PFLOTRAN Update

Code Enhancements, Documentation and QA

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Sandia National Laboratories

SFWD

Spent Fuel & Waste Disposition

Annual Working Group Meeting
UNLV-SEB – *Las Vegas, Nevada*
May 21-23, 2019

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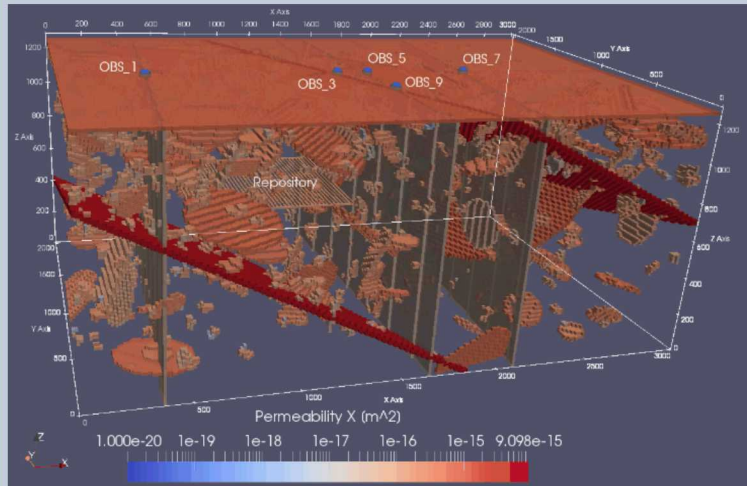


PFLOTRAN Developments

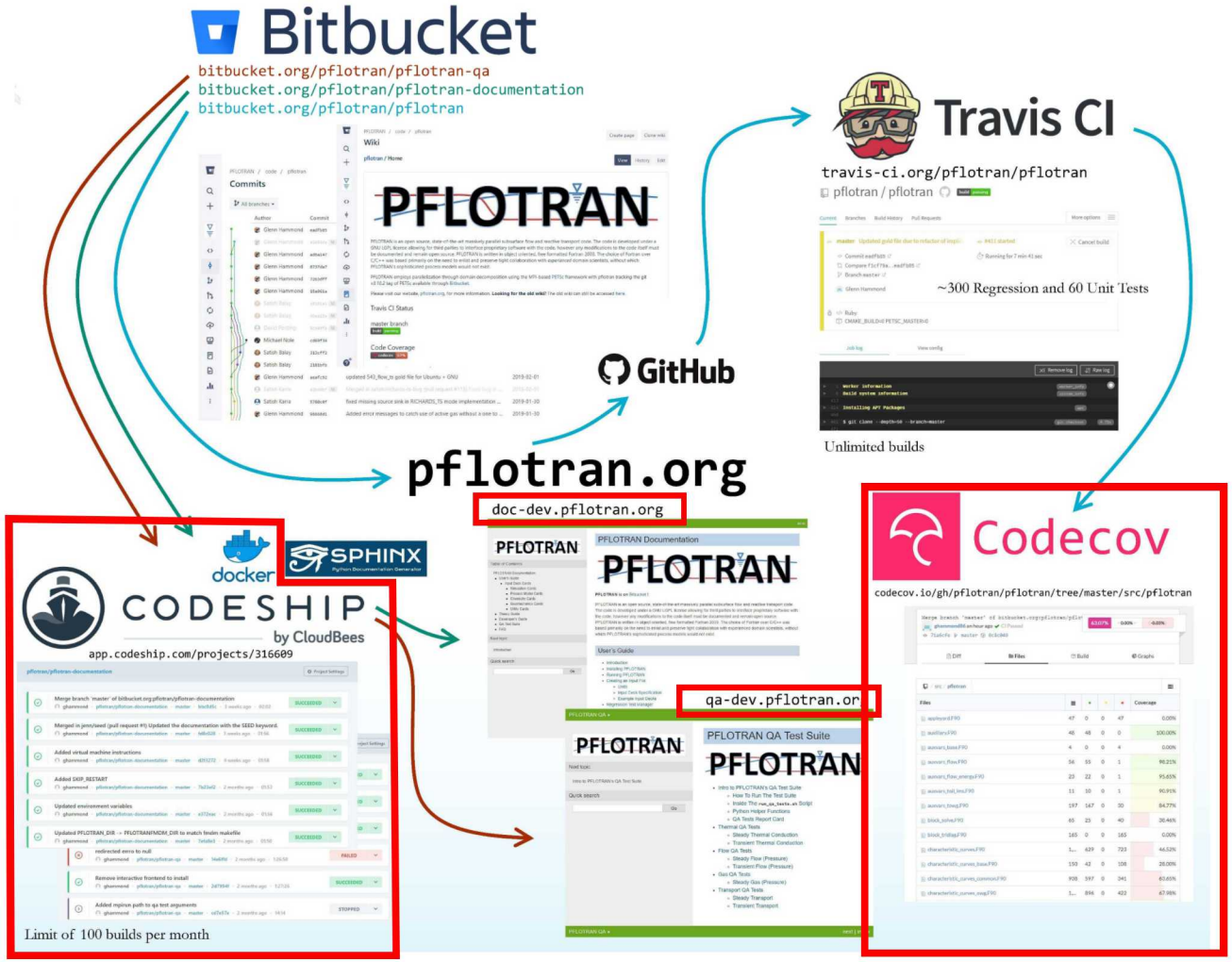
- Code enhancements
  - Multiphase solution controls (convergence) – Michael N.
  - IF97 EOS – Michael N.
    - Relative to IFC67, smoother, cheaper and valid for a larger range of temperature and pressure
  - Linear[1]/nonlinear solvers – Heeho
    - CPR (constrained pressure-residual)-based solvers[1]
    - Line search and trust region algorithms to improve convergence
  - NW-transport[1] – Jenn
    - Chemistry that accommodates dry grid cells
    - Decay and ingrowth in all phases
  - Short courses: Vanderbilt, CSIRO[2], IHLRWM, Uni Bern

