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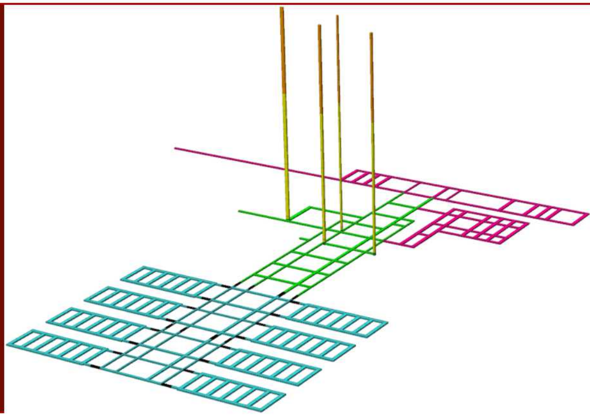

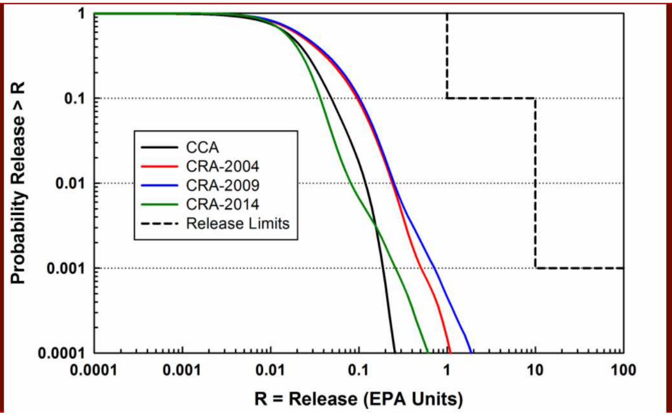

PFLOTRAN Code Development for Waste Isolation Pilot Plant Performance Assessment

James Bethune

8800 Energy and Earth Systems Symposium 2019

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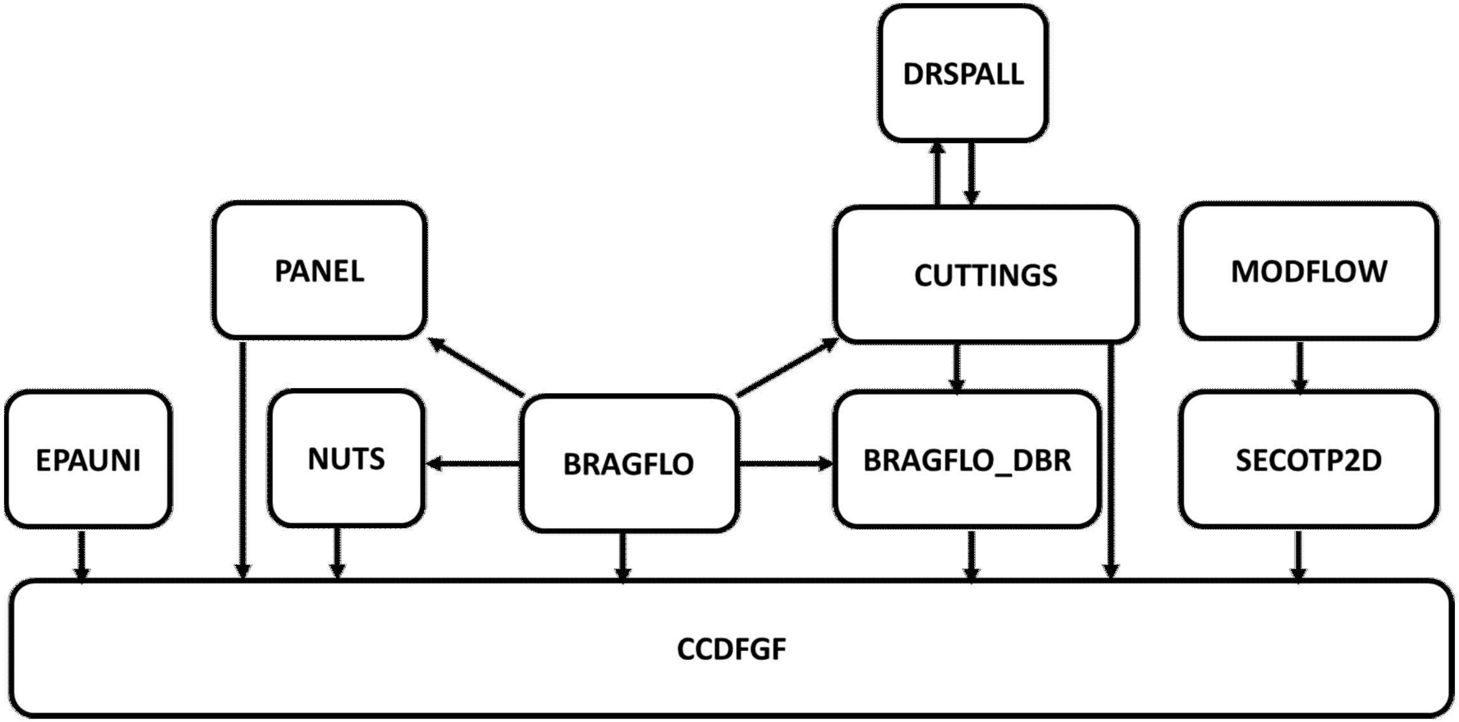
Outline

- Motivation for Considering a New PA Code
  - Current Representation of WIPP Repository in WIPP PA
  - Challenges of potential repository layout changes
- PFLOTRAN—What is it?
- PFLOTRAN Development for WIPP PA
  - Long-term integration plan
  - Code replacements
  - Code testing
- Summary

WIPP Performance Assessment

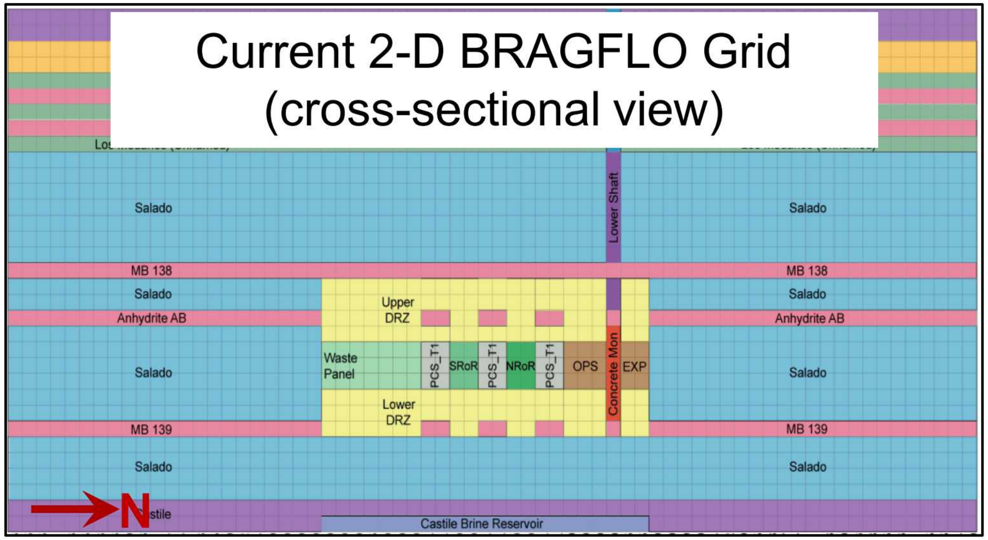
Performance Assessment:

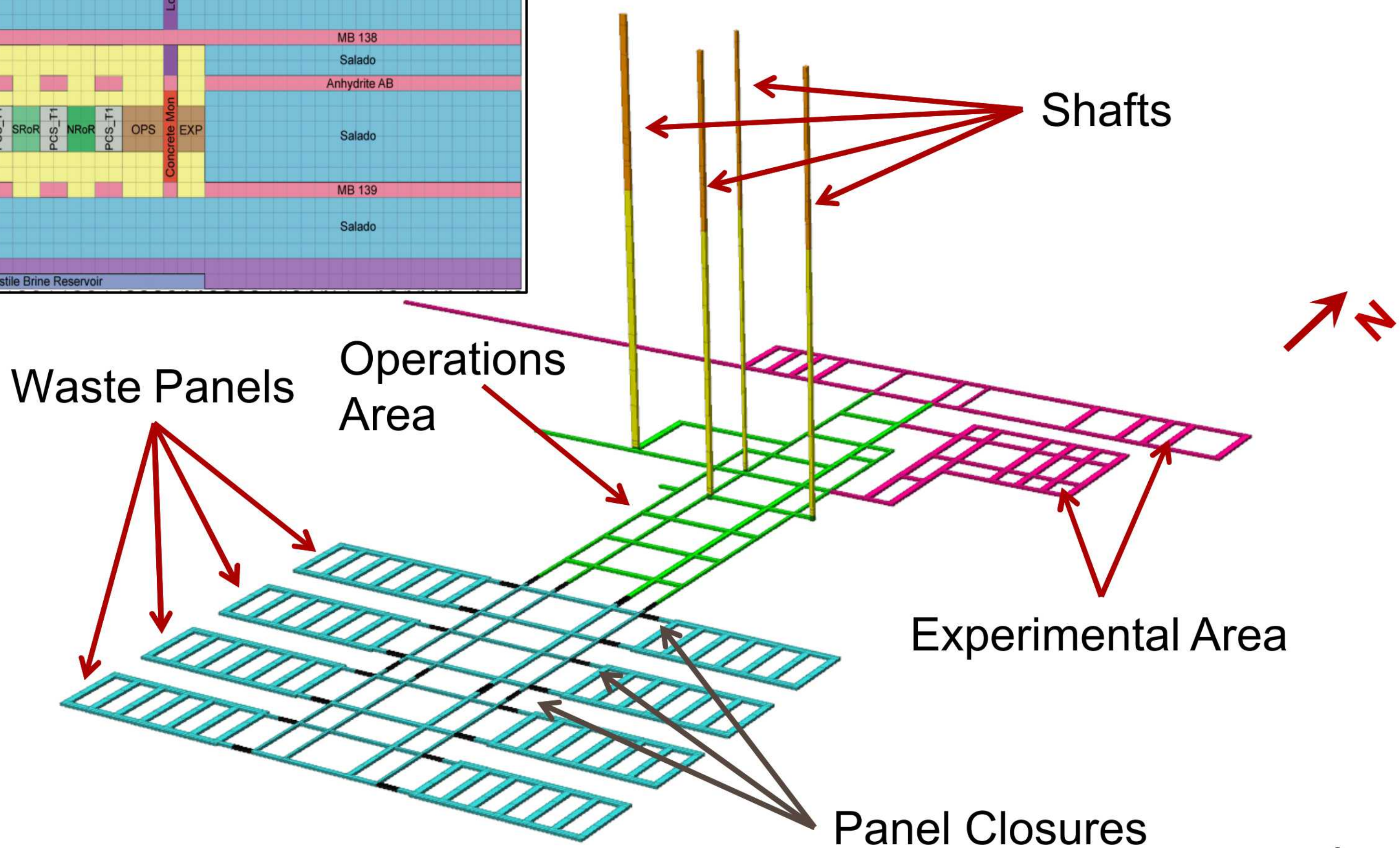
- considers 245 Features, Events, and Processes
- covers 24 peer-reviewed conceptual models
- includes 10 principal codes and many utility codes



