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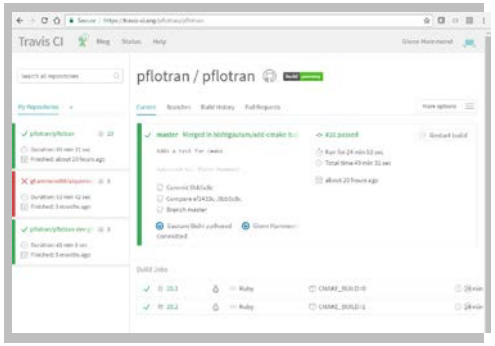

PFLOTRAN Support Infrastructure

U.S. DEPARTMENT OF ENERGY
National Nuclear Security Administration

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PFLOTRAN Support Infrastructure

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- www.pflotran.org: documentation and overview
- Git: distributed source control management tool
- Bitbucket: online PFLOTRAN repository
  - git clone https://bitbucket.org/pflotran/pflotran
  - Source tree
  - Commit logs
  - Pull requests
  - Issue tracker
  - Wiki
    - Link to documentation.pflotran.org
      - Developer/Theory/User guides
      - FAQ (entries motivated by questions on mailing list)
- Travis CI: automated building and testing (regression and unit)
- Google Groups: pflotran-users and pflotran-dev mailing lists
- Google Analytics: tracks behavior on Bitbucket

www.pflotran.org

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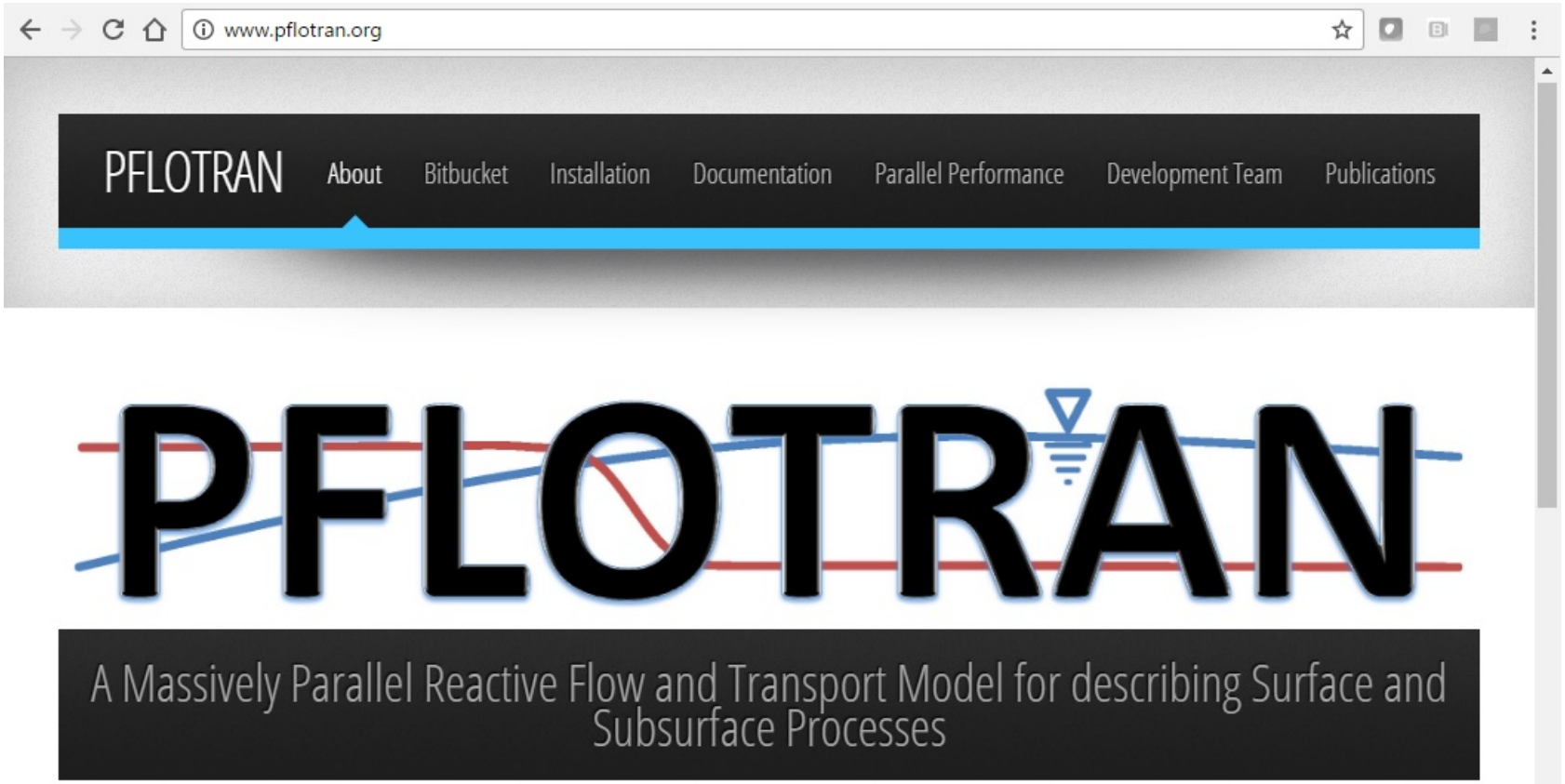
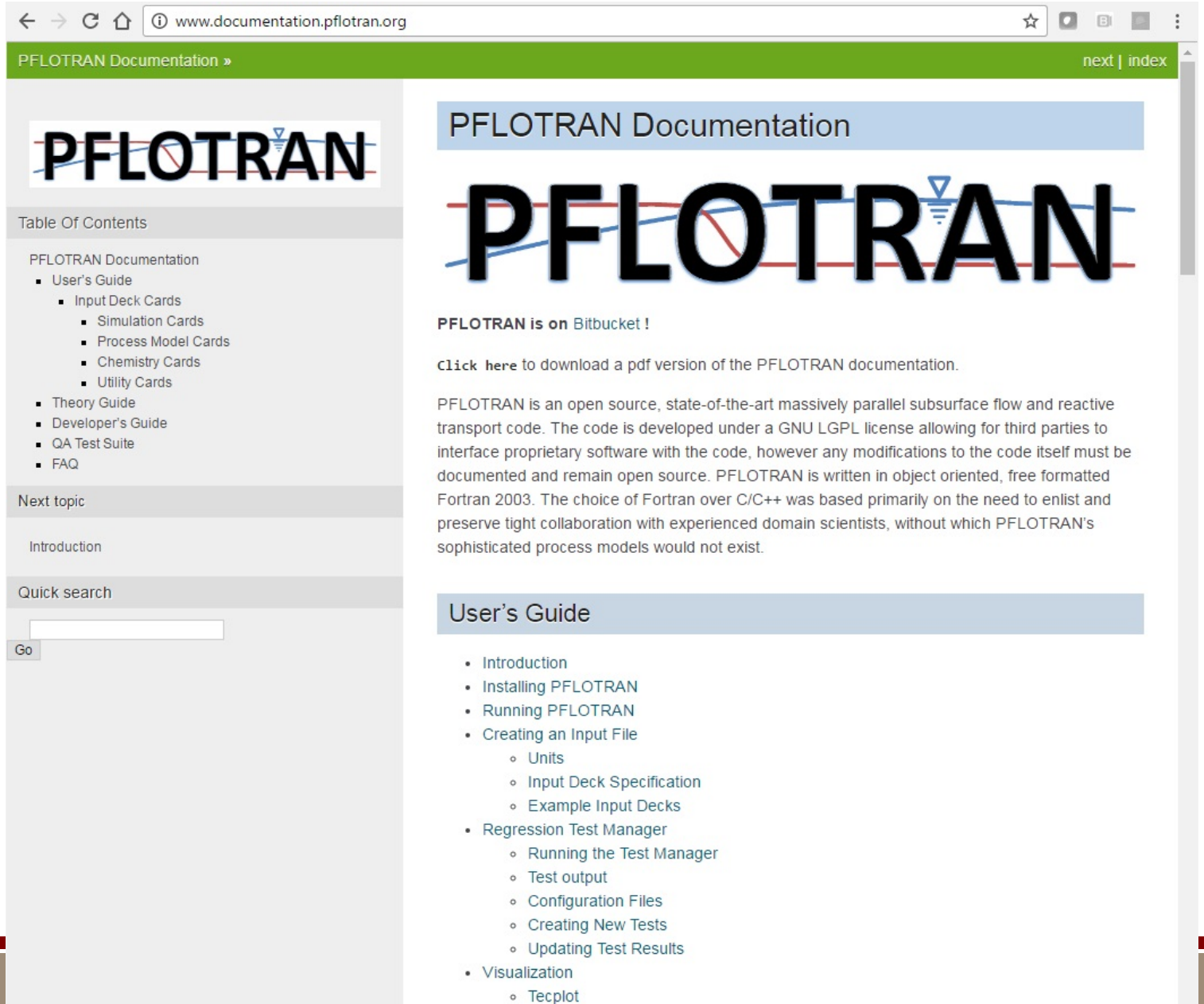