[1] WIPP-sponsored
[2] Sandia-sponsored

PFLOTRAN Developments (cont.)

- Quality Assurance (QA)
  - Streamlined updating of PFLOTRAN documentation
  - Initiated QA documentation
  - Refactoring automated QA testing framework

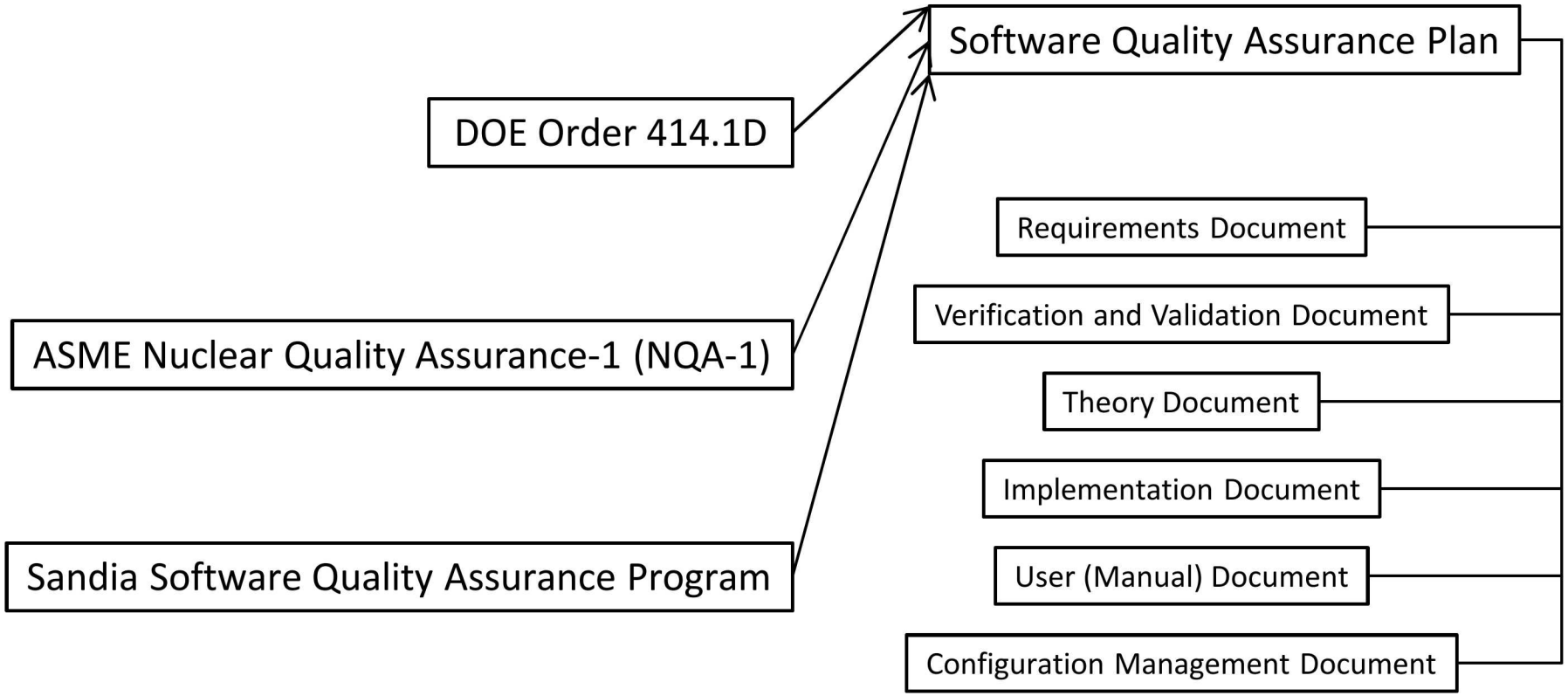
PFLOTRAN's Cloud-based Continuous Integration



