Used Fuel Disposition Campaign

GDSA Simulation Framework: PFLOTRAN

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PFLOTRAN

- **Petascale reactive multiphase flow and transport code**
- **Open source license (GNU LGPL 2.0)**
- **Object-oriented Fortran 2003/2008**
  - Pointer to procedures
  - Classes (extendable derived types with member procedures)
- **Founded upon well-known (supported) open source libraries**
  - MPI – parallel communication
  - PETSc – parallel data structures/solvers
  - HDF5 – Binary parallel I/O
  - METIS/ParMETIS/CMAKE – unstructured domain decomposition
- **Demonstrated performance**
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom
  - Scales well to over 10K cores

Advantages of Open Source

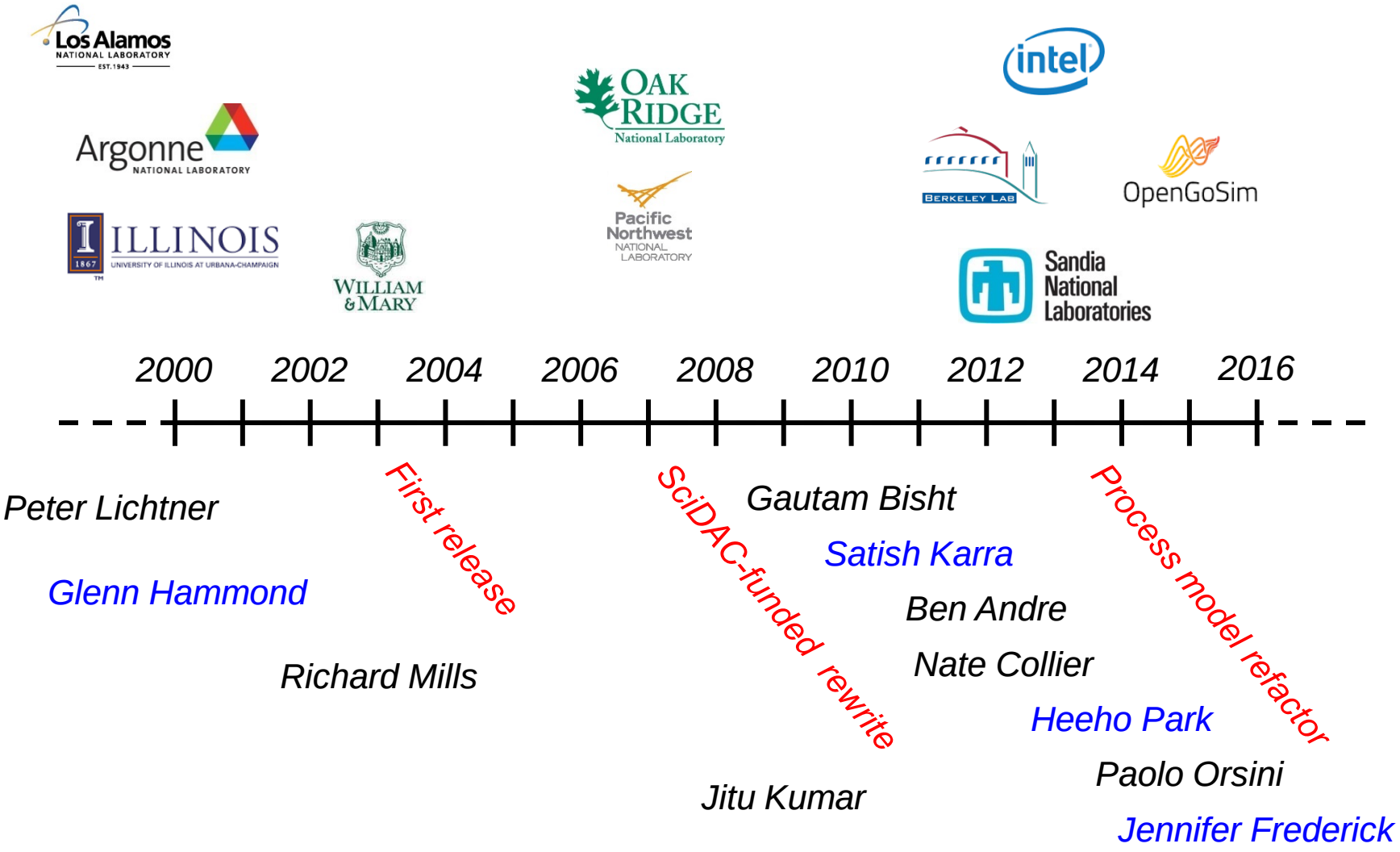
- **Encourages collaboration**
  - Development
  - Testing
  - Debugging
- **Transparency exposes implementation details critical to scientific reproducibility, but excluded by journal publications.**
- **More optimal use of funding**
  - Funding pooled across diverse set of projects/budgets.
  - What would have been spent on licensing fees can be redirected toward development.
  - Infinite benefit to those unfunded
- **The open source community can drive the code to evolve beyond the original vision (evolution).**
- **The most fit codes tend to survive (natural selection)**