documentation.pflotran.org



documentation.pflotran.org/installation

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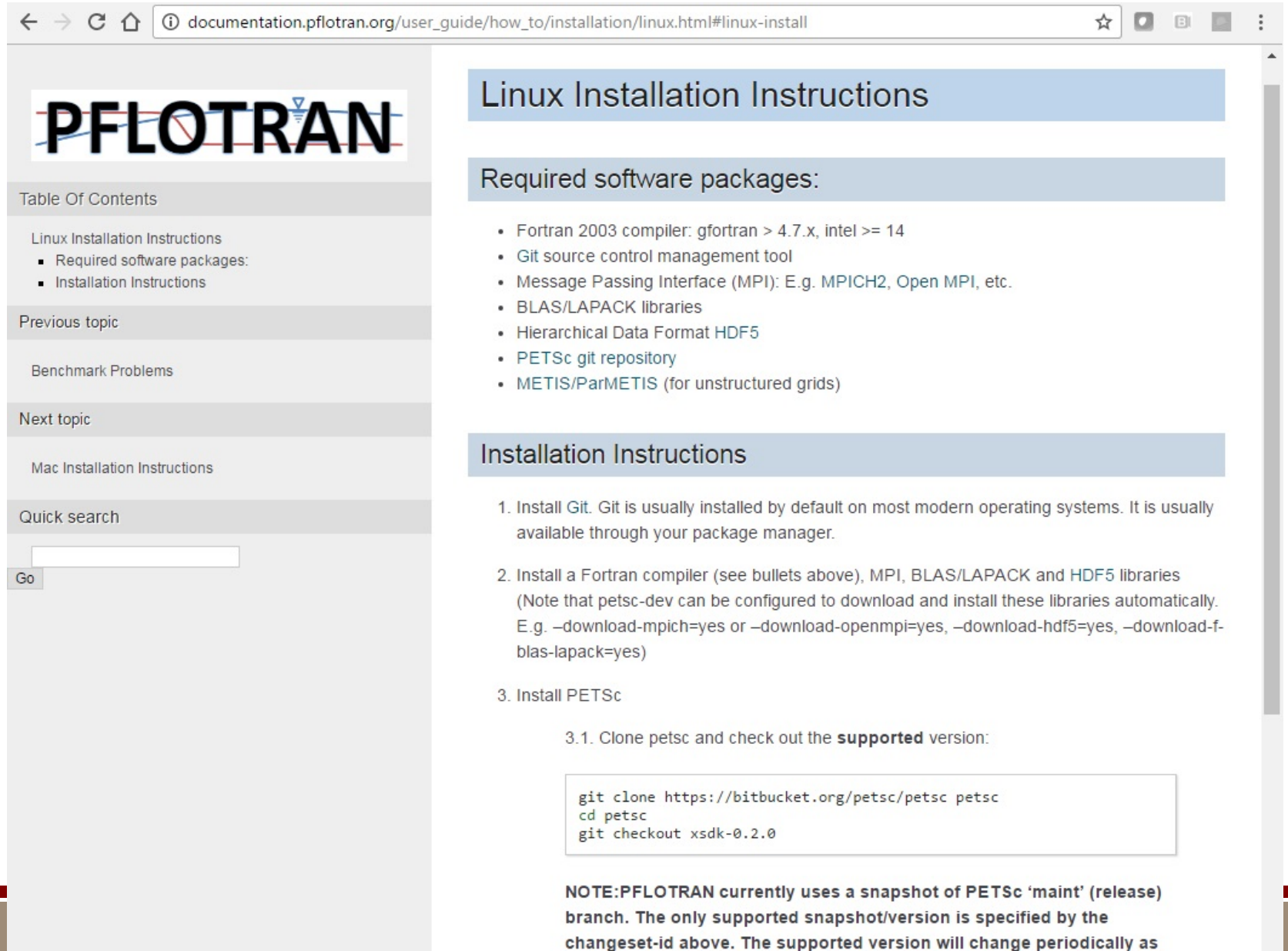

documentation.pflotran.org/chemistry

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www.documentation.pflotran.org/theory_guide/mode_reactive_transport.html

PFLOTRAN

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Mode: GEOMECHANICS

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Mode: REACTIVE TRANSPORT (Keyword CHEMISTRY)

The governing mass conservation equations for the geochemical transport mode for a multiphase system written in terms of a set of independent aqueous primary or basis species with the form

$$\frac{\partial}{\partial t}(\varphi \sum_{\alpha} s_{\alpha} \Psi_j^{\alpha}) + \nabla \cdot \sum_{\alpha} \Omega_j^{\alpha} = Q_j - \sum_m \nu_{jm} I_m - \frac{\partial S_j}{\partial t}, \quad (1)$$

and

$$\frac{\partial \varphi_m}{\partial t} = \overline{V}_m I_m, \quad (2)$$

for minerals with molar volume $\overline{V}_m$, mineral reaction rate I_m and mineral volume fraction φ_m referenced to an REV. Sums over α in Eqn. (1) are over all fluid phases in the system. The quantity Ψ_j^{α} denotes the total concentration of the jth primary species $\mathcal{A}_j^{\mathrm{pri}}$ in the αth fluid phase defined by

$$\Psi_j^{\alpha} = \delta_{l\alpha} C_j^l + \sum_{i=1}^{N_{\mathrm{sec}}} \nu_{ji}^{\alpha} C_i^{\alpha}, \quad (3)$$