Current generalized code map and run control configuration

Motivation for a New Code

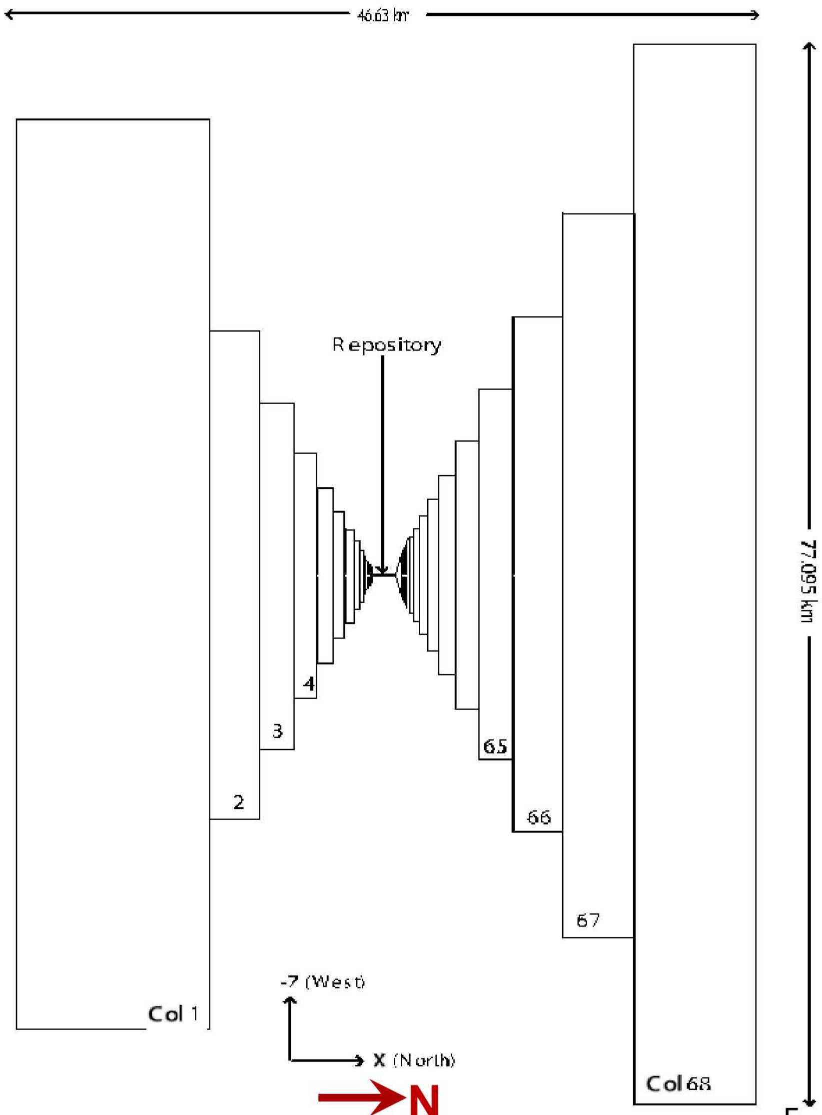




Motivation for a New Code

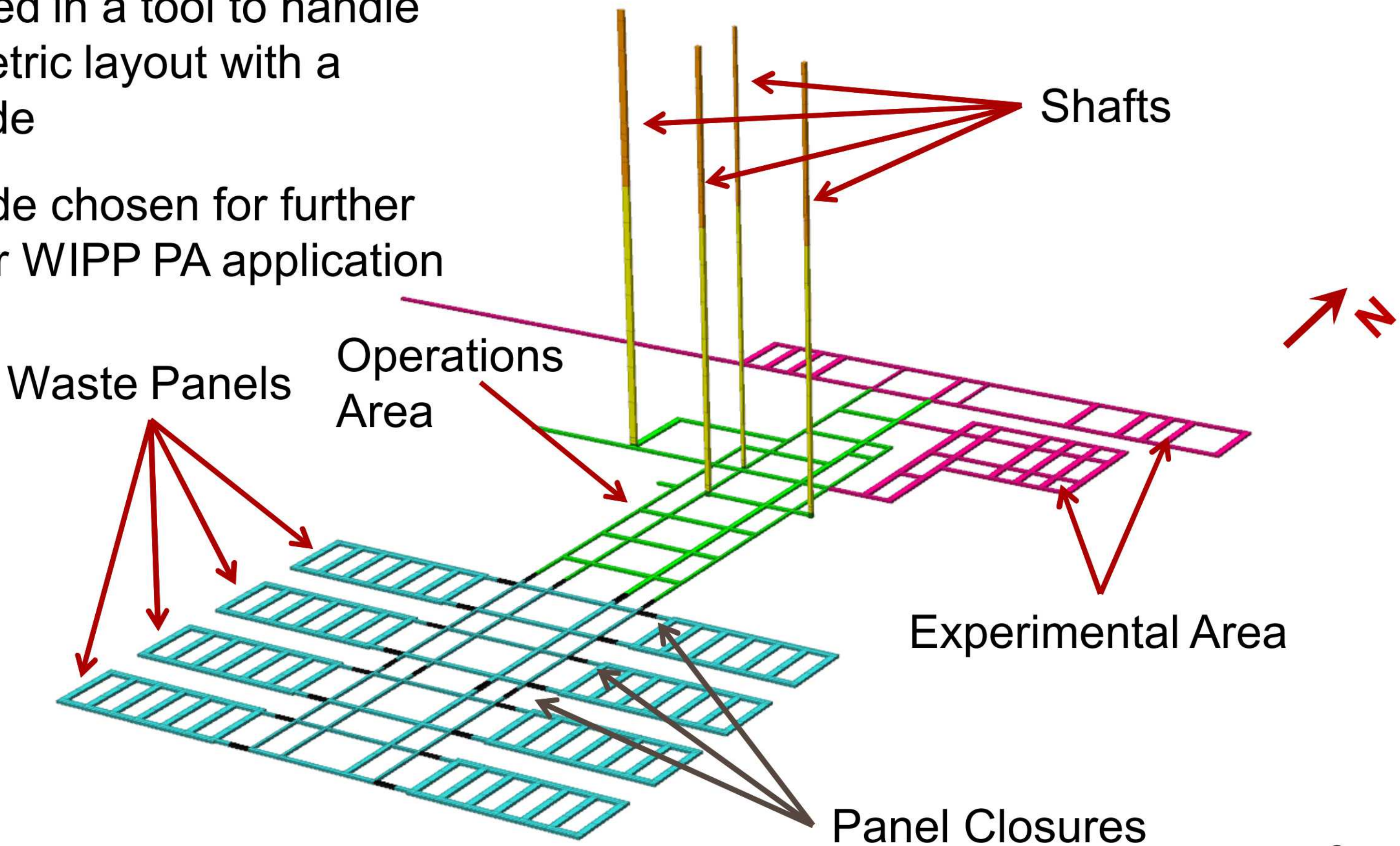
Current 2-D "Flared" Grid (plan view)

- One cell in width
- Width of each cell varies
- Approved for use in Compliance Certification Application (CCA)
- Shown to give similar results to a 3-D representation using BRAGFLO
- Radial concentric flow
  - No lateral flow
- Relies on (approximately) symmetric repository layout



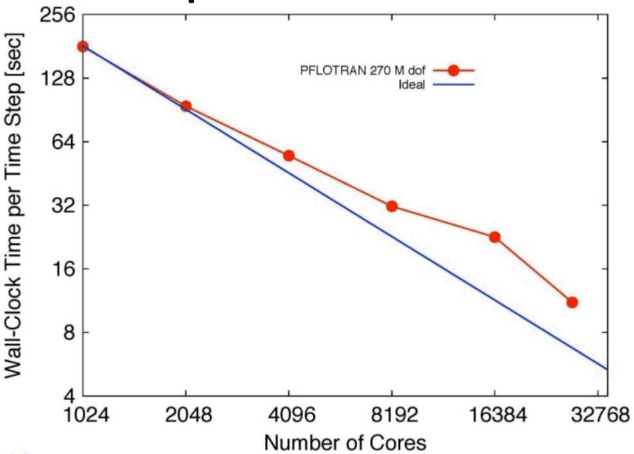
Motivation for a New Code

- Potential for additional waste panels challenges the radial concentric flow assumption
- DOE is interested in a tool to handle a more asymmetric layout with a modern 3-D code
- PFLOTRAN code chosen for further development for WIPP PA application



PFLOTRAN

- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)

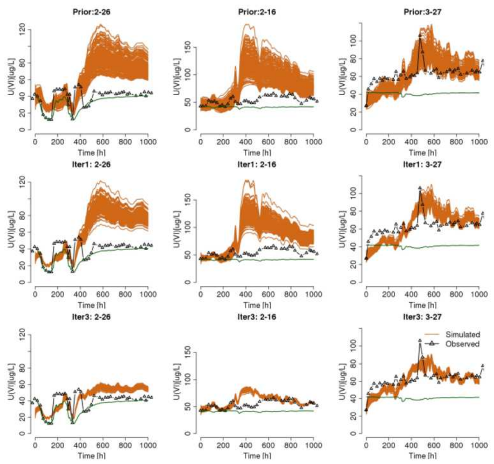


- Founded upon well-known (supported) open source libraries
  - MPI, PETSc, HDF5, METIS/ParMETIS/CMAKE
- Demonstrated performance
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom
  - Scales well to over 10K cores

PFLOTRAN Computing Capability

- High-Performance Computing (HPC)
  - Increasingly mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- Open Source Collaboration
  - Leverages a diverse scientific community
  - Sharing among subject matter experts and stakeholders from labs/universities
- Modern Fortran (2003/2008)
  - Domain scientists remain engaged
  - Modular framework for customization
- Leverages Existing Capabilities
  - Meshing, visualization, HPC solvers, etc.
  - Configuration management, testing, and QA

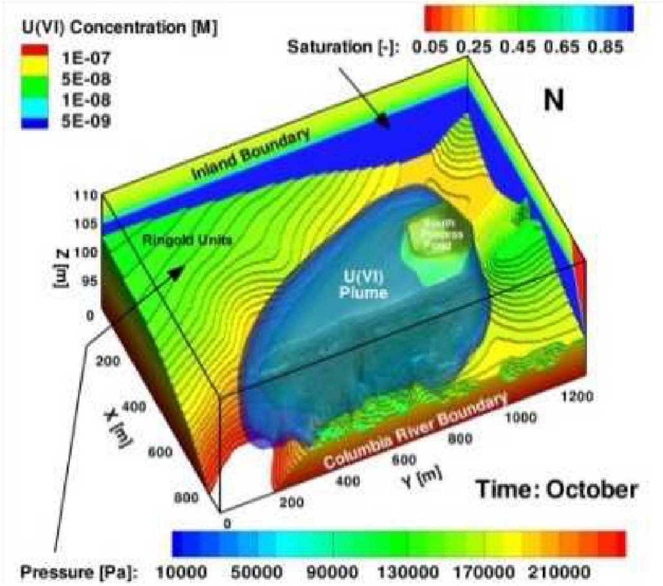
Data Assimilation



Xingyuan Chen, PNNL, 2011

Application of PFLOTRAN

- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - US DOE NE Spent Fuel and Waste Science and Technology (SFWST)
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos[21])
- Climate: coupled overland/groundwater flow; CLM
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- Biogeochemical transport modeling
  - U(VI) fate and transport at Hanford 300 Area
  - Hyporheic zone biogeochemical cycling
    - Columbia River, WA, USA
    - East River, CO, USA
- Oil & Gas (OpenGoSim.com)
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers