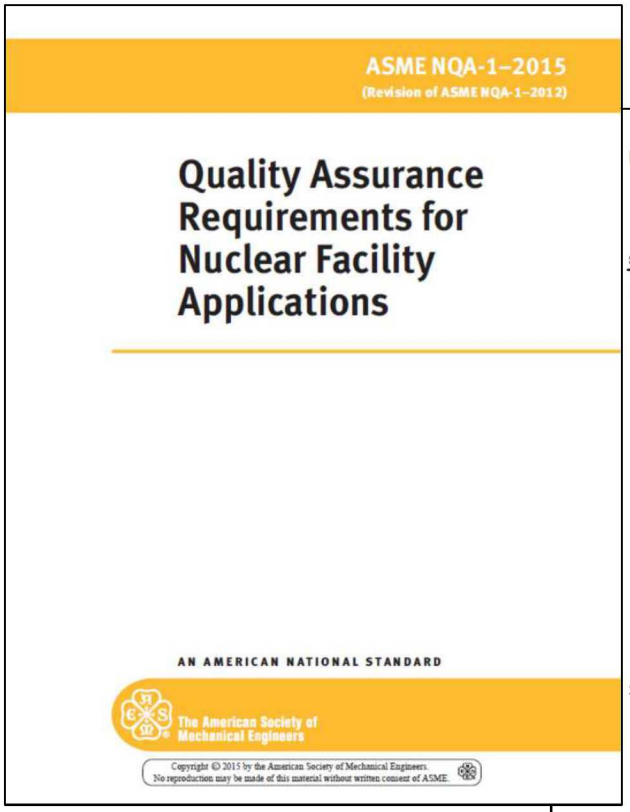
Hammond and Bisht, 2019

https://doi.org/10.6084/m9.figshare.7761950.v1

Software Quality Assurance Plan



NQA-1, DOE O 414.1D and SSQAP



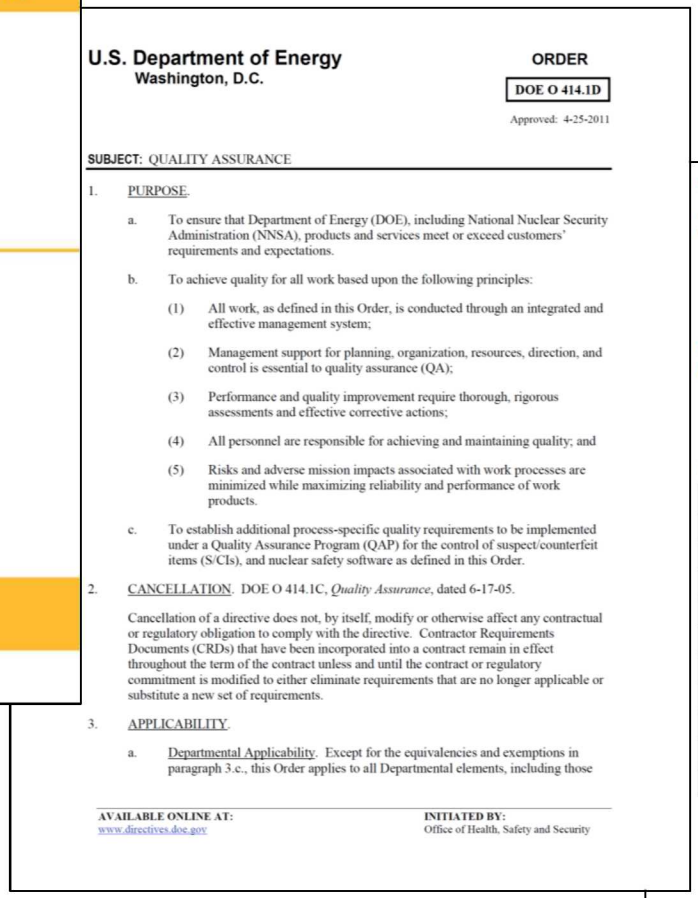
ASME NQA-1–2015
(Revision of ASME NQA-1–2012)