In this equation the subscript l represents the aqueous electrolyte phase from which the primary species are chosen. The secondary species concentrations C_i^{α} are obtained from mass action equations corresponding to equilibrium conditions of the reactions

$$\sum_j \nu_{ji}^{\alpha} \mathcal{A}_j^l \rightleftharpoons \mathcal{A}_i^{\alpha}, \quad (4)$$

yielding the mass action equations

$$C_i^{\alpha} = \frac{K_i^{\alpha}}{\gamma_i^{\alpha}} \prod_j \left(\gamma_j^l C_j^l\right)^{\nu_{ji}^{\alpha}}, \quad (5)$$

documentation.pflotran.org/input cards

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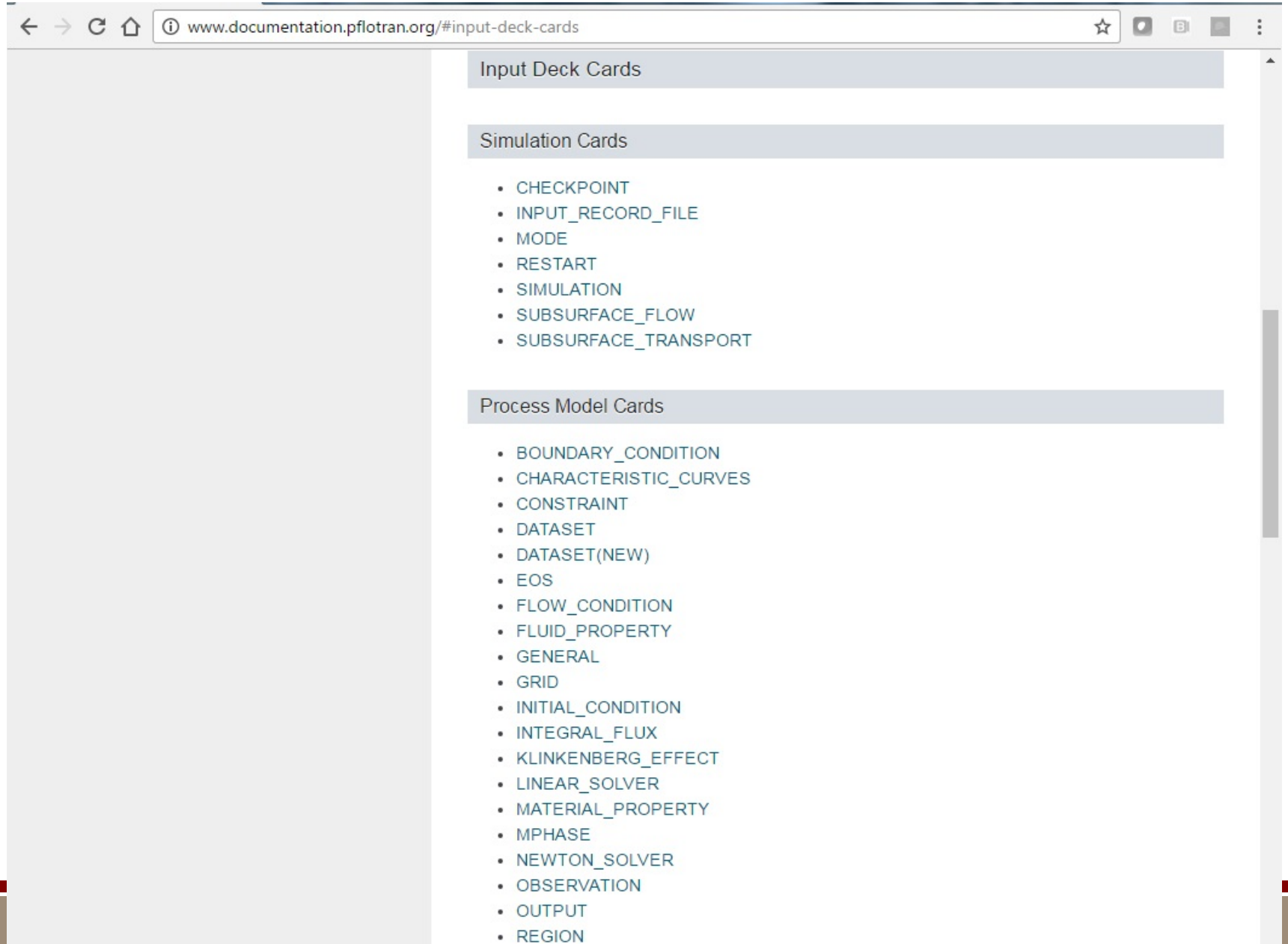
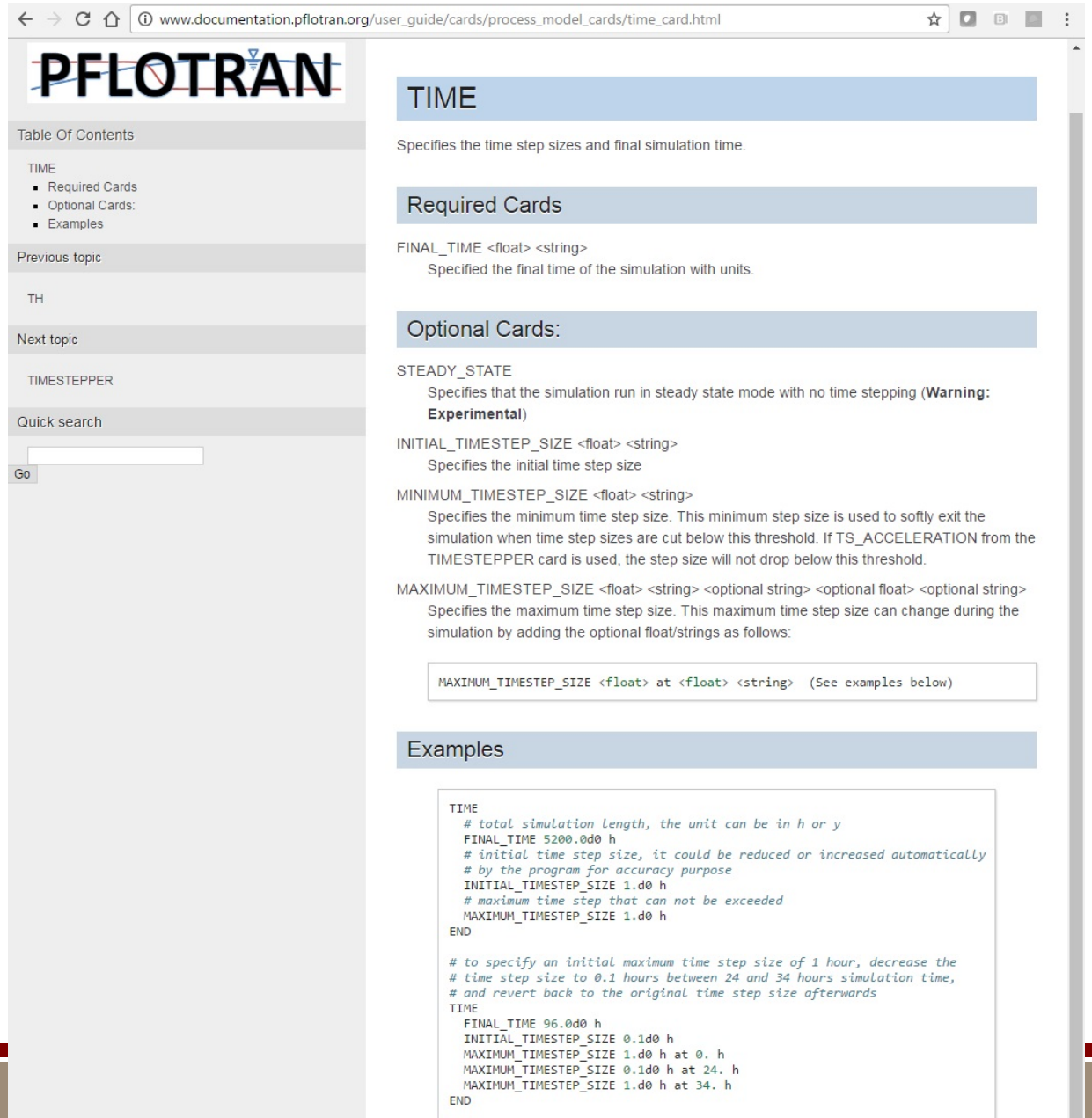


documentation.pflotran.org/TIME card



www.documentation.pflotran.org/user_guide/cards/process_model_cards/time_card.html

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TIMESTEPPER

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TIME

Specifies the time step sizes and final simulation time.