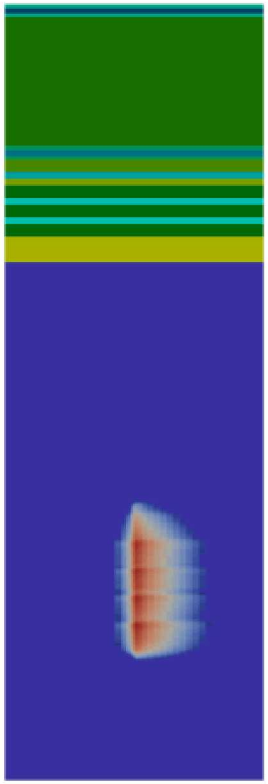


Hammond and Lichtner, WRR, 2010

Discretization and Numerical Methods

- Spatial discretization
  - Finite volume (2-point flux default)
  - Structured and unstructured grids
- Time discretization: fully-implicit backward Euler
- Nonlinear solver
  - Newton-Raphson
  - Line search/damping with custom convergence criteria
- Linear solver: direct (LU) or iterative (BiCGStab)
- Multi-physics coupling
  - Flow and transport/reaction: sequential
  - Transport and reaction: global implicit
  - Geomechanics and flow/transport: sequential
  - Geophysics and flow/transport: sequential

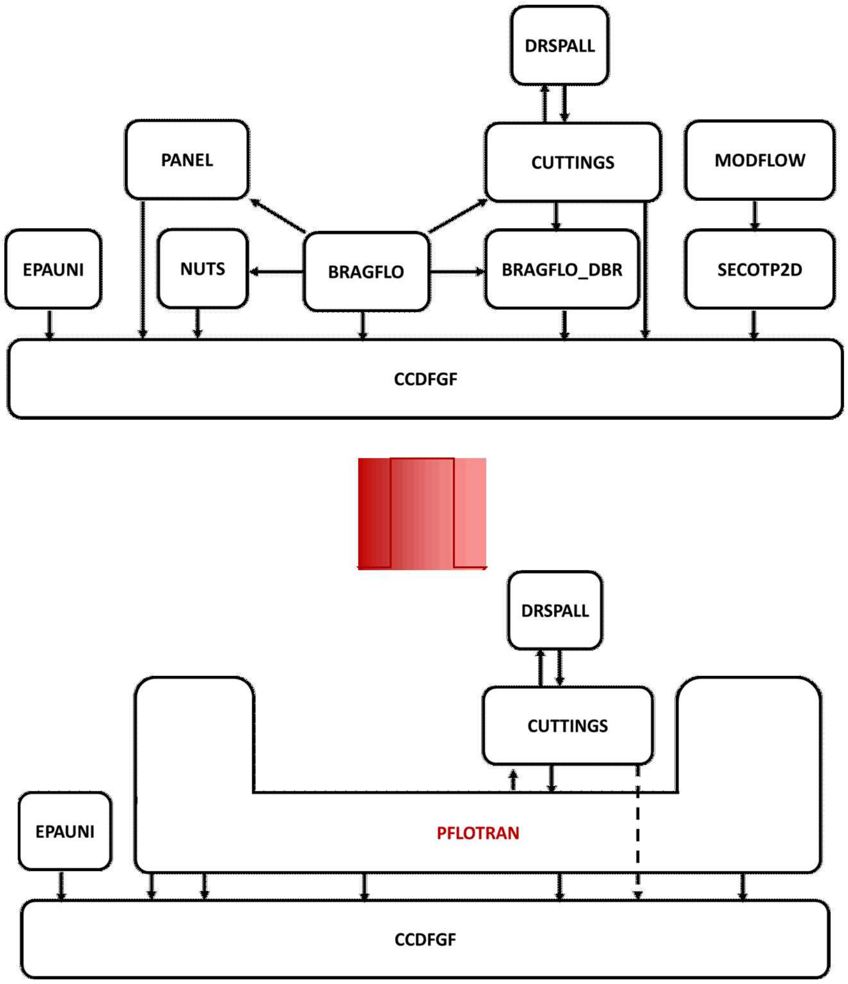
Deep Borehole Waste Disposal



Emily Stein, SNL, 2015

Long-term Approach to Integration

- Process model implementation
- Comparison of PFLOTRAN against BRAGFLO/NUTS for 2-D flared grid
  - Validates flow and transport
- Comparison of PFLOTRAN w/3-D representation against 2-D flared grid
  - Quantifies impact of 2-D→3-D
- Development of 3-D conceptualization
  - Grid resolution
  - Run-time
- Formal reviews
  - QA review
    - Formal testing
    - Code documentation
  - Peer review
  - EPA review

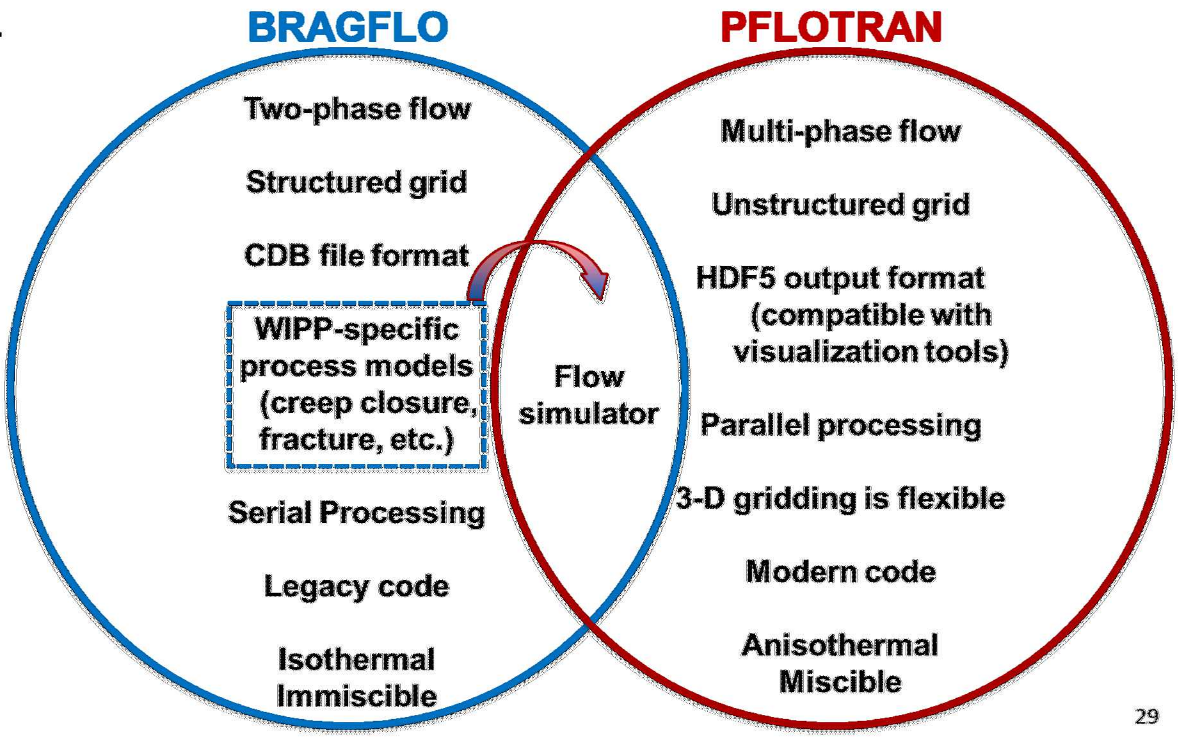


Generalized code map and run control configuration

Process Model Implementation

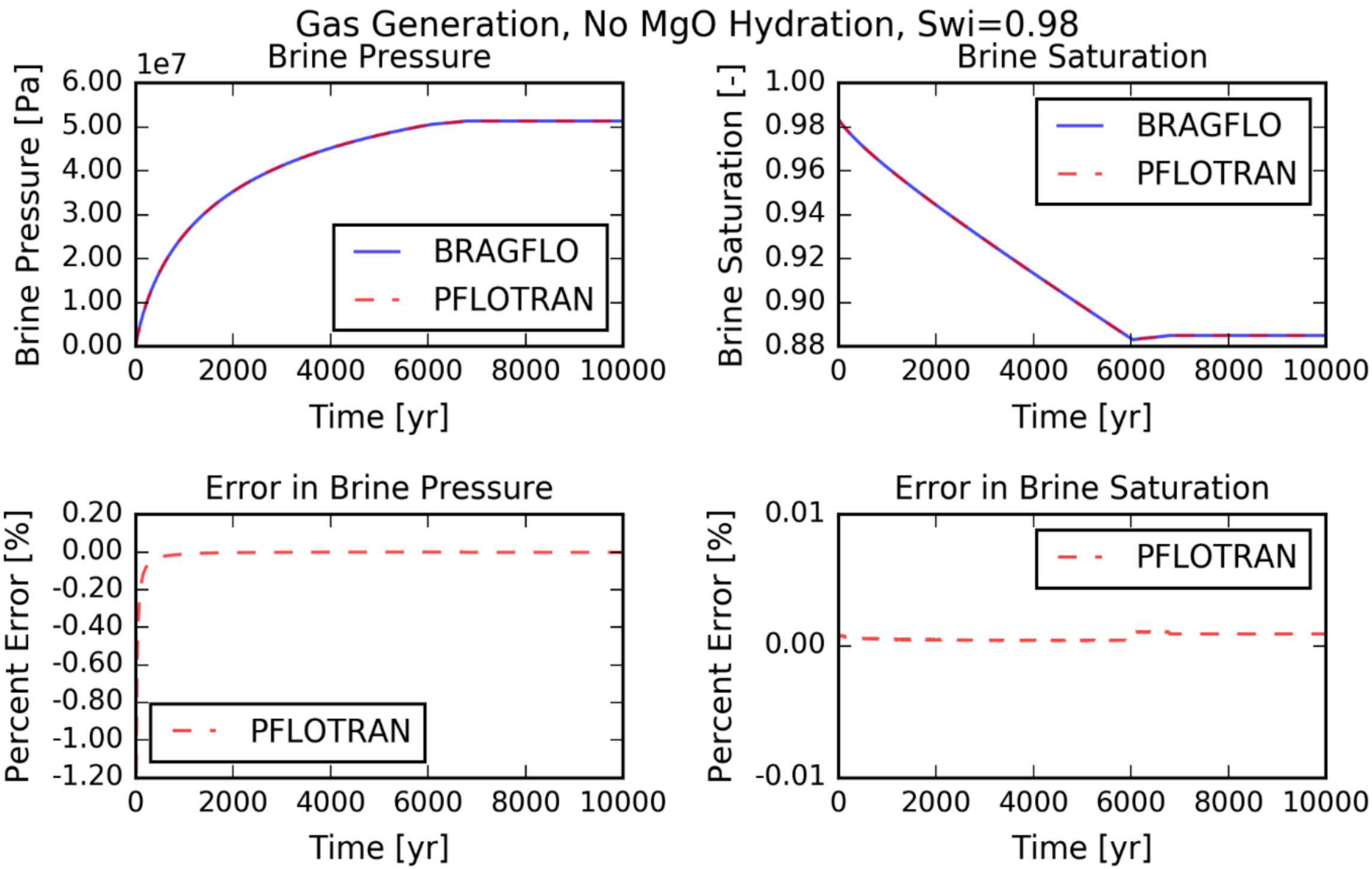
- Code development
  - Transport appears straight-forward
  - Flow has required more work
  - Transition to 3-D is still largely unknown

- Validation/Verification
  - Against BRAGFLO, NUTS, analytical solutions
  - Single-cell
  - Multi-cell
  - 2-D flared grid