Potential Disadvantages of Open Source

- **Potential time sinks**
  - Newbies
  - lookie-loos
- **Care must be taken to avoid exposing the details of unpublished research**
- **One's own capability can be leveraged against oneself by competitors**
  - competing proposals
- **Dissention among the ranks**
  - permanently forked repositories
- **Codes can be licensed as open source, but the source code remains private.**
  - disingenuous licensing

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PFLOTRAN Development Timeline



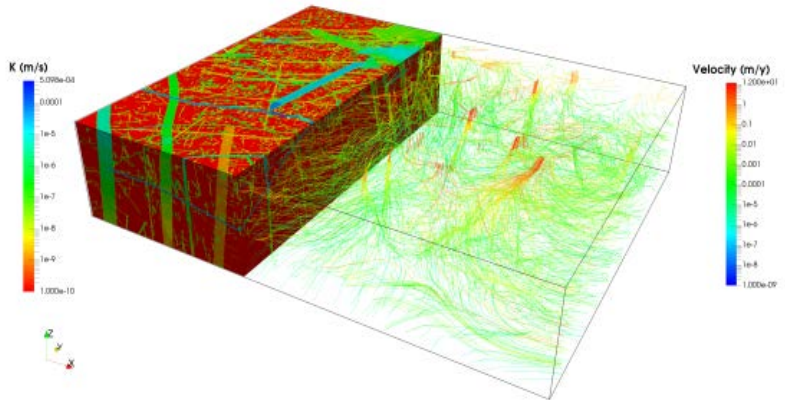
Core PFLOTRAN Capabilities

- **Groundwater Flow**
  - Single phase, variable-saturated
  - Multiphase liquid-gas
  - Extensible constitutive relation and equation of state classes
- **Energy**
  - Thermal convection
  - Thermal conduction
- **Multicomponent Transport**
  - Advection
  - Hydrodynamic dispersion
- **Geomechanics**
  - Elastic deformation
- **Geophysics**
  - Coupling to E4D
- **Biogeochemical Reaction**
  - Aqueous speciation
    - Ion activity models
  - Mineral precipitation-dissolution
  - Sorption
    - Isotherm-based
    - Ion exchange
    - Surface complexation
      - Equilibrium
      - Kinetic / multirate kinetic
  - Microbiological
    - Biomass
    - Inhibition
  - Radioactive decay with daughter products
  - Reaction sandbox

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Application of PFLOTRAN

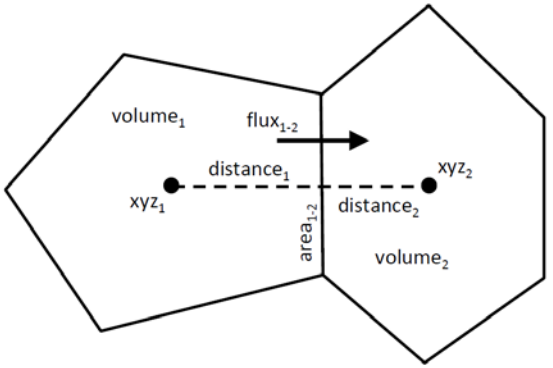
- **Nuclear waste disposal**
  - DOE Used Fuel Disposition Program
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Amphos[21])
- **Climate: coupled overland/groundwater flow; coupled to CLM**
  - DOE Subsurface Biogeochemical Research (SBR) Program (LBNL, PNNL)
  - DOE Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- **Fate and transport of contaminants**
  - U(VI) at Hanford 300 Area
- **CO_2 sequestration**
- **Enhanced geothermal energy**
- **Hydrogeophysics (coupled to E4D)**
  - River water intrusion at Hanford 300 Area
- **Radioisotope tracers**