Required Cards

FINAL_TIME <float> <string>
Specified the final time of the simulation with units.

Optional Cards:

STEADY_STATE
Specifies that the simulation run in steady state mode with no time stepping (**Warning: Experimental**)

INITIAL_TIMESTEP_SIZE <float> <string>
Specifies the initial time step size

MINIMUM_TIMESTEP_SIZE <float> <string>
Specifies the minimum time step size. This minimum step size is used to softly exit the simulation when time step sizes are cut below this threshold. If TS_ACCELERATION from the TIMESTEPPER card is used, the step size will not drop below this threshold.

MAXIMUM_TIMESTEP_SIZE <float> <string> <optional string> <optional float> <optional string>
Specifies the maximum time step size. This maximum time step size can change during the simulation by adding the optional float/strings as follows:

```
MAXIMUM_TIMESTEP_SIZE <float> at <float> <string>  (See examples below)
```

Examples

```
TIME
  # total simulation length, the unit can be in h or y
  FINAL_TIME 5200.0d0 h
  # initial time step size, it could be reduced or increased automatically
  # by the program for accuracy purpose
  INITIAL_TIMESTEP_SIZE 1.d0 h
  # maximum time step that can not be exceeded
  MAXIMUM_TIMESTEP_SIZE 1.d0 h
END

# to specify an initial maximum time step size of 1 hour, decrease the
# time step size to 0.1 hours between 24 and 34 hours simulation time,
# and revert back to the original time step size afterwards
TIME
  FINAL_TIME 96.0d0 h
  INITIAL_TIMESTEP_SIZE 0.1d0 h
  MAXIMUM_TIMESTEP_SIZE 1.d0 h at 0. h
  MAXIMUM_TIMESTEP_SIZE 0.1d0 h at 24. h
  MAXIMUM_TIMESTEP_SIZE 1.d0 h at 34. h
END
```

documentation.pflotran.org/FAQ

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How do I make any sense of the screen output, in particular Newton iteration convergence?

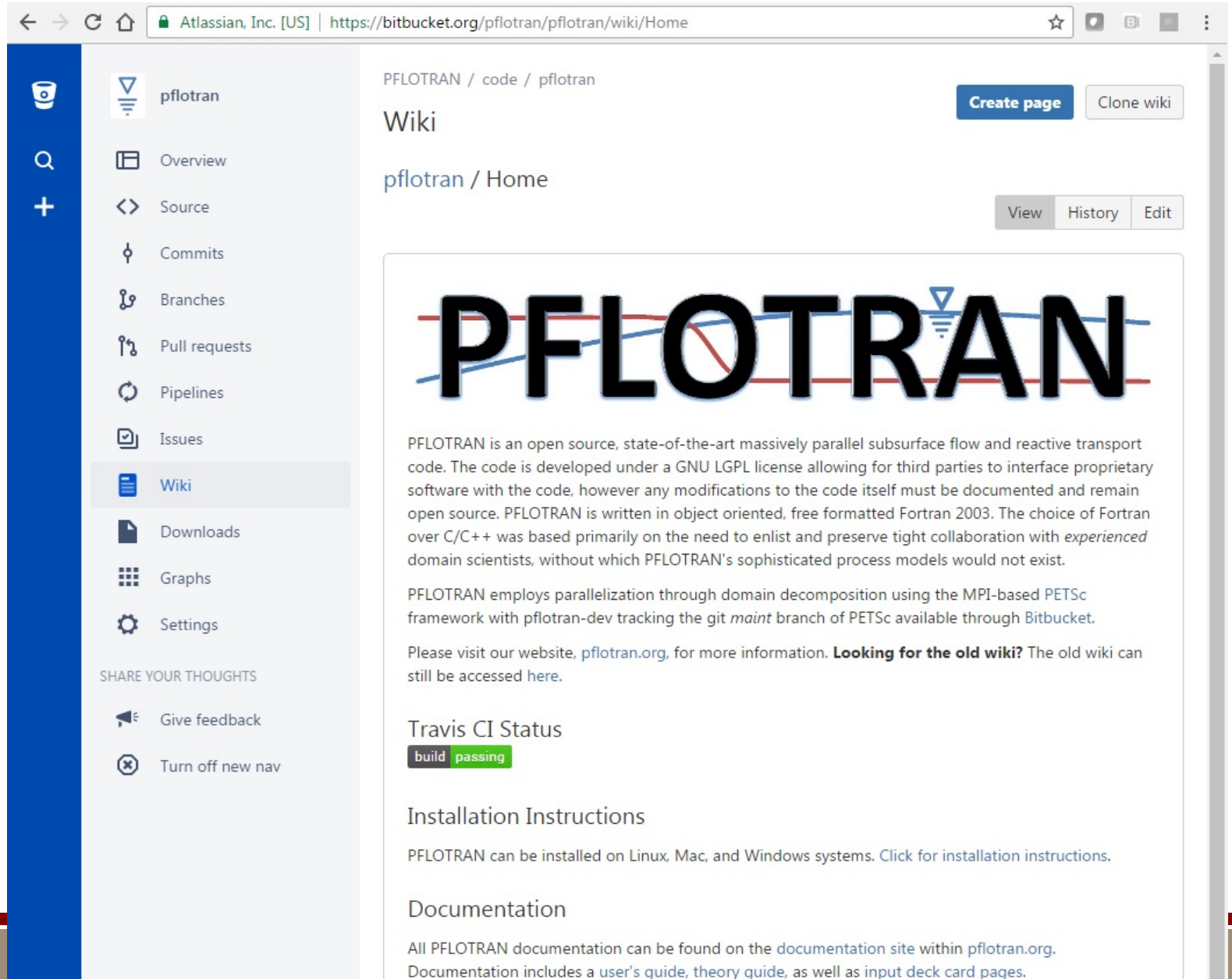
Standard Flow

```
== GENERAL FLOW ================================================================
  1 2r: 4.13E-13 2x: 1.30E+08 2u: 4.47E-01 ir: 4.42E-14 iu: 2.44E-02 rsn:   0
  2 2r: 6.06E-13 2x: 1.30E+08 2u: 5.63E-01 ir: 5.65E-14 iu: 5.23E-02 rsn:   0
  3 2r: 2.21E-13 2x: 1.30E+08 2u: 3.67E-01 ir: 1.90E-14 iu: 3.05E-02 rsn:   0
  4 2r: 2.45E-13 2x: 1.30E+08 2u: 3.33E-01 ir: 2.20E-14 iu: 2.42E-02 rsn: itol_post_che

 Step   5498 Time=  9.89040E+03 Dt=  1.04142E+01 [y] snes_conv_reason:   12
  newton =   4 [   31891] linear =    75 [    645652] cuts =  0 [ 915]
  --> SNES Linear/Non-Linear Iterations =           75  /            4
  --> SNES Residual:   2.452466E-13  2.335682E-16  2.200252E-14
  --> max chng: dpl=   2.7064E-03 dpg=   1.1357E-01 dpa=   1.1357E-01
                dxa=   1.3283E-11  dt=   0.0000E+00 dsg=   2.9327E-08
```