Process Model Implementation

- Example test for gas generation



BJ1

Process Model Implementation

- WIPP-specific BRAGFLO capabilities
  - Characteristic curves: capillary pressure, relative permeability
  - Creep closure: porosity
  - Fracture processes: permeability, porosity
  - $H_{2(g)}$ generation: gas source
  - Klinkenberg effect: gas permeability
  - Soil compressibility: porosity
  - Redlich-Kwong-Soave equation of state: gas density
  - Modification of material properties at select points in time
- Tested using existing BRAGFLO tests plus additional tests

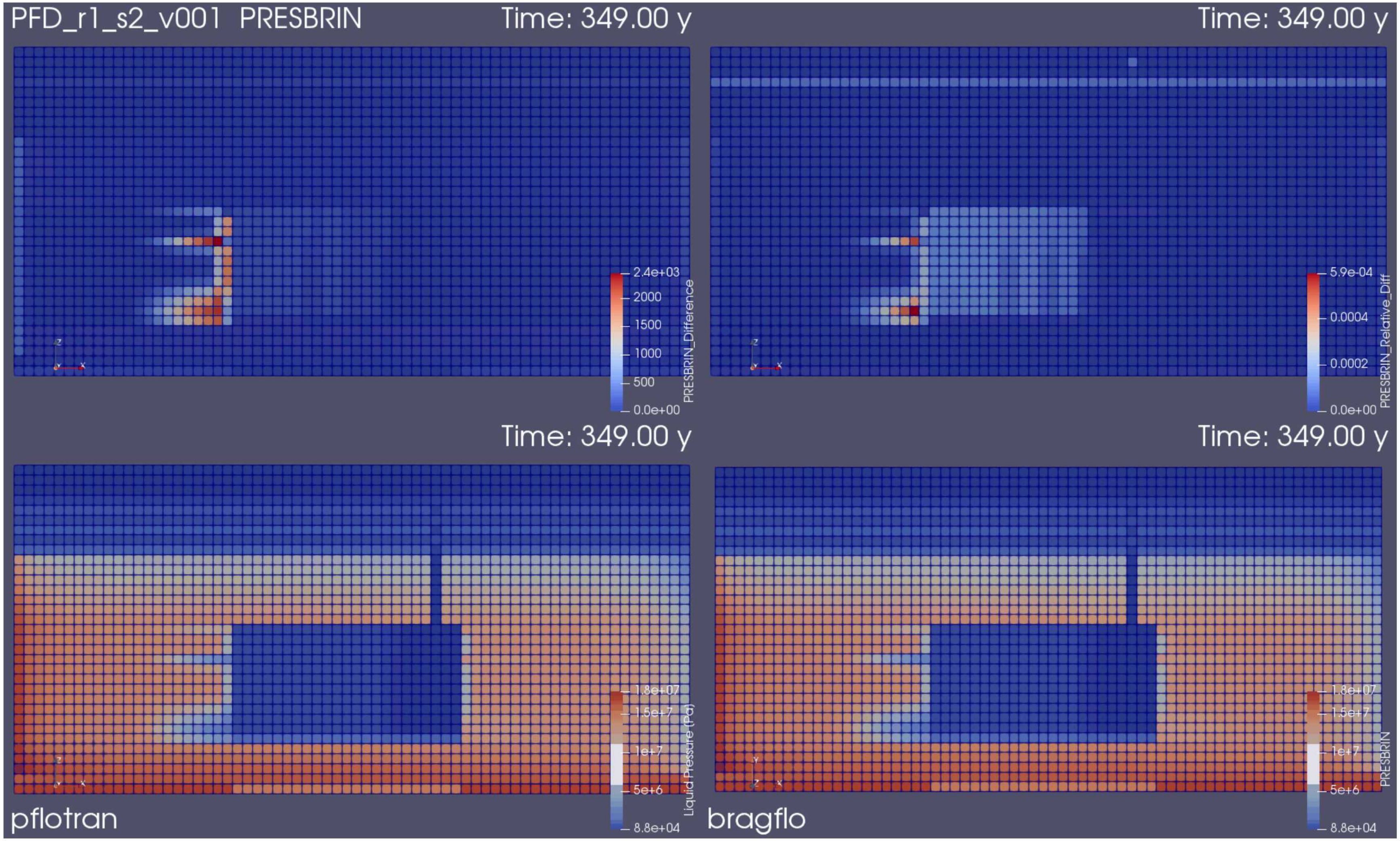
Slide 14

BJ1 Might remove this slide

Bethune, James, 9/13/2018

2-D Flared Grid Comparison

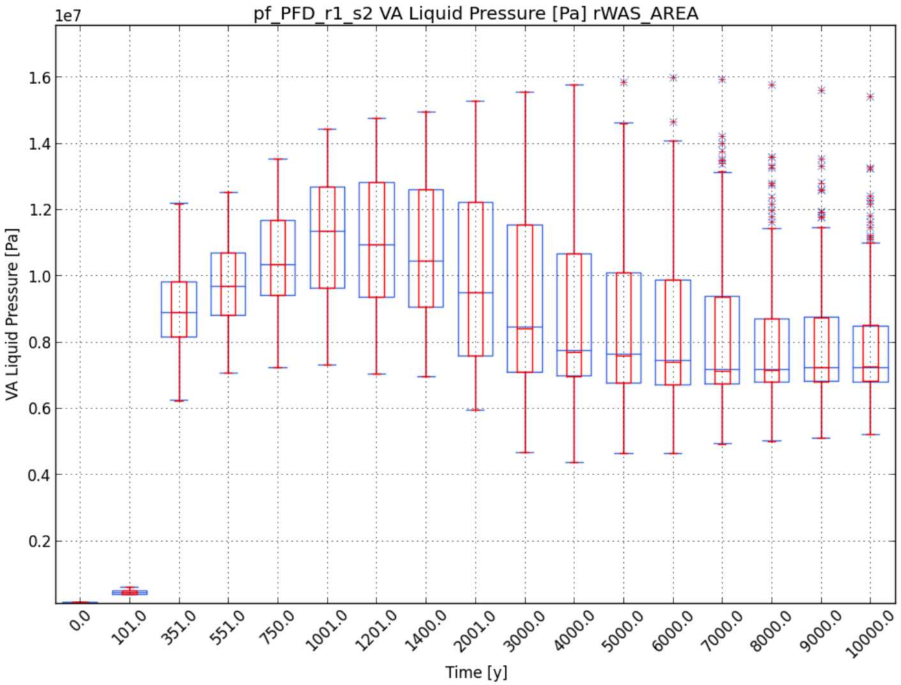
- Replicate 1, Scenario 2, vector 1



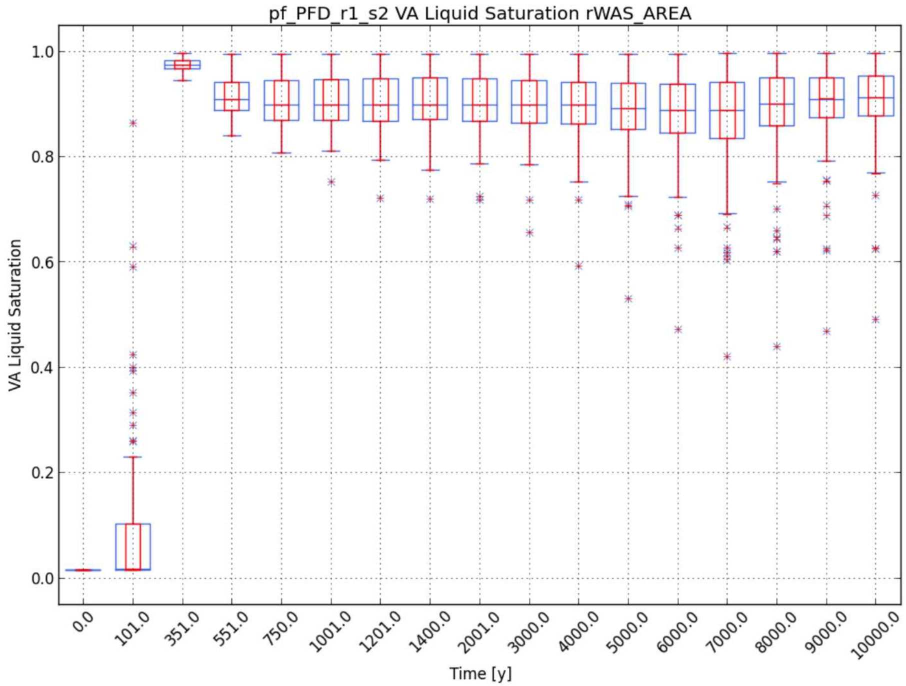
2-D Flared Grid Comparison

- Replicate 1, Scenario 2, all vectors, Waste Area

Liquid Pressure (Pa)



Liquid Saturation (--)



Summary

- SNL is further developing the existing PFLOTRAN code for application to WIPP PA
  - Potential repository layout changes require 3-D representation

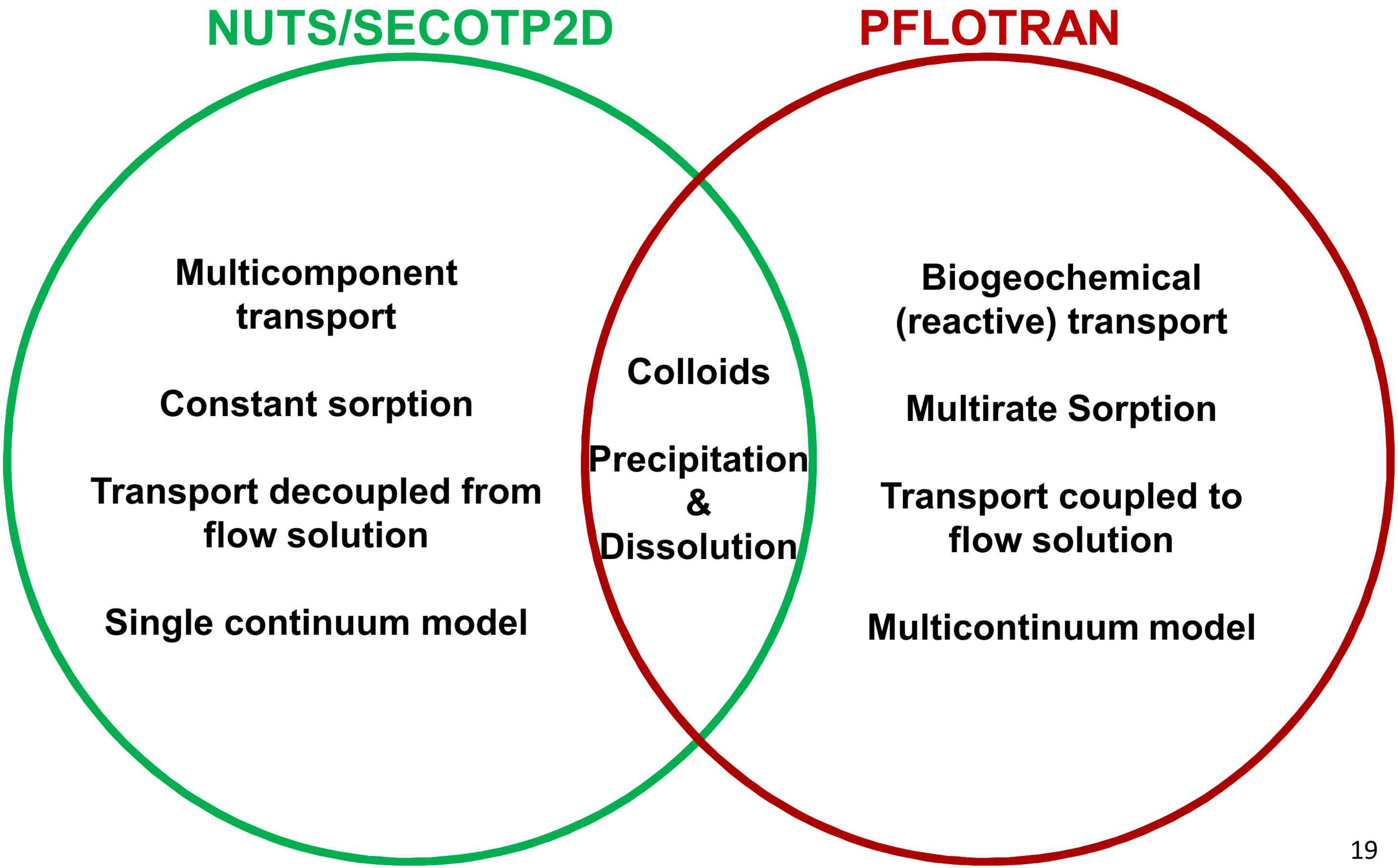
- PFLOTRAN comes with "upgraded" features
  - Enhanced 3-D capability
  - Integrated with existing postprocessing tools
  - Implementation of WIPP-specific capabilities required