Molinero et al., Amphos[21], 2015

PFLOTRAN Numerical Methods

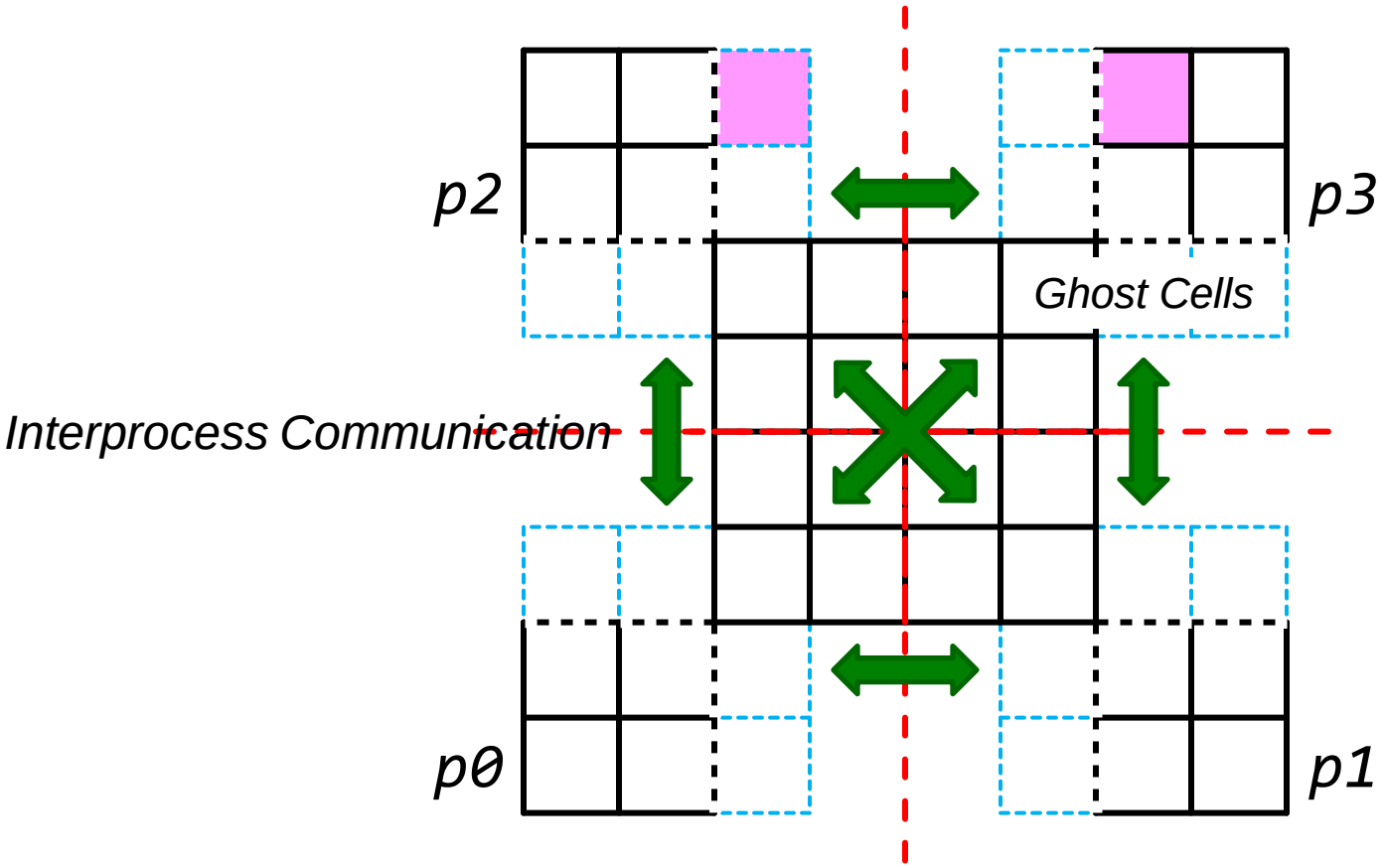
- **Spatial discretization**
  - Finite volume (default 2-point flux)
  - Finite element (geomechanics, geophysics)
  - Structured and unstructured grids
- **Time discretization**
  - Unconditionally stable backward Euler
  - Time step governors
- **Nonlinear solver**
  - Newton-Raphson
  - Custom convergence criteria
- **Linear solver**
  - Direct (LU)
  - Iterative Krylov (default BiCGStab)



PETSc

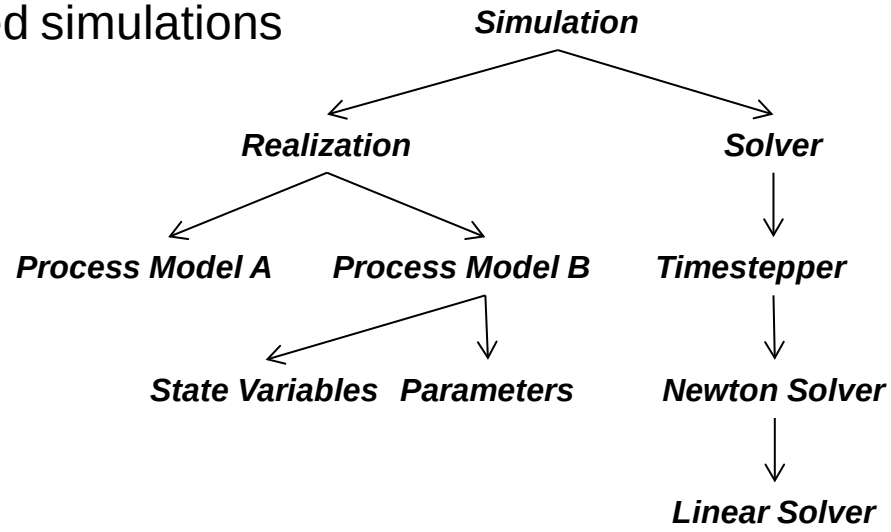
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PFLOTRAN Approach to Parallelization: Domain Decomposition



Why Object-Oriented Fortran 2003/2008?

