max error across all PKs being solved. Timestep is “converged” when this is less than the nonlinear tolerance.

Capillary pressure very negative, no water

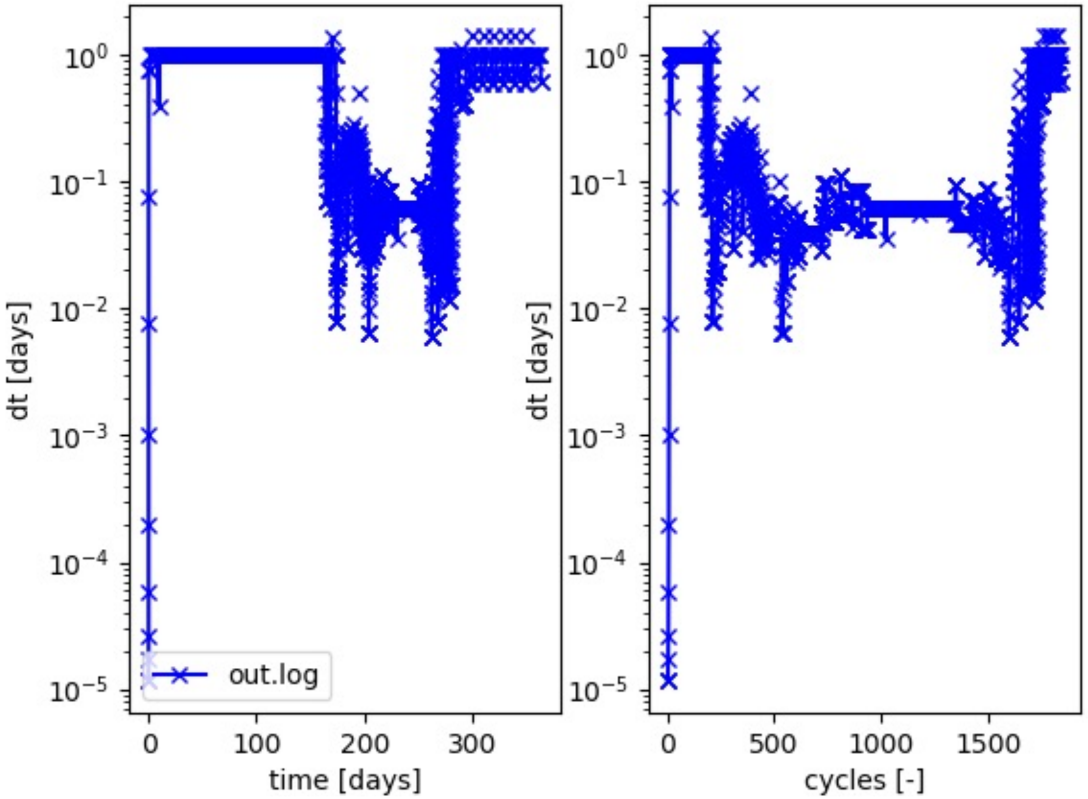
Saturation at residual

Source [mol / s] is negative and nonzero (small isn't good enough).



```
flow                |      ------------------------------------------------------------------
flow                |      Residual calculation: t0 = 40500000 t1 = 40500337.5 h = 337.5
flow                |       Debug Cells Information:
0: flow             |  Cell c(1314) centroid = 735 0 13.235
0: flow             |    neighbor face(1387) [dir=1] centroid = 735 0 13.25
0: flow             |    neighbor face(1388) [dir=-1] centroid = 735 0 13.22
0: flow             |    neighbor face(5860) [dir=-1] centroid = 735 -0.5 13.235
0: flow             |    neighbor face(5878) [dir=-1] centroid = 740 0 12.985
0: flow             |    neighbor face(5896) [dir=1] centroid = 735 0.5 13.235
0: flow             |    neighbor face(5824) [dir=1] centroid = 730 0 13.485
0: flow             |  p_old      ( 1314): -2448407.795744 -2448554.895494 -2448367.529694 -2448407.795744 -2448404.559568 -2448407.795744 -2448414.099179
0: flow             |  p_new      ( 1314): -2448408.754079 -2448555.853829 -2448368.690494 -2448408.754079 -2448405.527748 -2448408.754079 -2448415.518321
flow                |         BCs applied:
flow                |           pressure: 0
flow                |           head: 0
flow                |           head: 0
flow                |           mass_flux: 0
flow                |           standard seepage: 0
flow                |           seepage with infiltration: 0
flow                |           surface coupling (head): 0
flow                |           surface coupling (flux): 100
flow                |           default (zero flux): 3736
0: flow             |  BCs        ( 1314):  2(  -2.721932e-05) 0(       0.      ) 2(       0.      ) 0(       0.      ) 2(       0.      ) 0(       0.      )
0: flow             |  sl_old     ( 1314):         0.100014         0.100014         0.100014         0.100014
0: flow             |  sl_new     ( 1314):         0.100014         0.100014         0.100014         0.100014
0: flow             |  poro       ( 1314):         0.400000
0: flow             |  perm_K     ( 1314):     1.000000e-12
0: flow             |  k_rel      ( 1314):     3.920363e-17        6.179775    3.920363e-17    3.920363e-17
0: flow             |  wind       ( 1314):    -4.124701e-12       -0.714466        0.          -1.467229e-04        0.          -1.465109e-04
0: flow             |  uw_k_rel   ( 1314):         6.179775    3.920363e-17    3.920363e-17    3.920363e-17    3.920363e-17    3.920217e-17
0: flow             |  flux       ( 1314):    -3.799805e-11   -2.800965e-17        0.          -5.752070e-21        0.          -5.743545e-21
0: flow             |  res (diff) ( 1314):   -3.799805e-11   -2.725332e-04   -2.019484e-28        0.           1.540744e-33        0.          -7.703720e-34
0: flow             |  res (acc)  ( 1314):   -2.415035e-10   -2.725332e-04   -2.019484e-28        0.           1.540744e-33        0.          -7.703720e-34
0: flow             |    source   ( 1314):   -6.764538e-10
0: flow             |  res (src)  ( 1314):   -3.856735e-11
flow                |      ENorm (Infnorm) of: water_content:
```