Quality Assurance Requirements for Nuclear Facility Applications

AN AMERICAN NATIONAL STANDARD

The American Society of Mechanical Engineers

316 pages



U.S. Department of Energy
Washington, D.C.

ORDER
DOE O 414.1D
Approved: 4-25-2011

SUBJECT: QUALITY ASSURANCE

1. PURPOSE.

   a. To ensure that Department of Energy (DOE), including National Nuclear Security Administration (NNSA), products and services meet or exceed customers' requirements and expectations.

   b. To achieve quality for all work based upon the following principles:

      (1) All work, as defined in this Order, is conducted through an integrated and effective management system;

      (2) Management support for planning, organization, resources, direction, and control is essential to quality assurance (QA);

      (3) Performance and quality improvement require thorough, rigorous assessments and effective corrective actions;

      (4) All personnel are responsible for achieving and maintaining quality; and

      (5) Risks and adverse mission impacts associated with work processes are minimized while maximizing reliability and performance of work products.

   c. To establish additional process-specific quality requirements to be implemented under a Quality Assurance Program (QAP) for the control of suspect/counterfeit items (S/CIs), and nuclear safety software as defined in this Order.

2. CANCELLATION. DOE O 414.1C, *Quality Assurance*, dated 6-17-05.

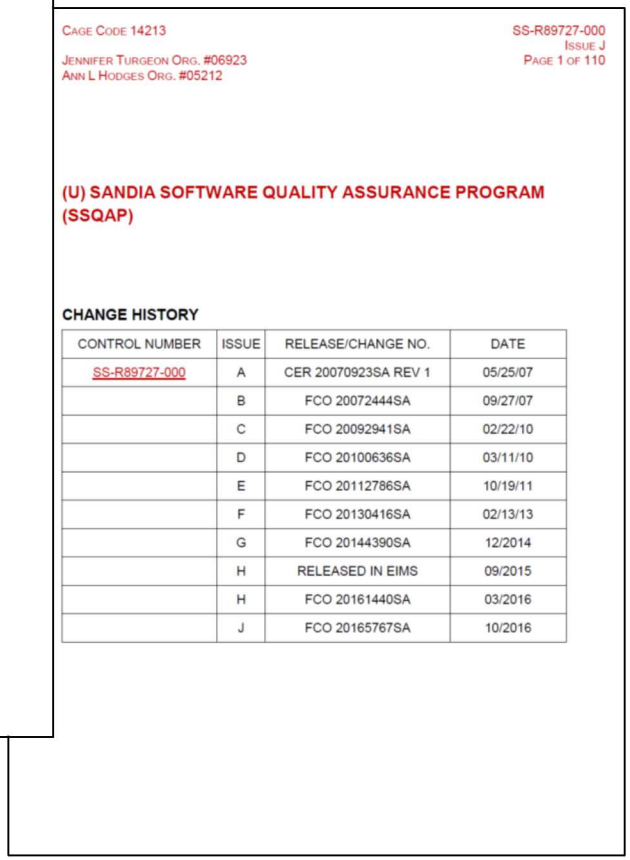
Cancellation of a directive does not, by itself, modify or otherwise affect any contractual or regulatory obligation to comply with the directive. Contractor Requirements Documents (CRDs) that have been incorporated into a contract remain in effect throughout the term of the contract unless and until the contract or regulatory commitment is modified to either eliminate requirements that are no longer applicable or substitute a new set of requirements.