- **Why Fortran?**
  - Experienced domain scientists remain engaged
  - Commonality among all domain scientists
- **Why object-oriented?**
  - Modular data structures
    - *Eases code development and debugging – data locality*
    - *Nesting of processes and data*
  - Tree structure enables self-contained simulations
- **Why Fortran 2003/2008?**
  - Classes (extendable derived types)
    - *Member functions*
    - *Inheritance*
  - Pointers to procedures
    - *E.g. swapping equations of state*



Object-Oriented Fortran

Fortran 77

```
subroutine X(a,b,c,d,e,f,…)

...

common/array/a(ncomp,ncell)



do icell = 1, ncell
  do icomp = 1, ncomp
    a(icomp,icell) = …
  enddo
enddo
```

OO Fortran 90

```
subroutine X(realization)

...

grid => realization%patch%grid
reaction => realization%reaction
cells => realization%patch…%cells

do icell = 1, grid%ncell
  do icomp = 1, reaction%ncomp
    cells(icell)%conc(icomp) = …
  enddo
enddo
```

Modern Fortran

Fortran 90

```
select case(eos_type)
  case(WATER)
    call EvaluateWater(p,t)
  case(AIR)
    call EvaluateAir(p,t)
  case(CO2)
    call EvaluateCO2(p,t)
  case(CH4)
    call EvaluateCH4(p,t)
end select
```

Fortran 2003/2008

```
type, extends(eos_base) :: eos_CO2
  …
contains
  procedure :: Evaluate => EvaluateCO2
end type eos_CO2

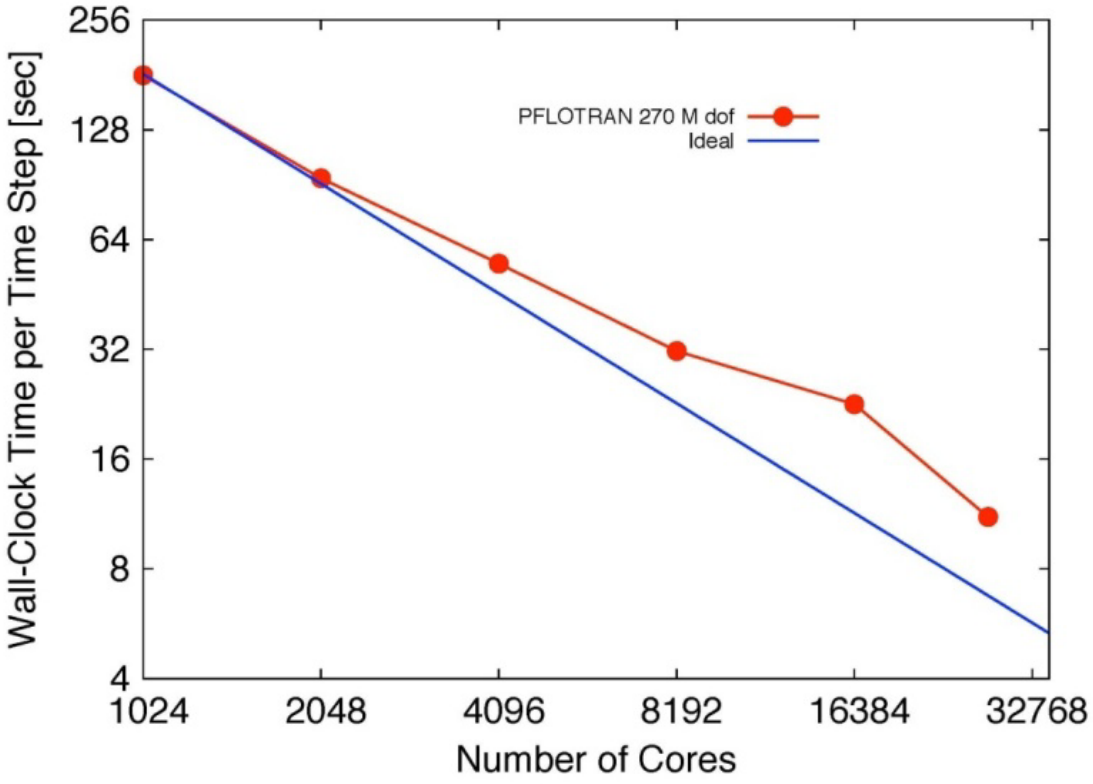
class(eos_CO2) :: eos

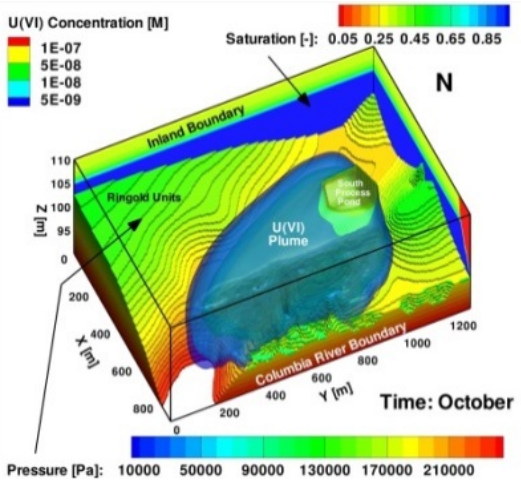
call eos%Evaluate(p,t)
```