- Large-scale testing of PFLOTRAN vs. current WIPP PA codes
  - Aid in validation during review process

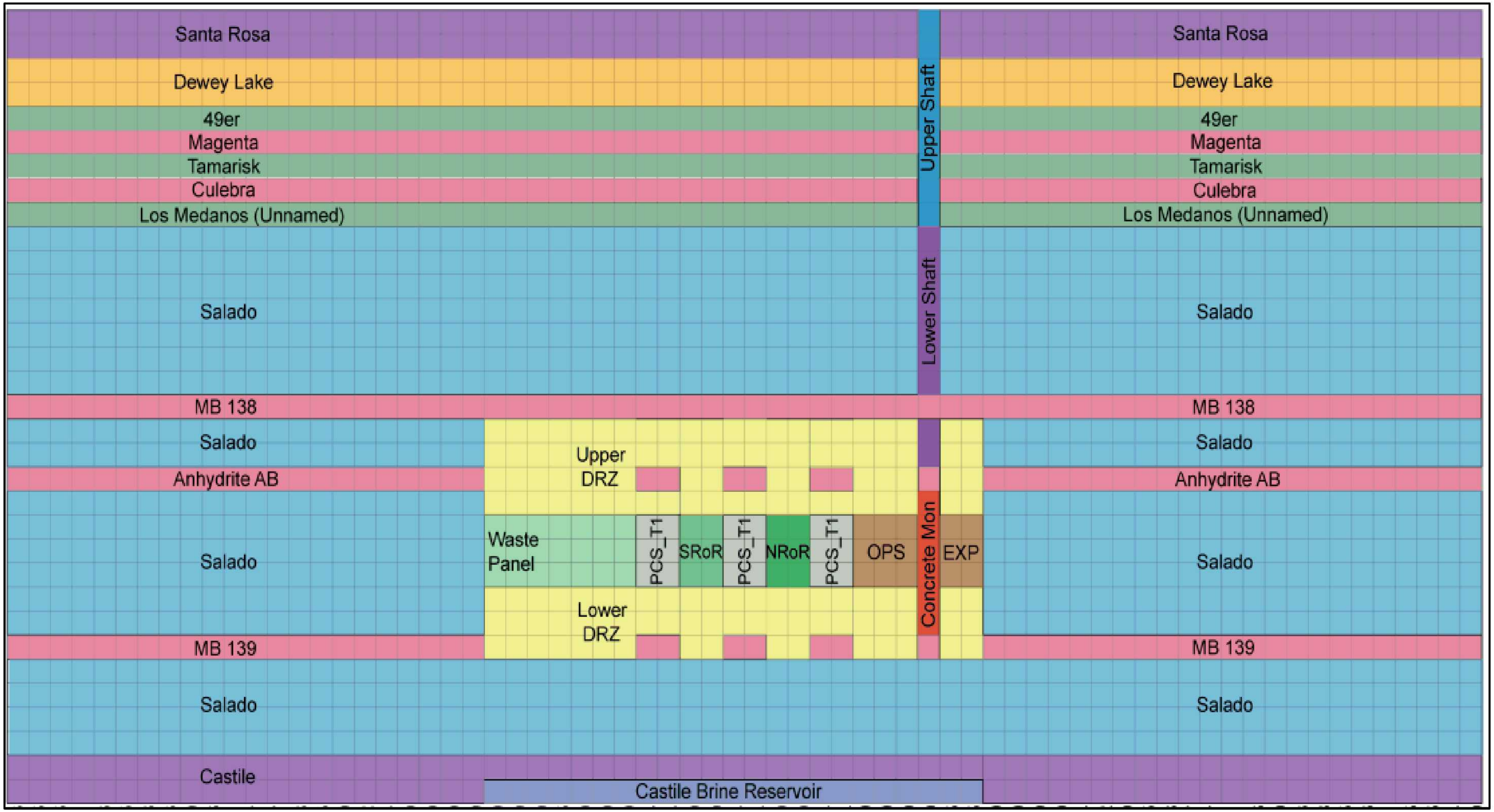
- PFLOTRAN to be integrated into WIPP PA for CRA-2024

Questions?

Code Features and Capabilities (Transport)



2D Representation of Repository

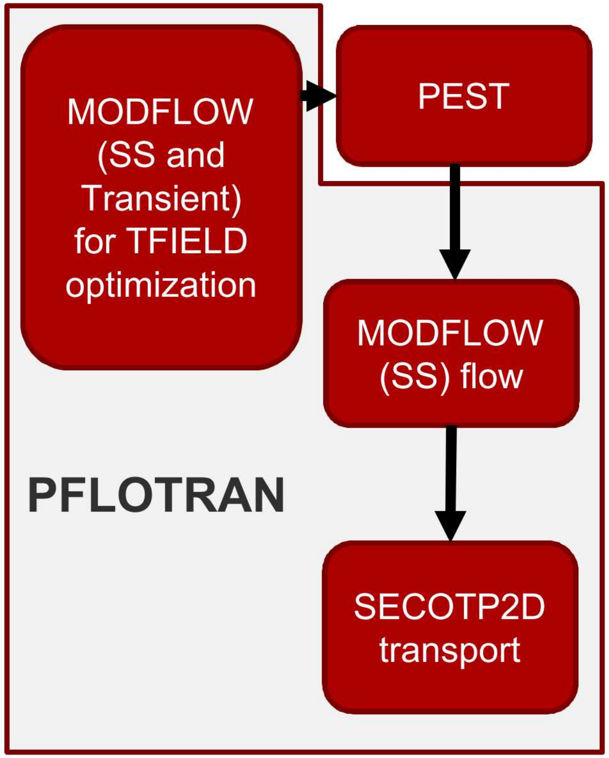


Current 2-D Grid
(cross-sectional view)

- Used by BRAGFLO
- Two-phase flow (brine and gas)

MODFLOW and SECOTP2D

Hydrology PA Workflow



- Streamlined hydrology PA workflow
  - Flow and transport calculations done with a single code (coupled)
  - Flow and transport calculations done potentially over a single grid
- TFIELDS can be recalculated with PFLOTRAN rather than MODFLOW2000.
- Other non-PA applications (ASER contour maps & COMPs) will also benefit from updated/streamlined process.

Code	PA Role	PFLOTRAN Replacement Capabilities
MODFLOW2000	Culebra flow	Provides similar fully saturated, 2-D transient flow solutions (steady state is just transient run out to long time)
SECOTP2D	Culebra transport	Has existing transport capability comparable to SECOTP2D. Some aspects (e.g., dual domain mass transport) may require some minor modifications.

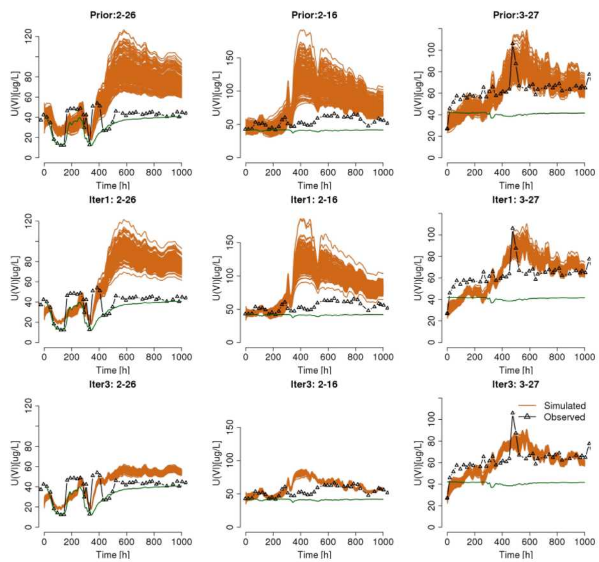
PFLOTRAN Reactive Transport

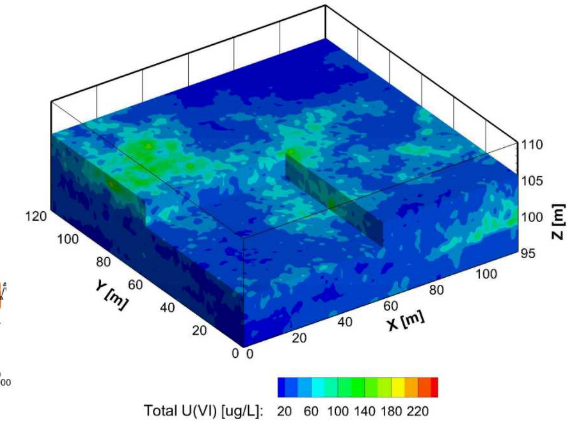
- Transport
  - Multicomponent
  - Mobile/immobile primary species
  - Advection (upwinding)
  - Hydrodynamic dispersion
- Reaction
  - Aqueous speciation
    - Ion activity models
  - General (A + B ↔ C)
    - N^{th} order kinetics
    - Reversible
  - Mineral precipitation-dissolution
    - Prefactors
- Microbiological
  - Michaelis–Menten kinetics
  - Biomass
  - Inhibition
- Radioactive decay with daughter products
- Sorption
  - Isotherm-based: linear, Langmuir, Freundlich
  - Ion exchange
  - Surface complexation
    - Equilibrium
    - Kinetic / multirate kinetic
- Reaction Sandbox

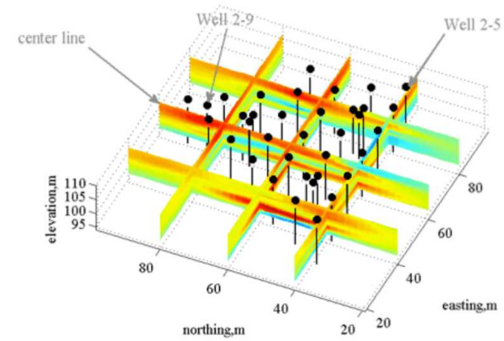
Benefits of Massively Parallel HPC

Data Assimilation at the Hanford 300 Area (Xingyuan Chen, 2011)