3. APPLICABILITY.

   a. Departmental Applicability. Except for the equivalencies and exemptions in paragraph 3.c., this Order applies to all Departmental elements, including those

AVAILABLE ONLINE AT:
www.directives.doe.gov

INITIATED BY:
Office of Health, Safety and Security



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JENNIFER TURGEON ORG. #06923
ANN L HODGES ORG. #05212

SS-R89727-000
ISSUE J
PAGE 1 OF 110

(U) SANDIA SOFTWARE QUALITY ASSURANCE PROGRAM (SSQAP)

CHANGE HISTORY

CONTROL NUMBER	ISSUE	RELEASE/CHANGE NO.	DATE
SS-R89727-000	A	CER 20070923SA REV 1	05/25/07
	B	FCO 20072444SA	09/27/07
	C	FCO 20092941SA	02/22/10
	D	FCO 20100636SA	03/11/10
	E	FCO 20112786SA	10/19/11
	F	FCO 20130416SA	02/13/13
	G	FCO 20144390SA	12/2014
	H	RELEASED IN EIMS	09/2015
	H	FCO 20161440SA	03/2016
	J	FCO 20165767SA	10/2016

SANDIA SOFTWARE QUALITY ASSURANCE PROGRAM

Graded Risk Level and Associated SSQAP Recommended Practice Level

Graded Risk Level (RL) Associated SSQAP Recommended Practice Level (PL)					
Likelihood Tier Undesirable event due to software failure	**Consequence Tier** Undesirable Event				
	C4 (Catastrophic)	**C3** (Severe)	**C2** (Moderate)	**C1** (Low)	**C0** (Negligible)
L4 (Very High)	RL = VH PL = P4	RL = VH PL = P4	RL = H PL = P3	RL = M PL = P2	RL = L PL = P1
L3 (High)	RL = VH PL = P4	RL = H PL = P3	RL = M PL = P2	RL = M PL = P2	RL = L PL = P1
L2 (Moderate)	RL = H PL = P3	RL = M PL = P2	RL = M PL = P2	RL = L PL = P1	RL = L PL = P1
L1 (Low)	RL = M PL = P2	RL = M PL = P2	RL = L PL = P1	RL = L PL = P1	RL = N PL = P0
L0 (Negligible)	RL = L PL = P1	RL = L PL = P1	RL = L PL = P1	RL = N PL = P0	RL = N PL = P0

Legend:

RL values: N = negligible, L = low, M = moderate, H = high, VH = very high

PL values: P0, P1, P2, P3, and P4 are defined in the Guidance to SSQAP Practice Levels. Practice activities related to these practice levels are provided in Table 3-3.

Sandia Software Quality Assurance Program

Table C-3. Practice Activities Based Upon Recommended PL Tier

Process Areas and Global Practices	Practice Activities Based upon Recommended Practice Level Tier				
	P0*	P1	P2	P3	P4
Project Planning [PP]	X	X	X	X	X
Project Monitoring and Control [PO]			X	X	X
Risk Management [RK]	X	X	X	X	X
Requirements Management [RM]	X	X	X	X	X
Requirements Development [RD]	X	X	X	X	X
Technical Solution [TS]		X	X	X	X
Verification [VE]	X	X	X	X	X
Validation [VA]			X	X	X
Deployment [DE]			X	X	X
Life Cycle Support [LS]			X	X	X
Configuration Management [CM]	X	X	X	X	X
Measurement & Analysis [MA]			X	X	X
Product Integration [PI]			X	X	X
Integrated Teaming [IT]				X	X
Stakeholder Involvement [SI]			X	X	X
Collecting Improvement Information [CI]				X	X
Objective Evaluation [OE]				X	X
Quantitative Objectives [QO]				X	X
Training [TR]	X	X	X	X	X
Problem Reporting and Corrective Actions[PR]			X	X	X

X – Suggested Practice Activities
- Existing Practice Activities
**P0 are "recommended" practices from SSQAP Table 3-3.*