- 2r: 2-norm of residual
- 2x: 2-norm of current solution
- 2u: 2-norm of update
- ir: inf-norm of residual
- iu: inf-norm of update
- rsn: converged reason (corresponding integer in brackets)
    - 0: iterating (not converged)
    - atol[2]: 2r < ATOL
    - rtol[3]: 2r < RTOL * 2r_initial
    - stol[4]: 2u < STOL * 2x
    - itol_res[10]: ir < ITOL_RES
    - itol_upd[11]: iu < ITOL_UPDATE

PFLOTRAN Bitbucket Site



Bitbucket → Github → Travis CI

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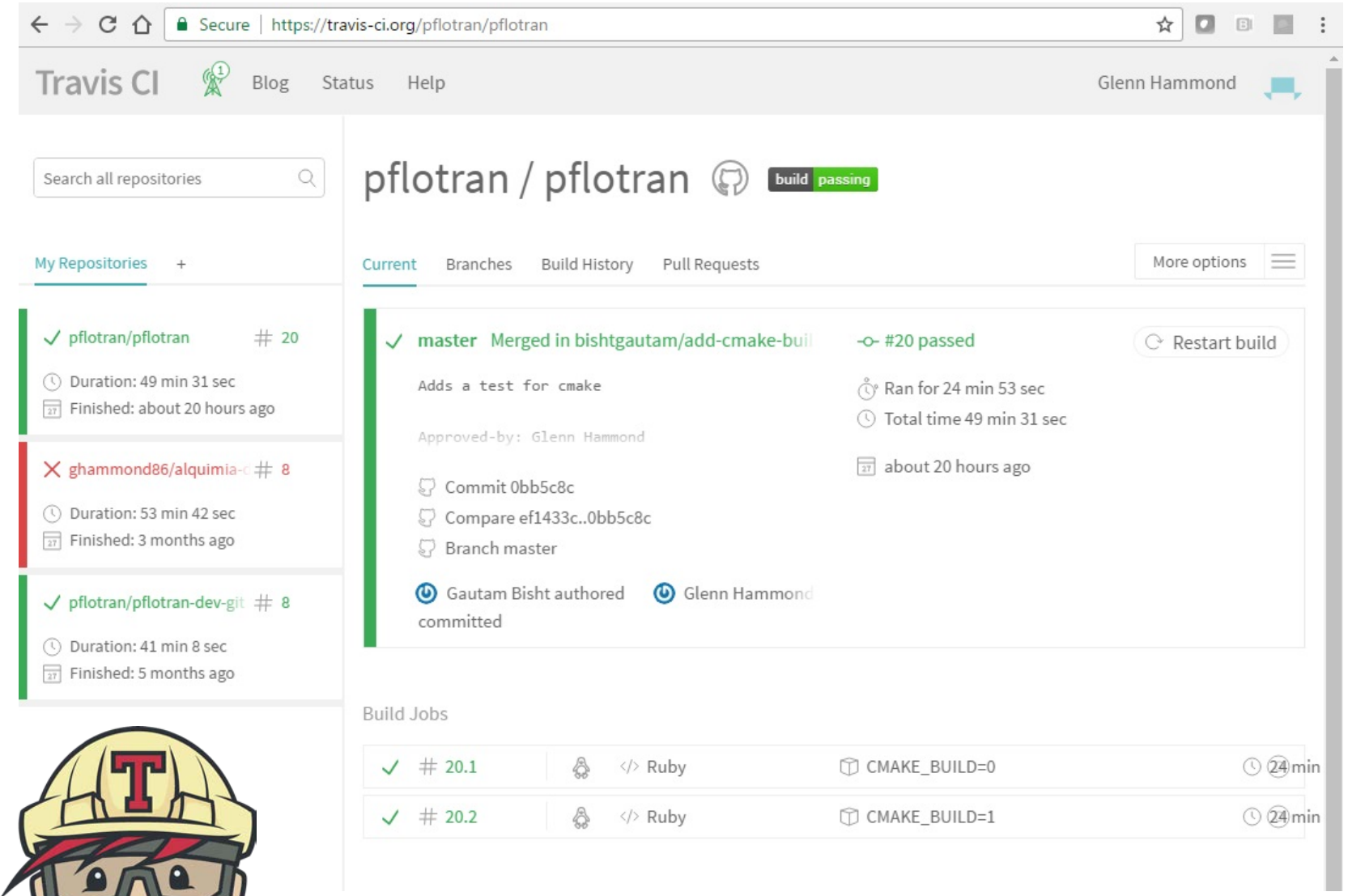

PFLOTRAN Bitbucket Commit Log

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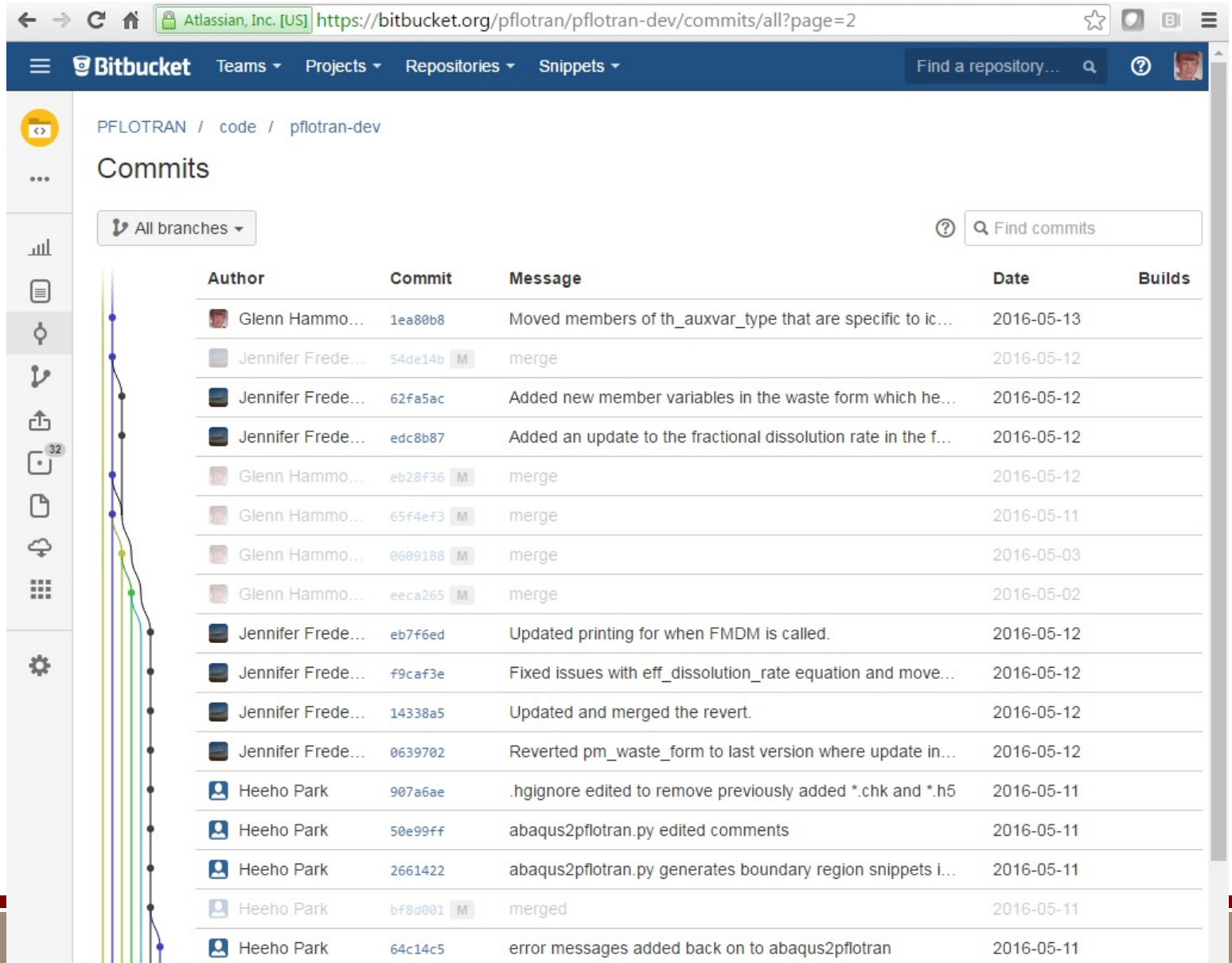