eos = equation of state

PFLOTRAN's Parallel Performance

High performance computing (HPC) enables larger simulations run in less time

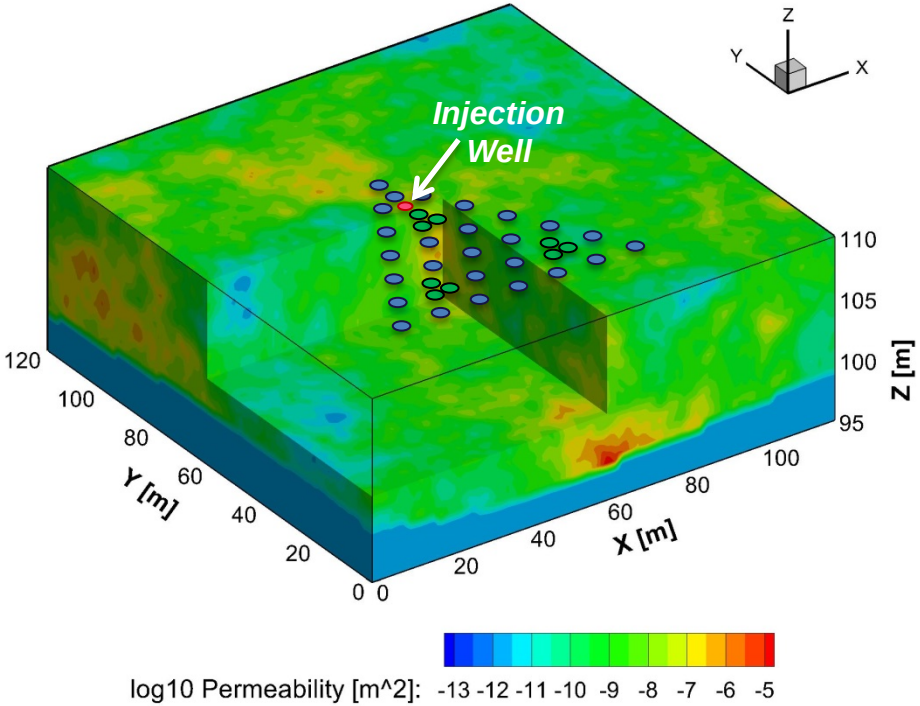


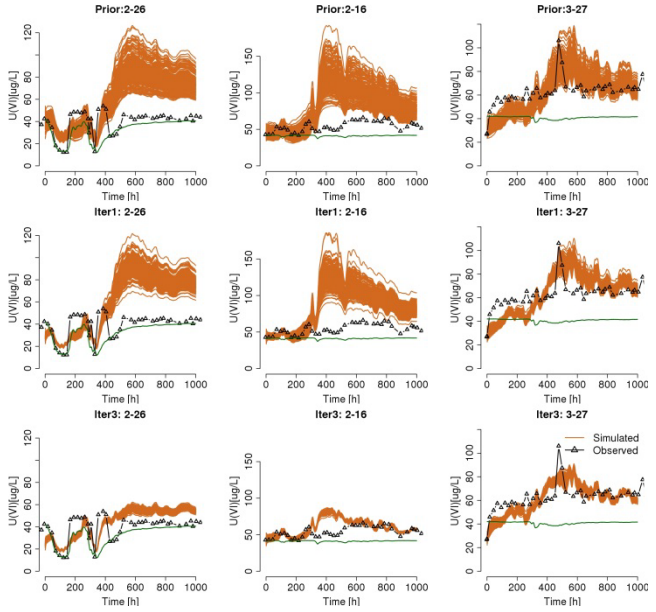


Hammond and Lichtner, WRR, 2010

HPC Empowers Scientific Discovery

Bayesian data assimilation with ensemble Kalman filters at the Hanford 300 Area Integrated Field Research Challenge site