Poor timestep size



Small timesteps when:

- Processes are fast (surface flow)
- Forcing is fast (hourly data)
- Physics is hard (cryosuction)
- *Model inconsistency (user error)*

```
$> python $ATS_SRC_DIR/tools/utils/plot_timestep_history.py out.log
```

Poor timestep size

Small timesteps when:

- Processes are fast (surface flow)

  Do you really need a small Manning coefficient (<1)?
- Forcing is fast (hourly data)

  Do you really need to resolve the diurnal cycle?
- Physics is hard (cryosuction)

  Do you really need that process?
- Model inconsistency (user error)
- Model performance problem

  Can we smooth a transition between physics?

Timesteps of ~0.1 to 0.01 days are typical. Less than this is atypical.

How to help yourself

Input spec problems: Read the manual

https://amanzi.github.io/ats/

Our goal: any “invalid” input spec should result in an error message that hints at both what to fix and where to fix it. *(We aren’t entirely there yet – send in examples of useless error messages!)*

How to help yourself

Start from a demo or test problem.

https://github.com/amanzi/ats-demos/

https://github.com/amanzi/ats-regression-tests/

- If you find a broken demo problem, we will fix it.
- If you can express your issue by changing a demo problem in a small way, we will help you sooner.
- If you compare your change to a known answer, you may find your own mistake!

How to get Help

- See the Frequently Asked Questions: https://github.com/amanzi/ats/wiki/FAQs
- Ask the user's mailing list: ats-users@googlegroups.com
- Submit a GitHub Issue: https://github.com/amanzi/ats/issues

How to get *Better* Help…

- Don’t be afraid to ask for help at conceptualization time.
- Start from a demo and change one thing at a time. If something breaks, back up and try again from the demo problem changing just the last thing.
- Think critically about your problem and describe not just what is your problem but *why is your problem?* What are you doing different from a demo problem?
- How to ask:
  - https://stackoverflow.com/help/how-to-ask
  - What version of the code are you using? `ats --print_version`
  - Reproduce it on `master` or latest release.
  - Include all required input – mesh, forcing files, input data – and set it up to run out of the box (e.g. all paths are correct)

Debugging

- Healthy skepticism will serve you well
- Mass balances and other simple heuristics are extremely valuable
- Predict the answer – what is your hypothesis?
- Visualize the answer – does it make sense?
- If things break, dig into the details. What is happening when and where the problem is occurring?

AMANZI ATS

Closing & Wrap-Up

Ethan Coon

Oak Ridge National Laboratory

Connect and Contribute

Amanzi–ATS Users Group: ats-users@googlegroups.com

- https://groups.google.com/g/ats-users

Source code, Wiki, Issue tracking

- https://github.com/amanzi/amanzi
- https://github.com/amanzi/ats

Demos, Example problems, Tests

- https://github.com/amanzi/ats-demos
- https://github.com/amanzi/ats-regression-tests

Users' Guide, FAQs

- https://amanzi.github.io/ats
- https://github.com/amanzi/ats/wiki/FAQs