Author	Commit	Message	Date	Builds
Glenn Hammo...	1ea80b8	Moved members of th_auxvar_type that are specific to ic...	2016-05-13	
Jennifer Frede...	54de14b M	merge	2016-05-12	
Jennifer Frede...	62fa5ac	Added new member variables in the waste form which he...	2016-05-12	
Jennifer Frede...	edc8b87	Added an update to the fractional dissolution rate in the f...	2016-05-12	
Glenn Hammo...	eb28f36 M	merge	2016-05-12	
Glenn Hammo...	65f4ef3 M	merge	2016-05-11	
Glenn Hammo...	0609188 M	merge	2016-05-03	
Glenn Hammo...	eeca265 M	merge	2016-05-02	
Jennifer Frede...	eb7f6ed	Updated printing for when FMDM is called.	2016-05-12	
Jennifer Frede...	f9caf3e	Fixed issues with eff_dissolution_rate equation and move...	2016-05-12	
Jennifer Frede...	14338a5	Updated and merged the revert.	2016-05-12	
Jennifer Frede...	0639702	Reverted pm_waste_form to last version where update in...	2016-05-12	
Heeho Park	907a6ae	.hgignore edited to remove previously added *.chk and *.h5	2016-05-11	
Heeho Park	50e99ff	abaqus2pflotran.py edited comments	2016-05-11	
Heeho Park	2661422	abaqus2pflotran.py generates boundary region snippets i...	2016-05-11	
Heeho Park	bf8d001 M	merged	2016-05-11	
Heeho Park	64c14c5	error messages added back on to abaqus2pflotran	2016-05-11	

PFLOTRAN Bitbucket Commit

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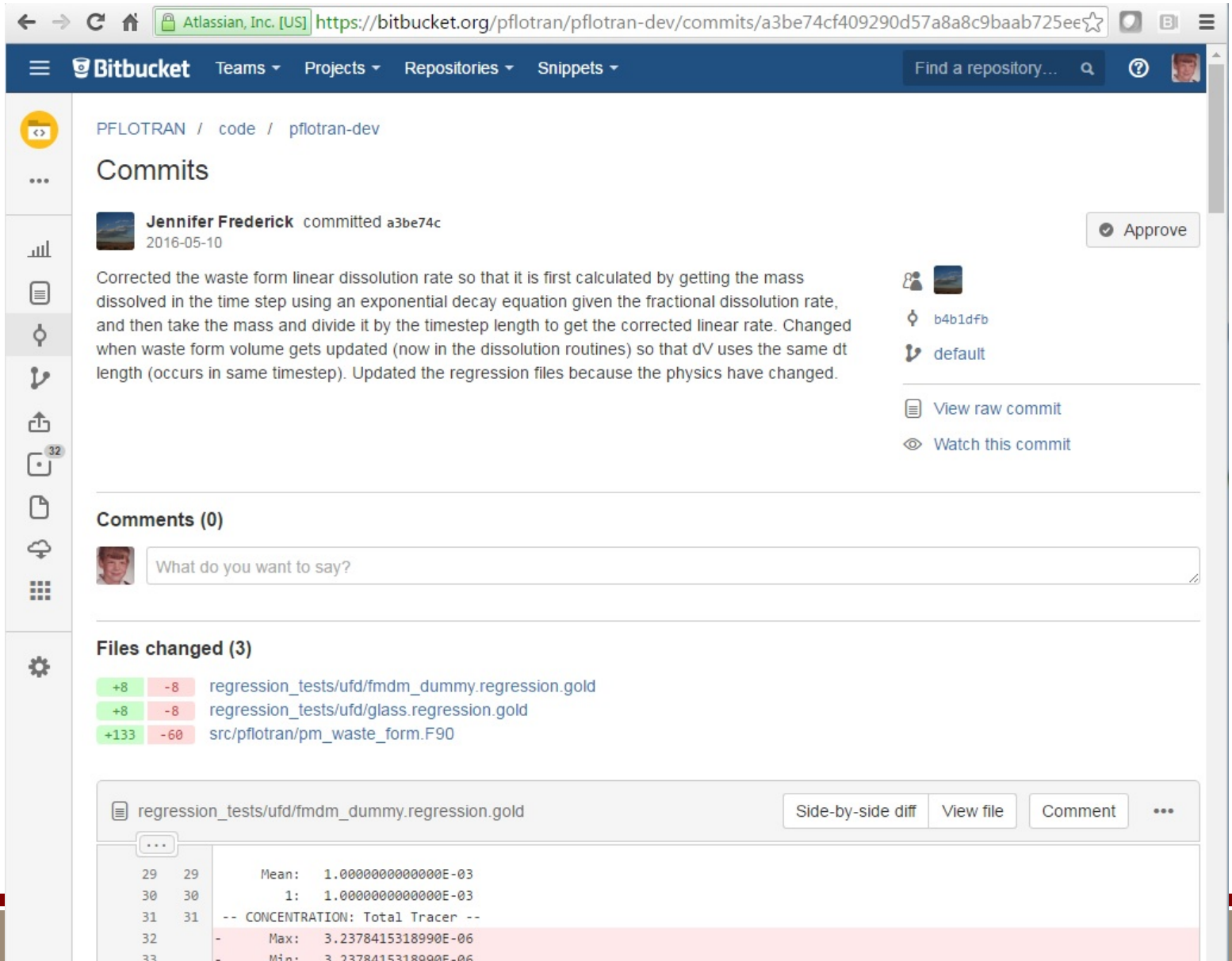