Xingyuan Chen, PNNL



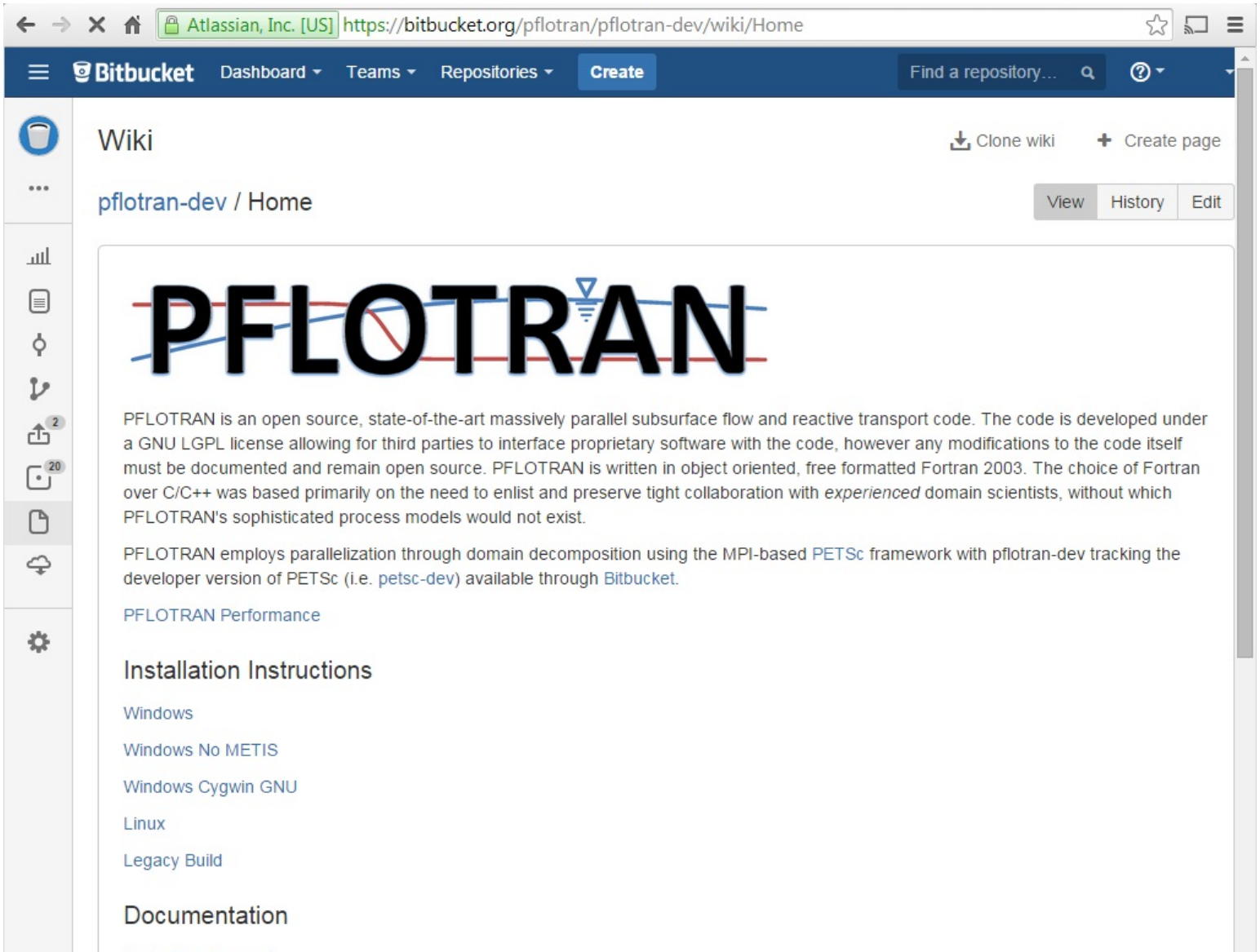
64,000 processes
500 realizations
~1 hour runtime