Table C-6. Developed Software Level of Formality

Process Areas and Global Practices	Developed Software Level of Formality				
	P0*	P1	P2	P3	P4
Project Planning [PP]	L	M	M	H	H
Project Monitoring and Control [PO]	L	M	M	H	H
Risk Management [RK]	L	M	M	H	H
Requirements Management [RM]	L	M	M	H	H
Requirements Development [RD]	L	M	M	H	H
Technical Solution [TS]	L	M	M	H	H
Verification [VE]	L	M	M	H	H
Validation [VA]	L	L	M	H	H
Deployment [DE]	L	M	M	H	H
Life Cycle Support [LS]	L	M	M	H	H
Configuration Management [CM]	L	M	M	H	H
Measurement & Analysis [MA]	L	M	M	H	H
Product Integration [PI]	L	M	M	H	H
Integrated Teaming [IT]	L	L	M	H	H
Stakeholder Involvement [SI]	L	M	M	H	H
Collecting Improvement Information [CI]	L	L	M	H	H
Objective Evaluation [OE]	L	L	M	H	H
Quantitative Objectives [QO]	L	L	M	H	H
Training [TR]	L	M	M	H	H
Problem Reporting and Corrective Actions[PR]	L	M	M	H	H

Legend:
L: Low formality guidelines for overall practice level and/or individual practice activities
M: Medium formality guidelines for overall practice level and/or individual practice activities
H: High formality guidelines for overall practice level and/or individual practice activities
- Existing Practice Activities **P0 are "recommended" practices from SSQAP Table 3-3*

QA Documentation

Software Quality Assurance Plan

Requirements Document

Verification and Validation Document

Theory Document

Implementation Document

User (Manual) Document

Configuration Management Document

Complete

Nearly Complete

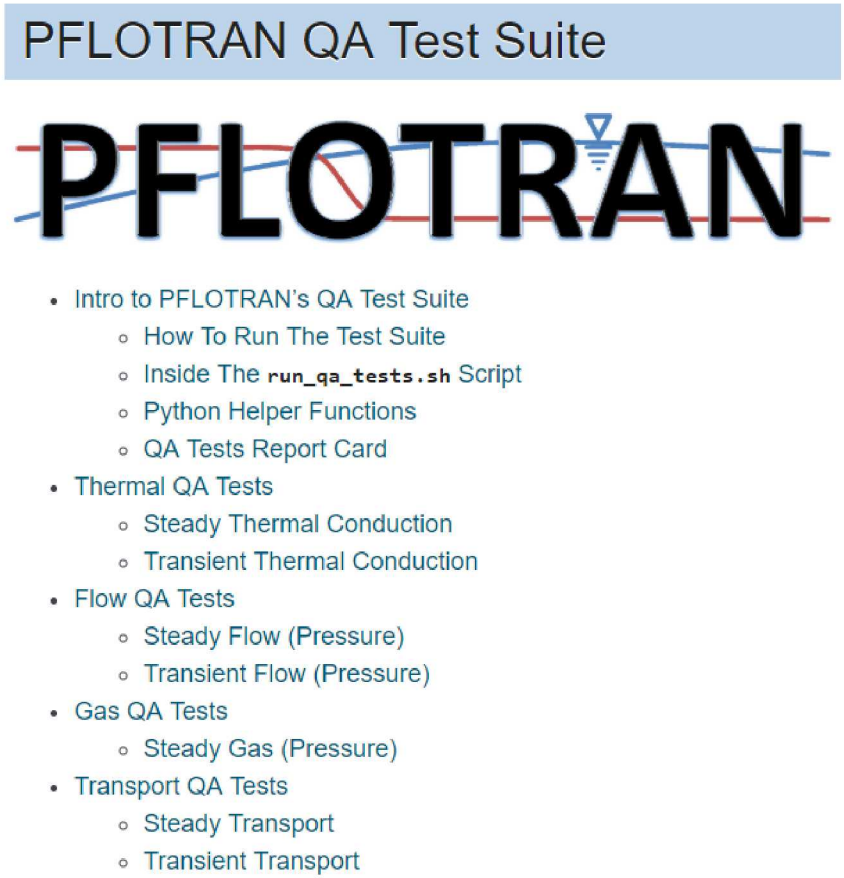
In Progress

Nonexistent

QA Test Suite Refactor

Jenn Frederick et al.