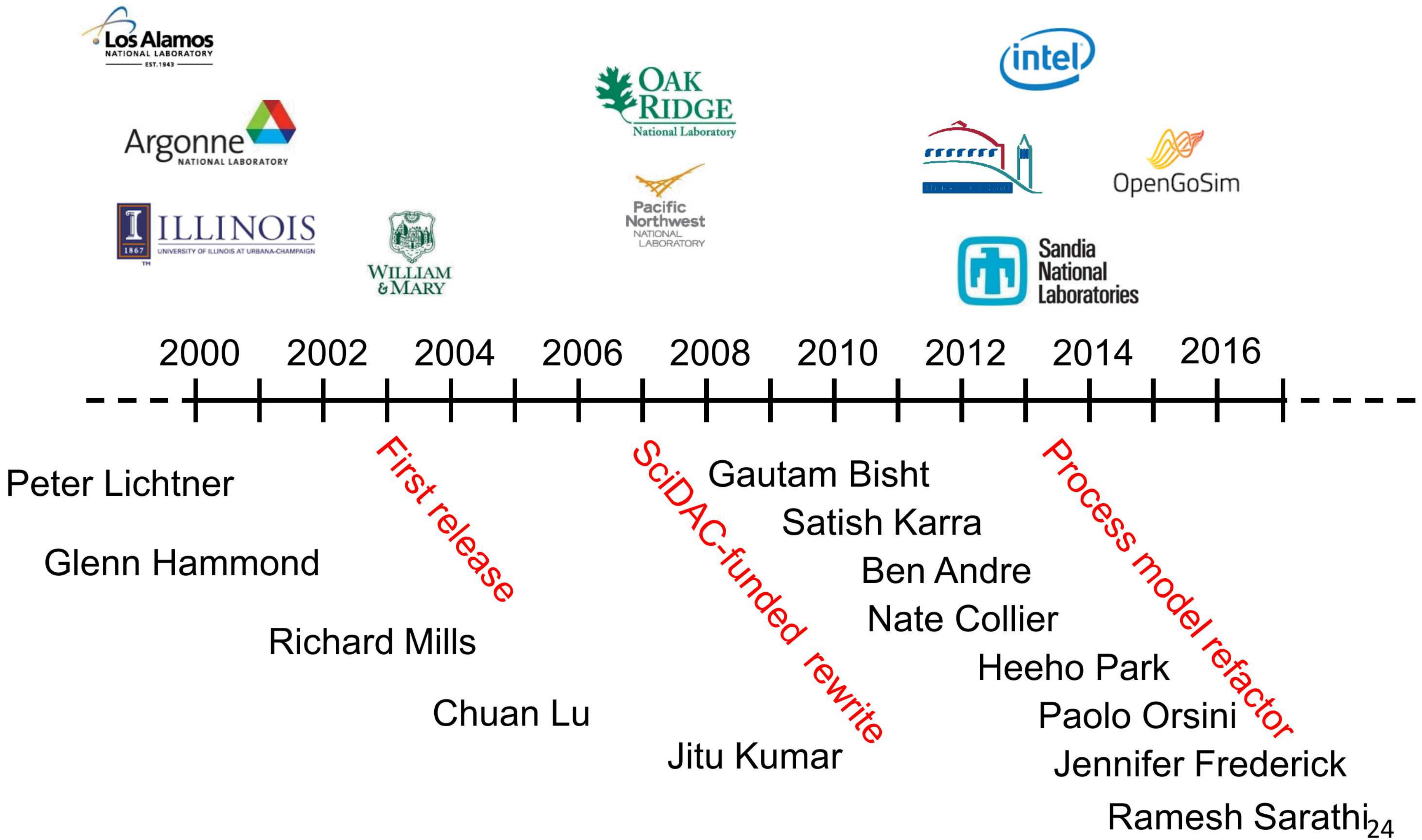
- Problem domain:
  - 120×120×15m
  - $\Delta x, \Delta y, \Delta z$ = 1,1,0.5 m
  - 432K grid cells
  - 15 chemical species
  - 6.48M dofs total
- 1-2 month simulation:
  - Δt = 1 hour
- Computing, e.g.
  - 128 cores (single realization)
  - 64,000 cores (500 realizations)
  - 1 hour wallclock runtime
  - ~7 cpu years







PFLOTRAN Development Timeline



PFLOTRAN Developers

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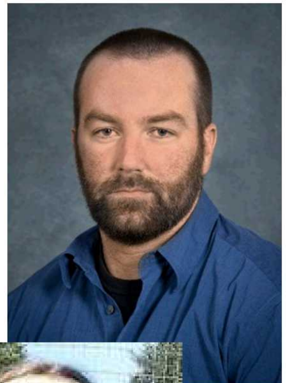
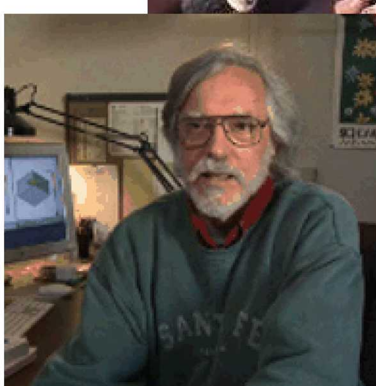
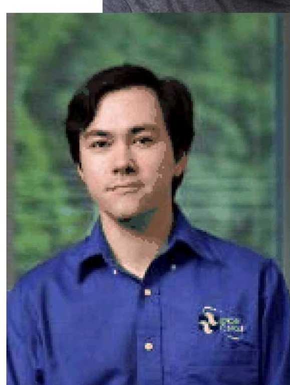






Governing Equations

GENERAL Mode (miscible air-water-energy)

Water Mass
$$\frac{\partial \phi (s_l \rho_l X_w^l + s_g \rho_g X_w^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_w^l \boldsymbol{q}_l + \rho_g X_w^g \boldsymbol{q}_g + \boldsymbol{J}_w^l + \boldsymbol{J}_w^g\right) + q_w$$

Air Mass
$$\frac{\partial \phi (s_l \rho_l X_a^l + s_g \rho_g X_a^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_a^l \boldsymbol{q}_l + \rho_g X_a^g \boldsymbol{q}_g + \boldsymbol{J}_a^l + \boldsymbol{J}_a^g\right) + q_a$$

Energy
$$\frac{\partial \phi \left(s_l \rho_l U_l + s_g \rho_g U_g\right) + (1-\phi) C_p^{\text{rock}} \rho_{\text{rock}} T}{\partial t} = -\nabla \cdot \left(\rho_l H_l \boldsymbol{q}_l + \rho_g H_g \boldsymbol{q}_g - \kappa_{\text{eff}} \nabla T\right) + q_e$$

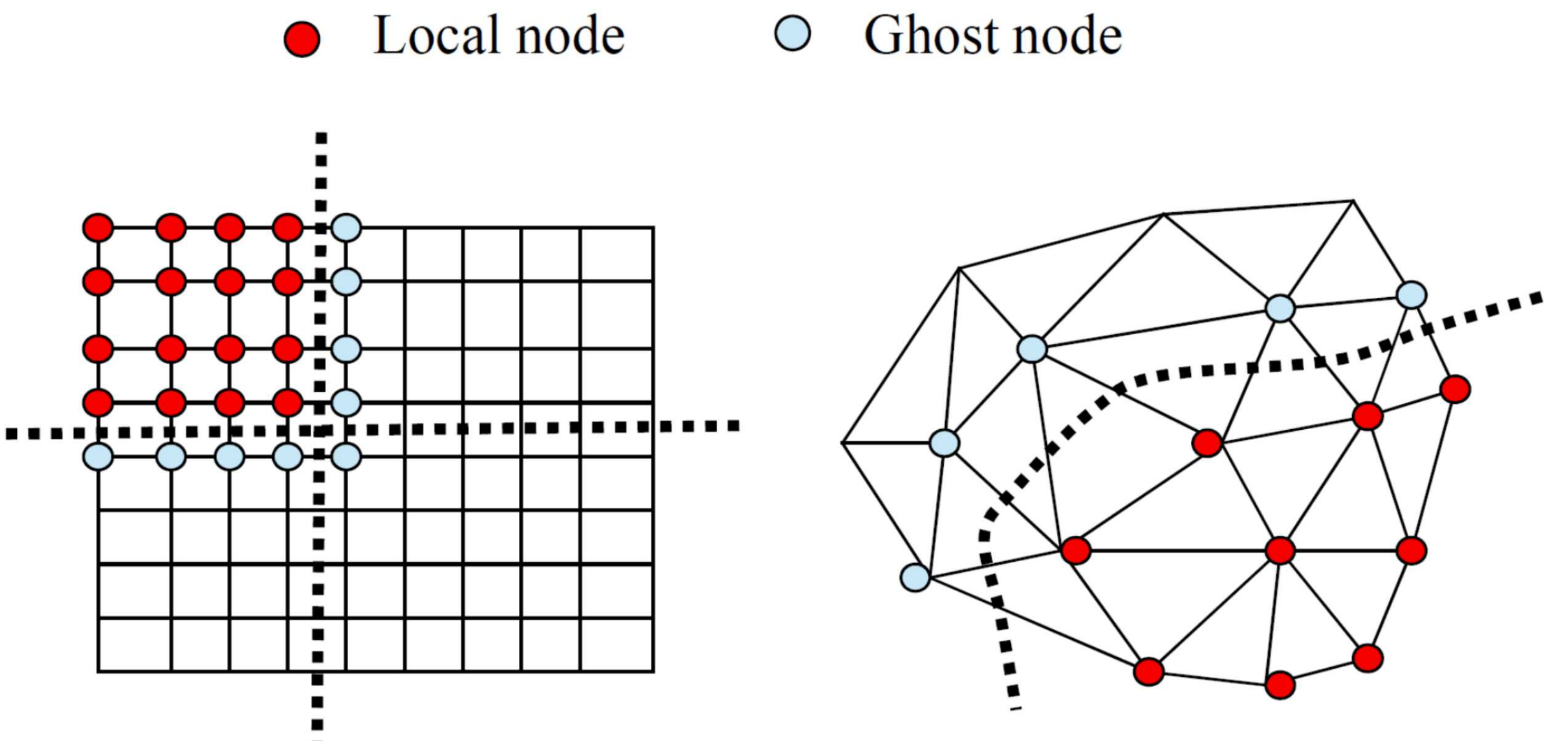
WIPP_FLOW Mode (immiscible air-water)

Water Mass
$$\frac{\partial \phi (s_l \rho_l)}{\partial t} = -\nabla \cdot (\rho_l \boldsymbol{q}_l) + q_w^G$$

Air Mass
$$\frac{\partial \phi (s_g \rho_g)}{\partial t} = -\nabla \cdot \left(\rho_g \boldsymbol{q}_g\right) + q_a^G$$