>7 years to run on desktop

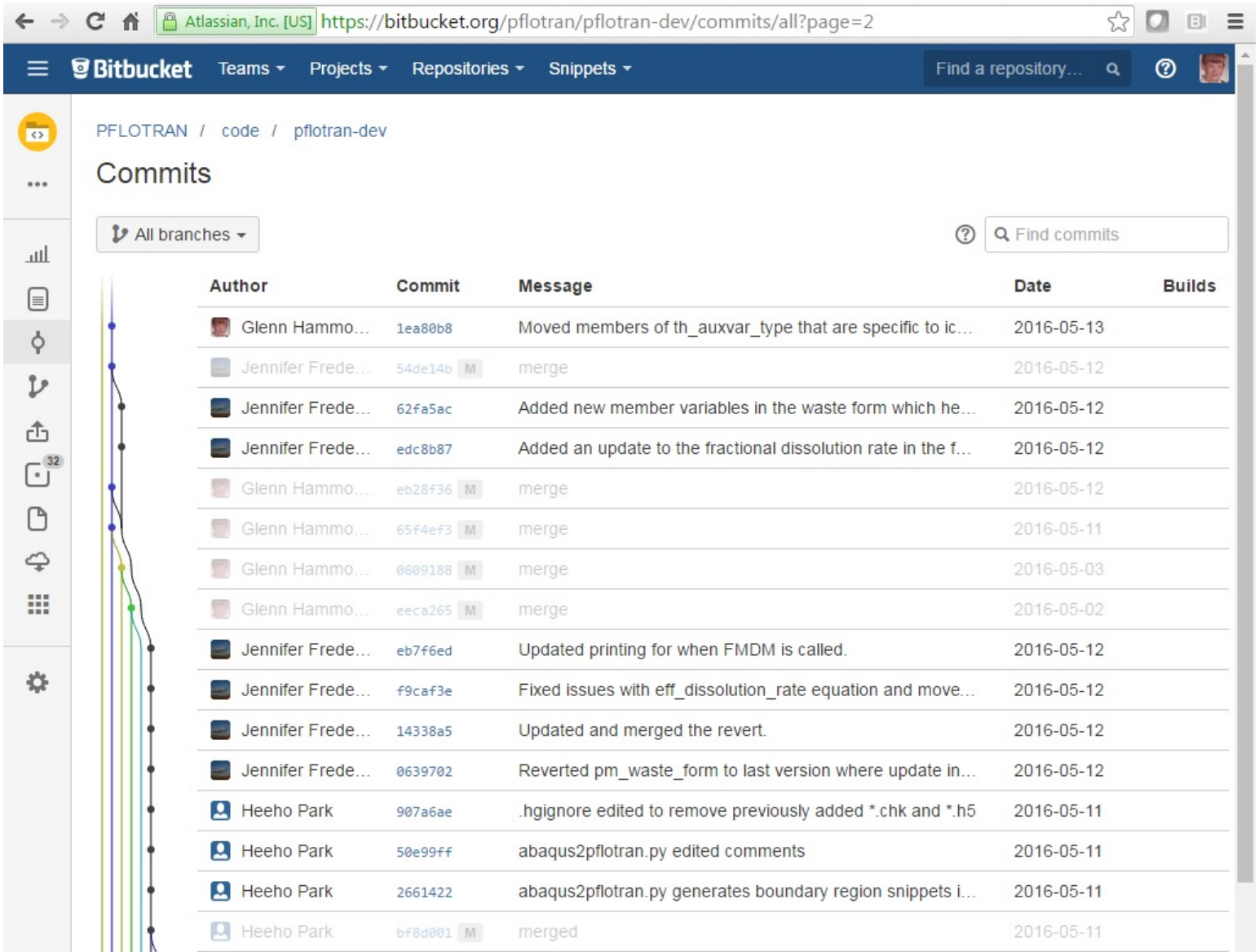
PFLOTRAN Support Infrastructure

- **Mercurial: distributed source control management tool**
- **Bitbucket: online PFLOTRAN repository**
  - hg clone https://bitbucket.org/pflotran/pflotran-dev
  - Source tree
  - Commit logs
  - Wiki
    - *Installation instructions*
    - *Quick guide*
    - *FAQ (entries motivated by questions on mailing list)*
  - Pull requests
  - Issue tracker
- **Buildbot: automated building and testing (regression and unit)**
- **Google Groups: pflotran-users and pflotran-dev mailing lists**
- **Google Analytics: tracks behavior on Bitbucket**