PFLOTRAN Bitbucket Pull Request

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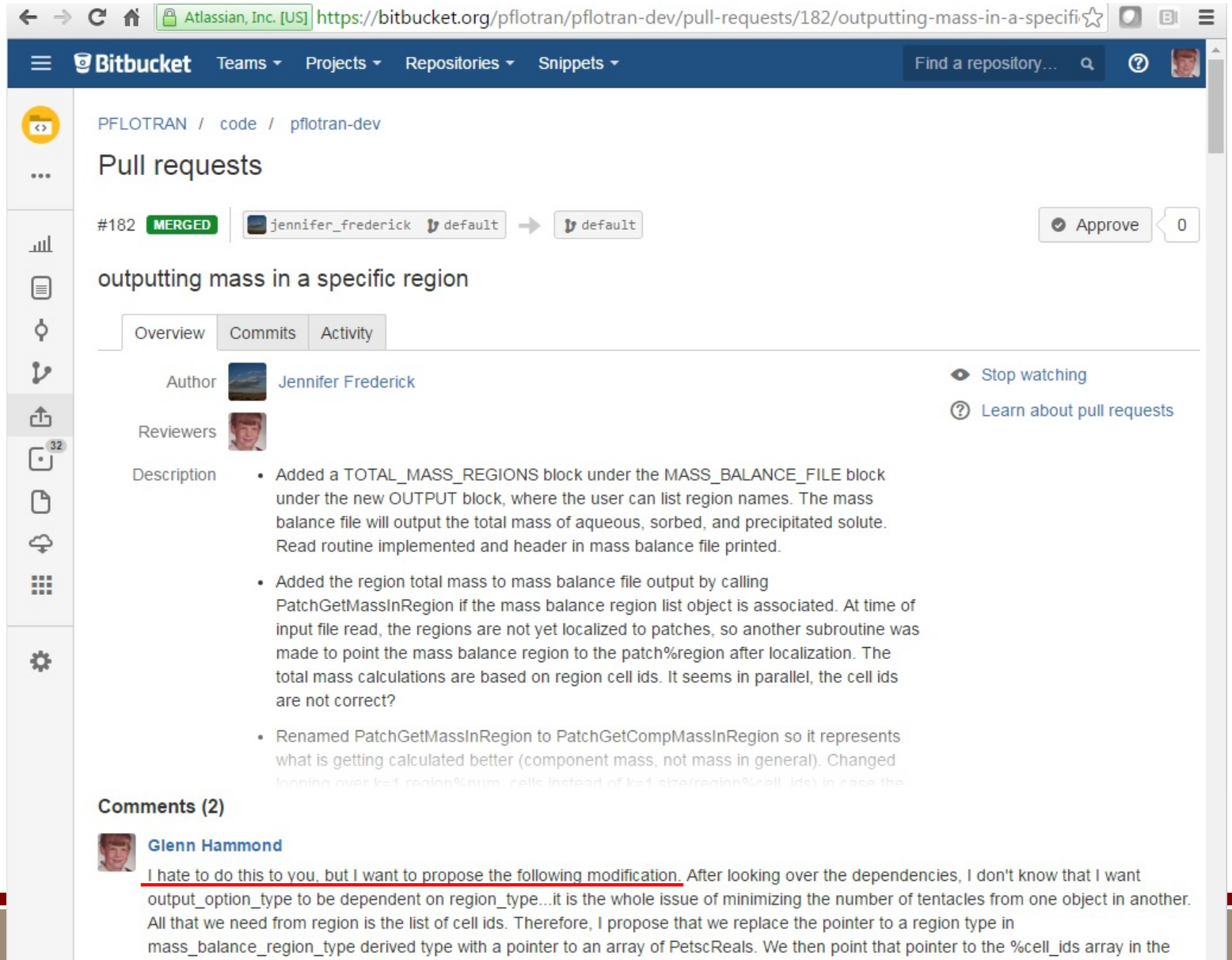
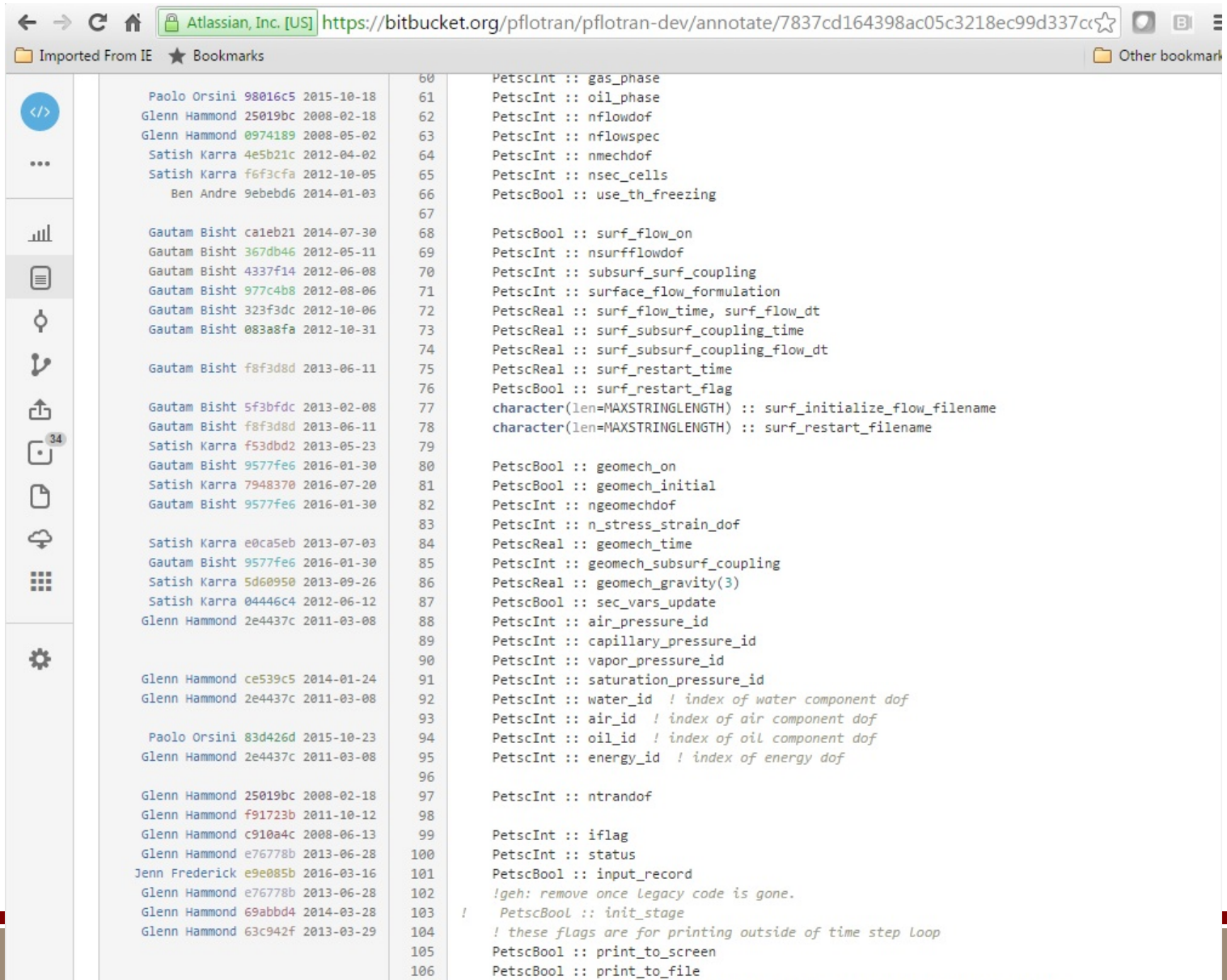
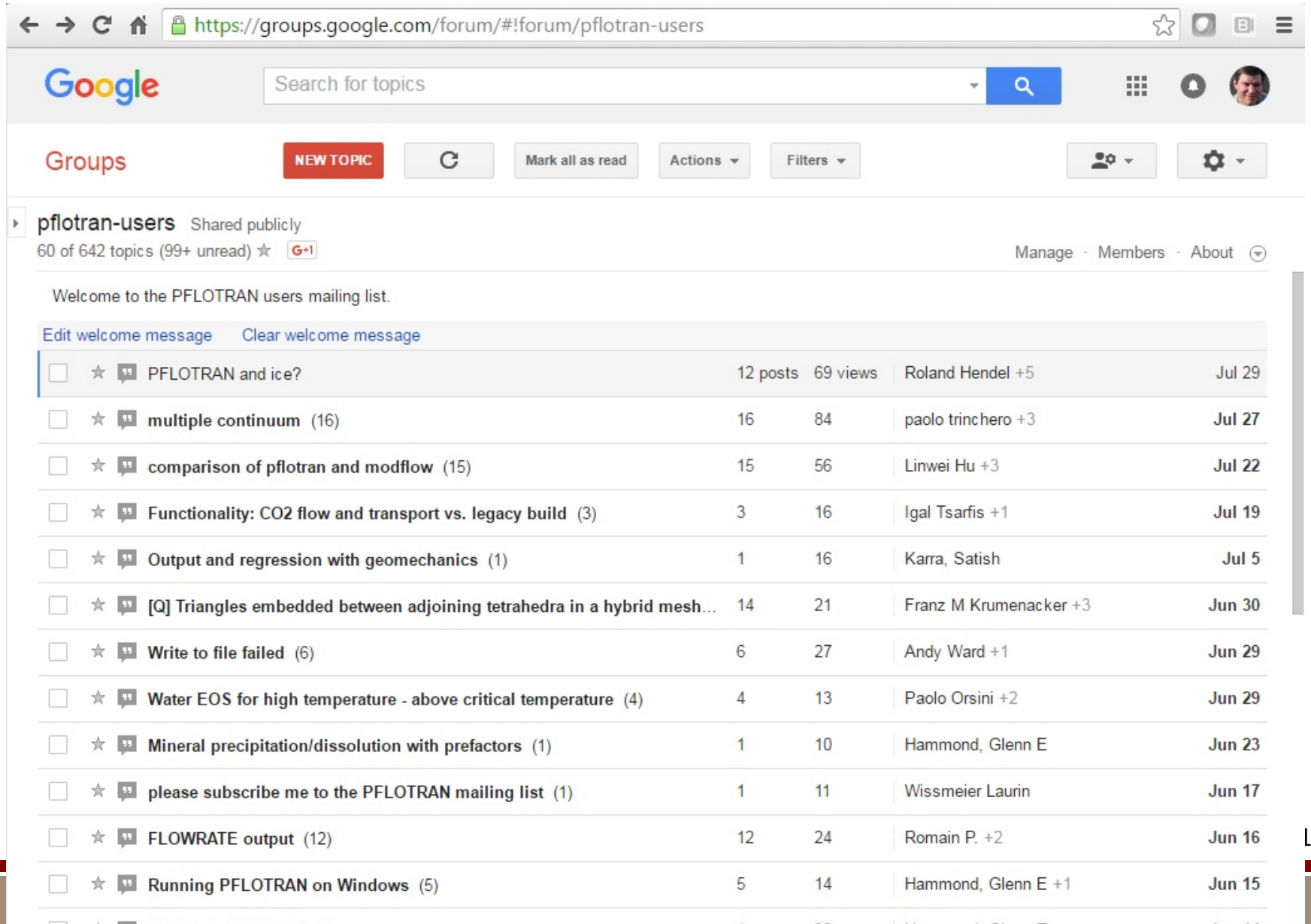