Approach to Parallelization

Domain Decomposition

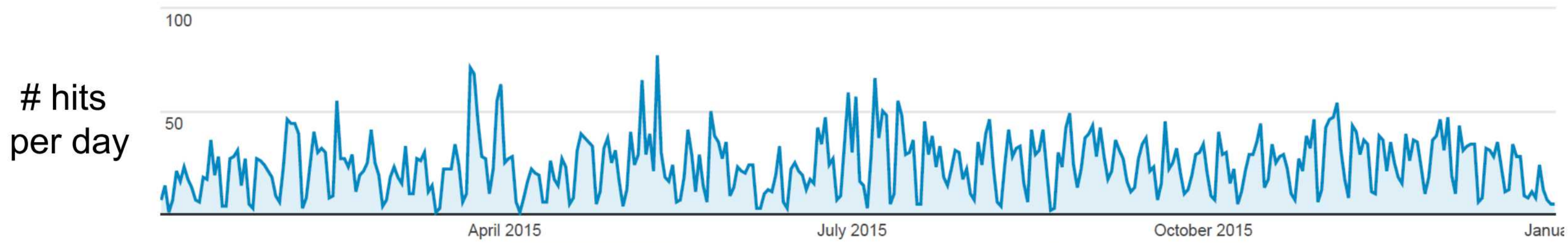


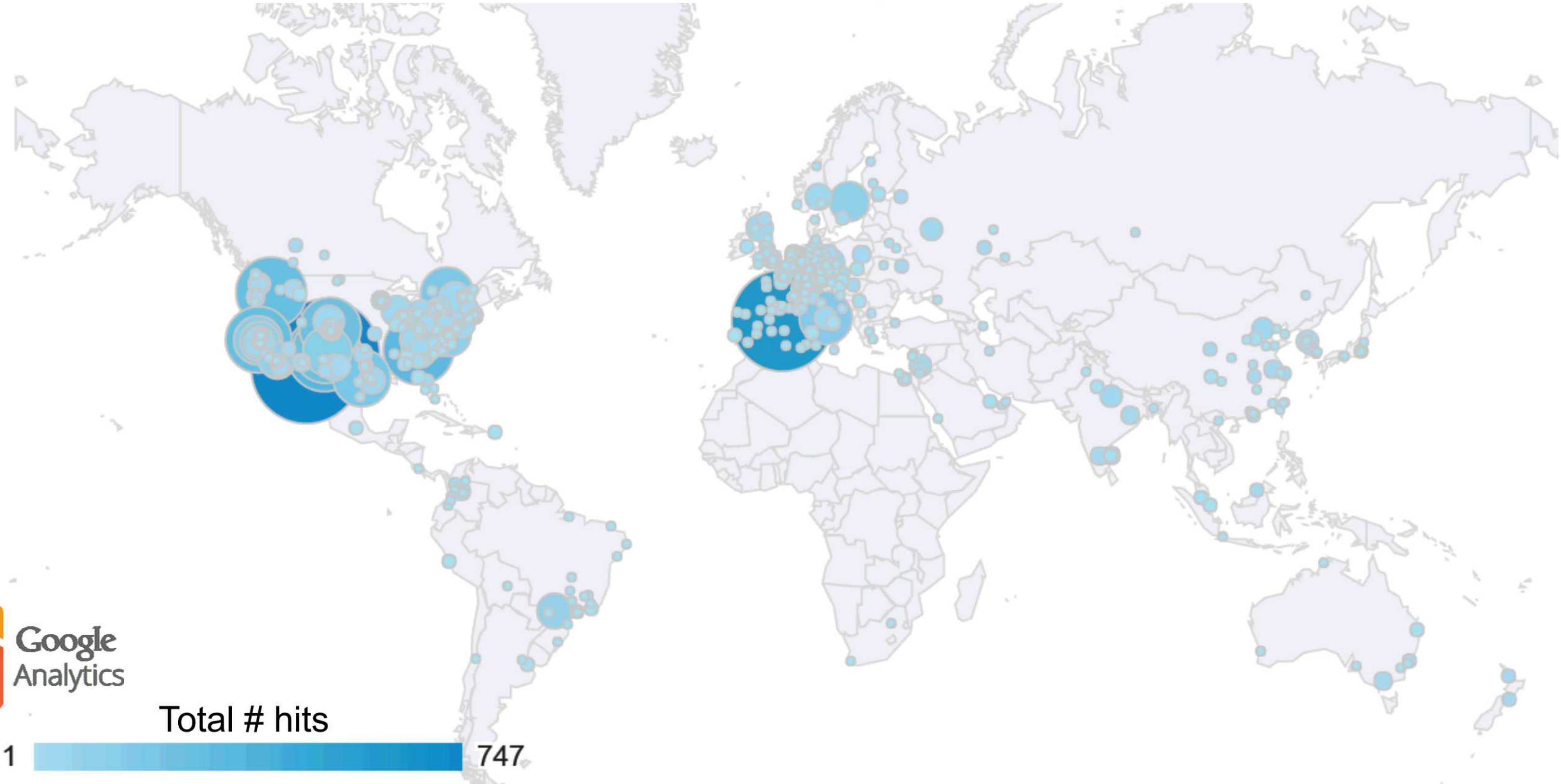
Ghost node information used only in flux calculations.

PFLOTRAN Support Infrastructure

- 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

Hits on PFLOTRAN Bitbucket Site in 2015





Hits on PFLOTRAN Bitbucket Site in 2016

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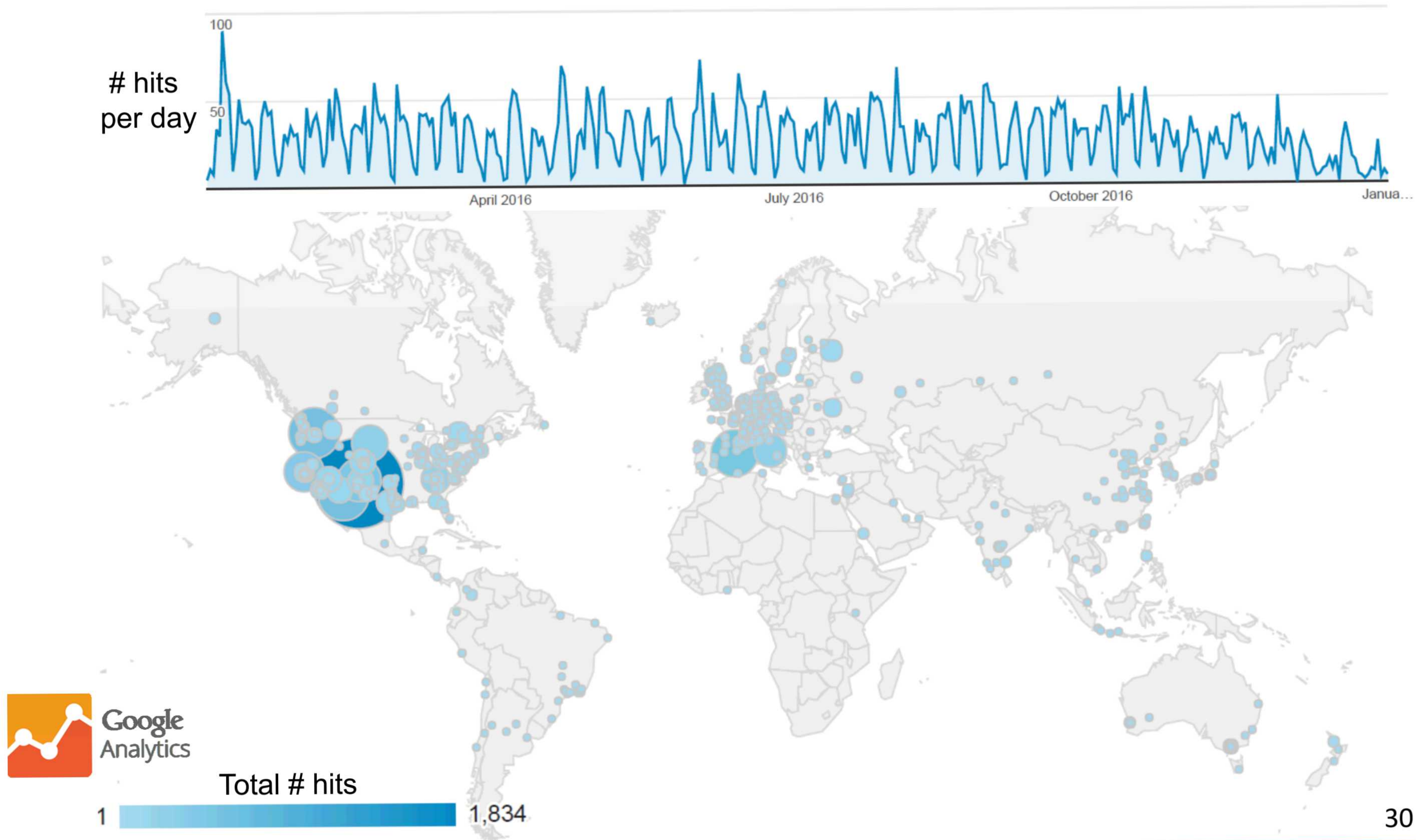
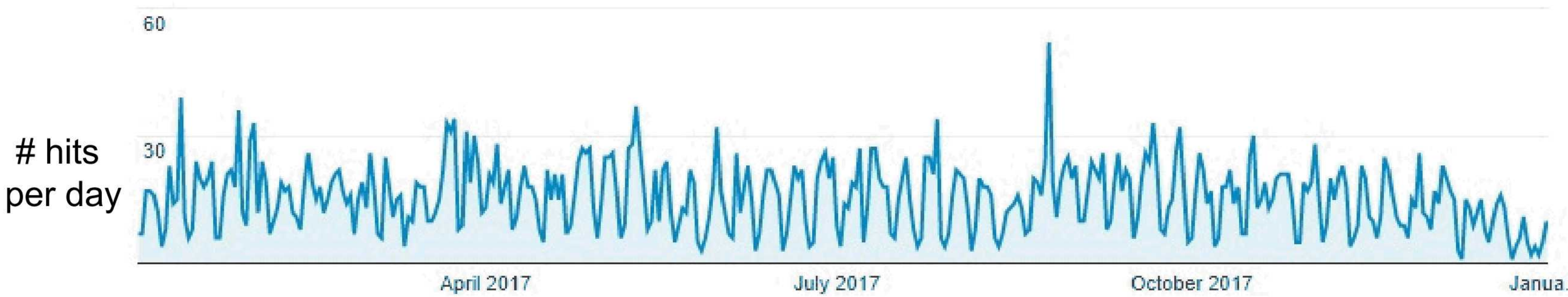
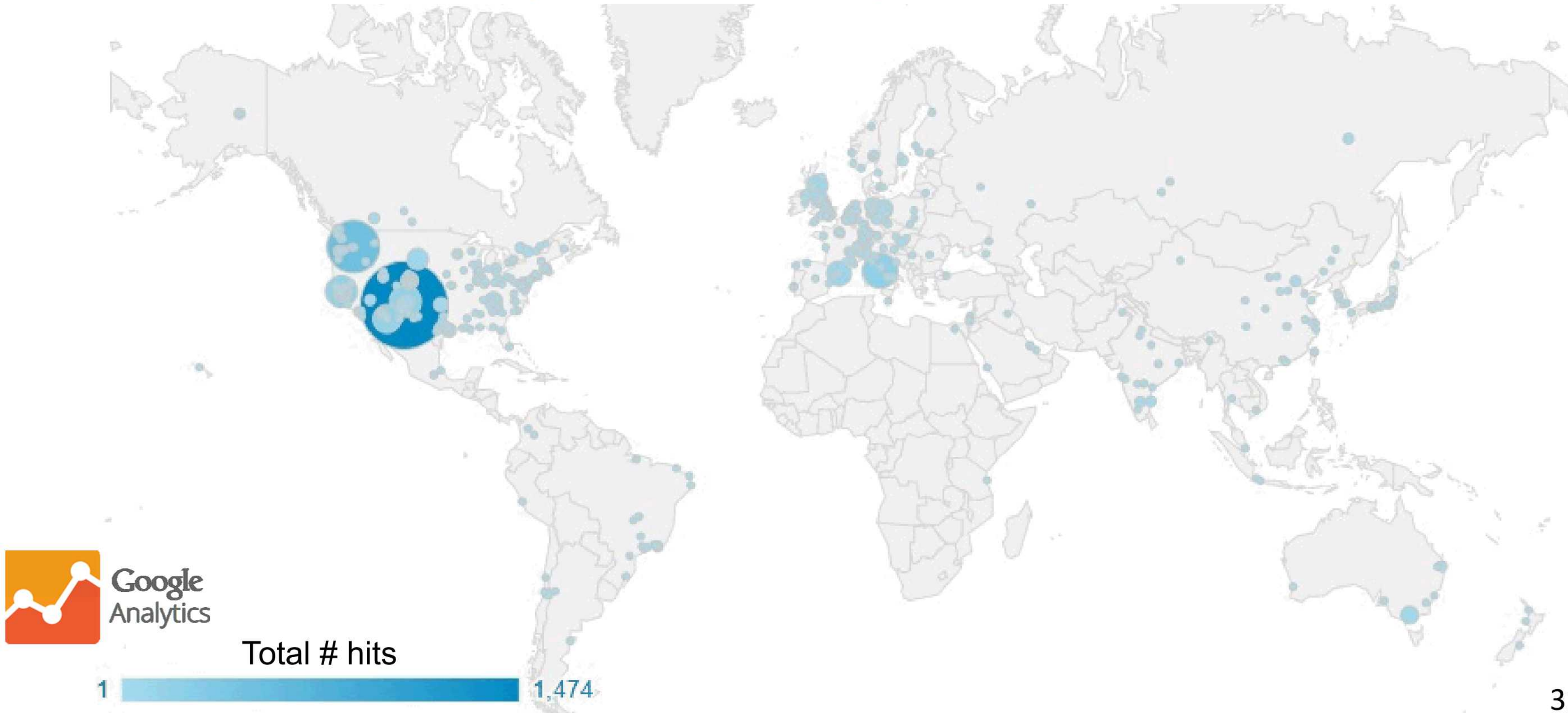