PFLOTRAN Bitbucket Site

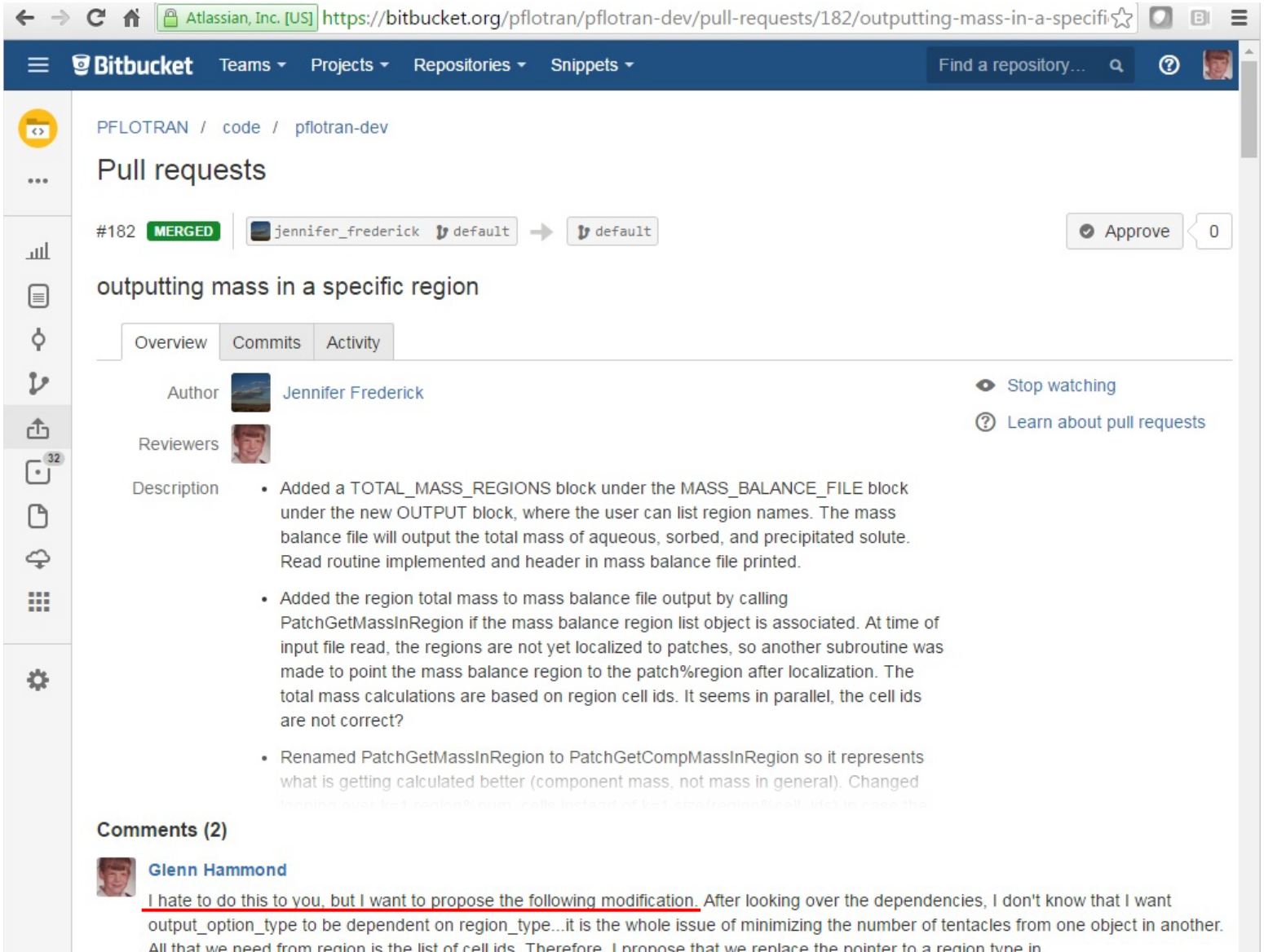


PFLOTRAN Bitbucket Commit Log



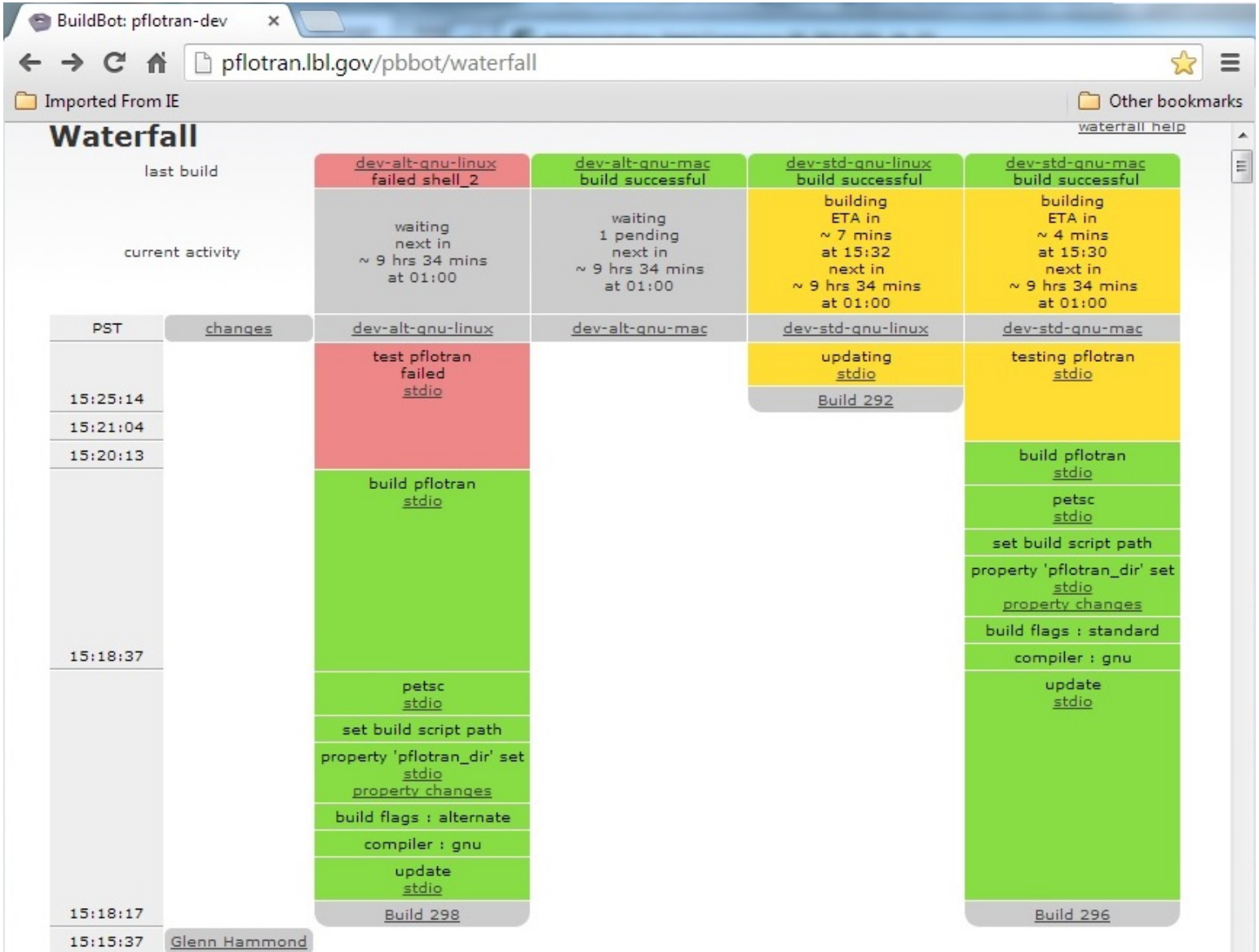
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PFLOTRAN Bitbucket Pull Request



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PFLOTRAN Buildbot



Hits on PFLOTRAN Bitbucket Site in 2015