PFLOTRAN Bitbucket Blame



PFLOTRAN User Support



Hits on PFLOTRAN Bitbucket Site in 2015

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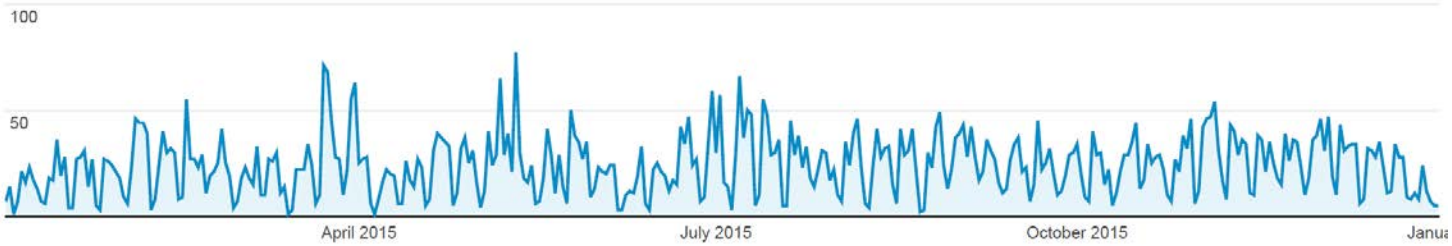
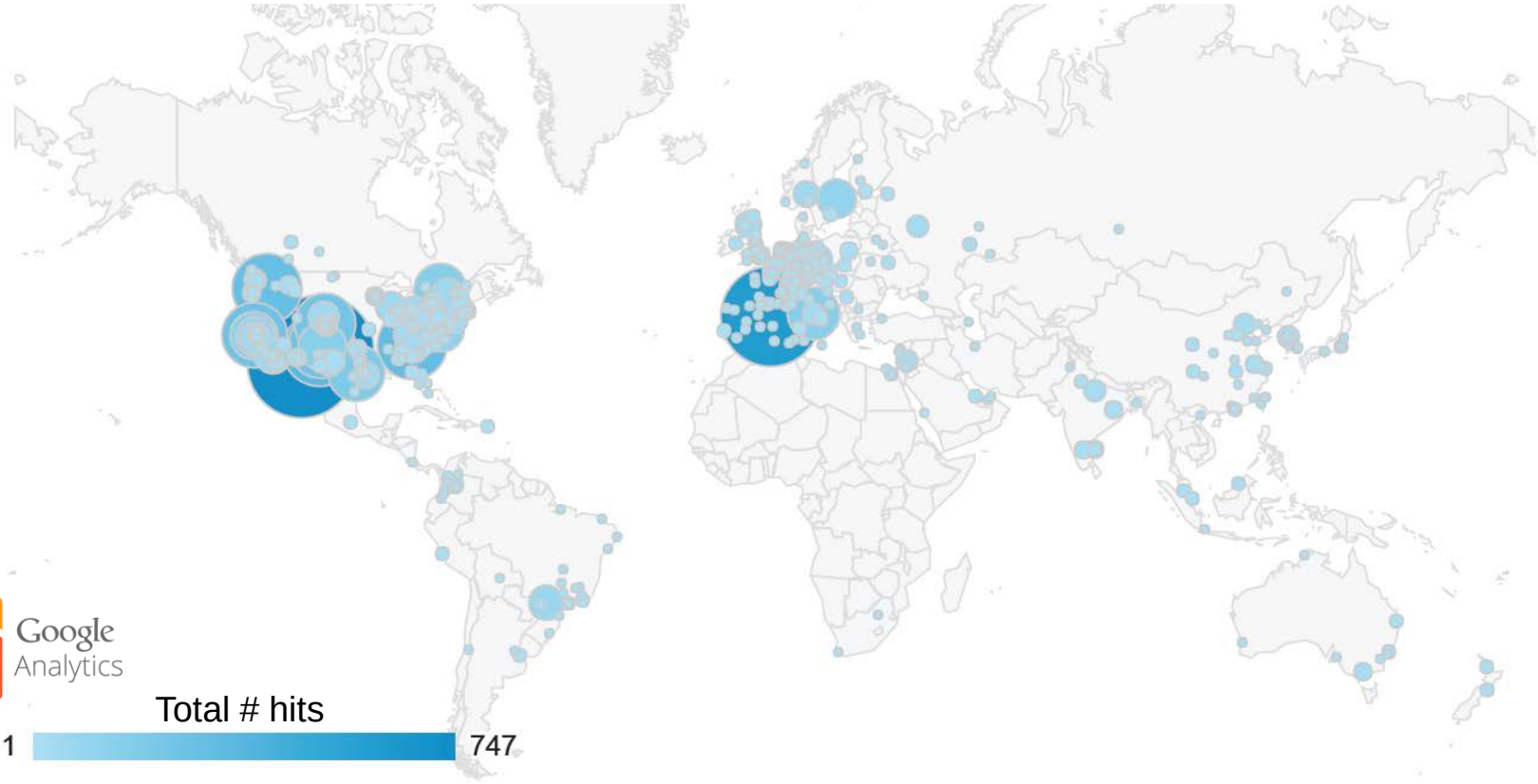
hits per day





Google Analytics

Total # hits

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Hits on PFLOTRAN Bitbucket Site in 2016

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