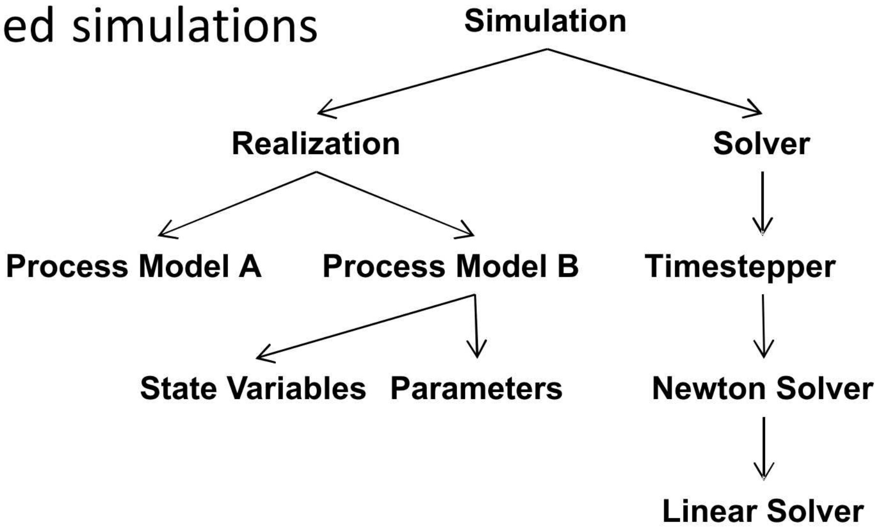
Hits on PFLOTRAN Bitbucket Site in 2017





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



PFLOTRAN Flow Modes

- RICHARDS: variably-saturated water
- TH: variably-saturated water-energy
- GENERAL: multiphase air-water-energy
- WIPP_FLOW: immiscible air-water
- MPHASE: supercritical CO2-water-energy
- FLASH2: supercritical CO2-water-energy (experimental)
- IMMIS: air-water (experimental)
- MISCIBLE: X-water-energy (experimental)
- TOIL_IMS: oil-water-energy (experimental)

Governing Equations

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GENERAL Mode (air-water-energy)

Water Mass
$$\frac{\partial \phi (s_l \rho_l X_w^l + s_g \rho_g X_w^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_w^l \boldsymbol{q}_l + \rho_g X_w^g \boldsymbol{q}_g + \boldsymbol{J}_w^l + \boldsymbol{J}_w^g\right) + q_w$$

Air Mass
$$\frac{\partial \phi (s_l \rho_l X_a^l + s_g \rho_g X_a^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_a^l \boldsymbol{q}_l + \rho_g X_a^g \boldsymbol{q}_g + \boldsymbol{J}_a^l + \boldsymbol{J}_a^g\right) + q_a$$

Energy
$$\frac{\partial \phi \left(s_l \rho_l U_l + s_g \rho_g U_g\right) + (1-\phi) C_p^{\text{rock}} \rho_{\text{rock}} T}{\partial t} = -\nabla \cdot \left(\rho_l H_l \boldsymbol{q}_l + \rho_g H_g \boldsymbol{q}_g - \kappa_{\text{eff}} \nabla T\right) + q_e$$

ϕ = effective porosity [-]
s_l = liquid saturation [-]
s_g = gas saturation [-]
ρ_l = liquid phase density [kmol/m^3]
ρ_g = gas phase density [kmol/m^3]
X_w^l = mole fraction of water in the liquid phase [-]
X_w^g = mole fraction of water in gas phase [-]
X_a^l = mole fraction of air in the liquid phase [-]
X_a^g = mole fraction of air in gas phase [-]
$\boldsymbol{q}_l$ = liquid phase Darcy flux [m/sec]
$\boldsymbol{q}_g$ = gas phase Darcy flux [m/sec]
$\boldsymbol{J}_w^l$ = water diffusive flux in liquid phase [kmol/m^2/sec]
$\boldsymbol{J}_a^l$ = air diffusive flux in liquid phase [kmol/m^2/sec]
$\boldsymbol{J}_w^g$ = water vapor diffusive flux in gas phase [kmol/m^2/sec]
$\boldsymbol{J}_a^g$ = air diffusive flux in gas phase [kmol/m^2/sec]
q_w = water source/sink [kmol/sec]
q_a = air source/sink [kmol/sec]
q_e = energy source/sink [MJ/sec]
U_l = liquid phase internal energy [MJ/kmol]
U_g = gas phase internal energy [MJ/kmol]
H_l = liquid phase enthalpy [MJ/kmol]
H_g = gas phase enthalpy [MJ/kmol]
C_p^{rock} = rock heat capacity [MJ/kg rock-K]
ρ_{rock} = rock particle density [kg/m^3 rock]
T = temperature [C]
κ_{eff} = effective thermal conductivity [W/K-m]

Governing Equations

Darcy Flux

$$\boldsymbol{q}_\alpha = -\frac{k k_\alpha}{\mu_\alpha} \nabla (p_\alpha - \gamma_\alpha g z), \quad (\alpha = l,\, g)$$

Air Diffusion in Liquid Phase

$$\boldsymbol{J}_a^l = -\tau \phi s_l D_l \rho_l \boldsymbol{\nabla} X_a^l$$

Air Diffusion in Gas Phase

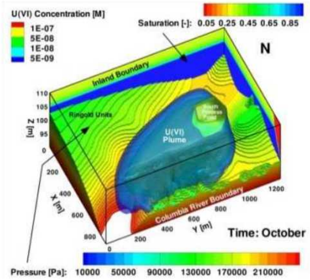
$$\boldsymbol{J}_a^g = -\tau \phi s_g D_g^0 \left(\frac{T}{T_K}\right)^\theta \frac{p_0}{p_g} \rho_g \nabla X_a^g$$

$\boldsymbol{q}_\alpha$ = Darcy flux for phase α [m/s]
k = intrinsic permeability [m^2]
k_α = relative permeability for phase α [-]
μ_α = viscosity for phase α [Pa-s]
p_α = pressure for phase α [Pa]
γ_α = density for phase α [kg/m^3]
g = gravity [m/s^2]

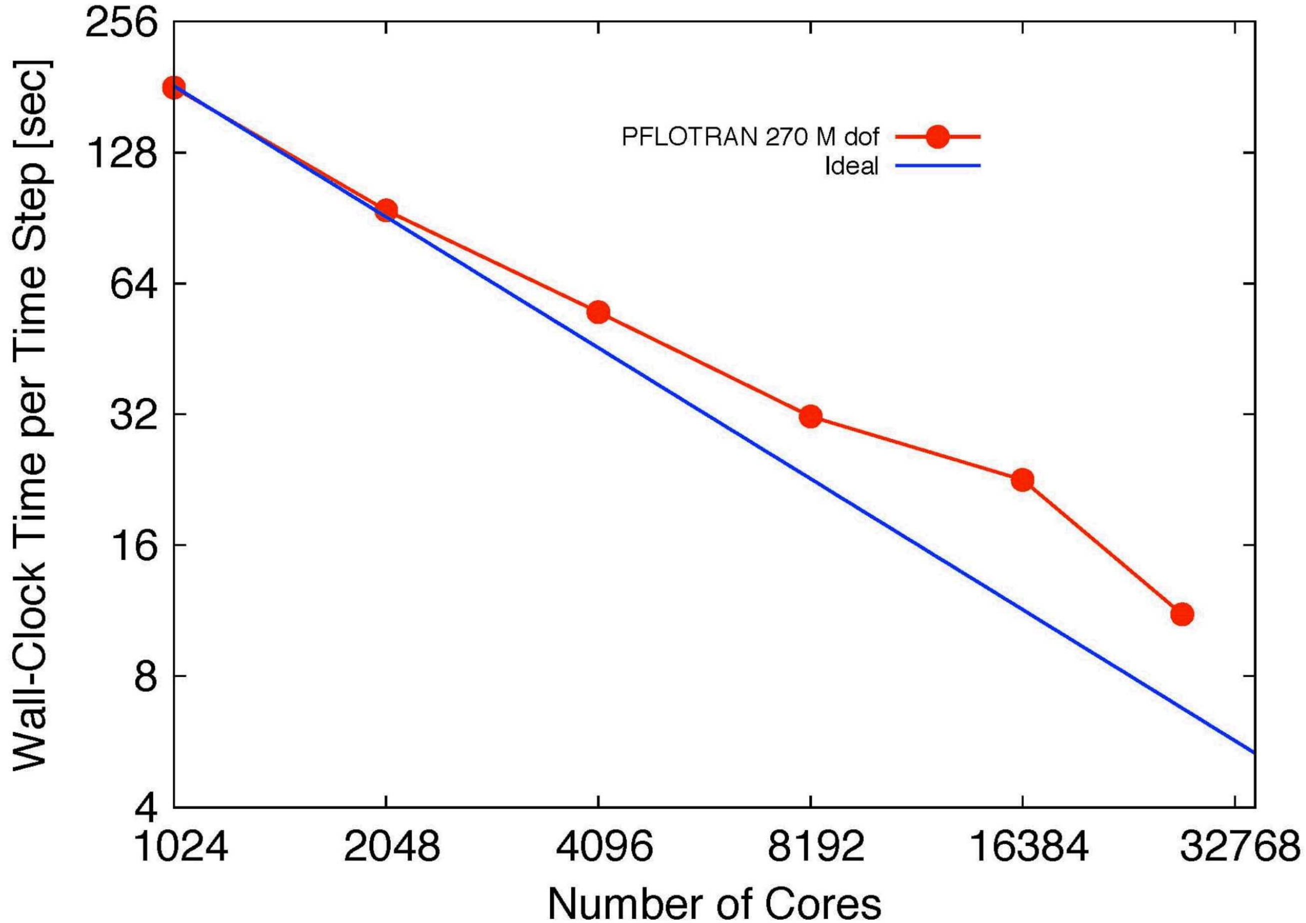
z = elevation [m]
$\boldsymbol{J}_a^l$ = diffusive flux of air in liquid phase [kmol/m^2-s]
τ = tortuosity [-]
D_l = aqueous diffusivity [m^2/s]
$\boldsymbol{J}_a^g$ = diffusive flux of air in gas phase [kmol/m^2-s]
D_g^0 = gas diffusivity [m^2/s]
p_0 = reference pressure [Pa]

PFLOTRAN Parallel Performance

Hanford 300 Area



Hammond and Lichtner, WRR, 2010



3-D Capability Development Timeline