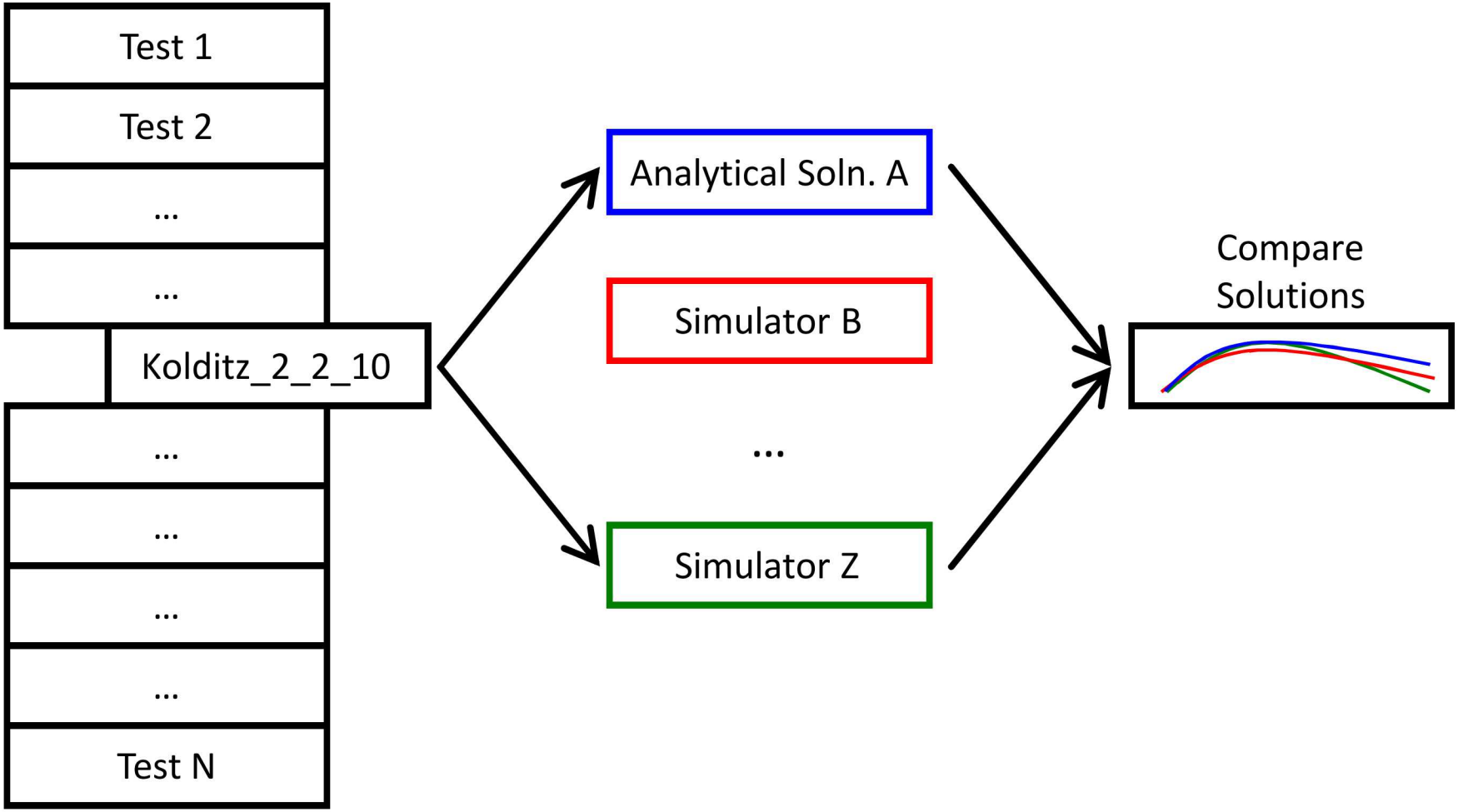
- Challenge: Sequential implementation of current test suite is difficult to maintain
- Solution:
  - Refactor test suite into an object oriented stack of tests
  - Leverage proven approach in regression testing suite



Object-Oriented QA Testing Framework

- Tests are managed by an outer test manager class.
- Separate driver interfaces control each simulator.
- Test classes are extensions of a base class written in python.
- Each test is generated from a configuration file with simulator-specific templates and a shared dictionary of parameters that feed into the templates.
- Solutions are compared qualitatively (plotting) and quantitively (absolute and relative error metrics).

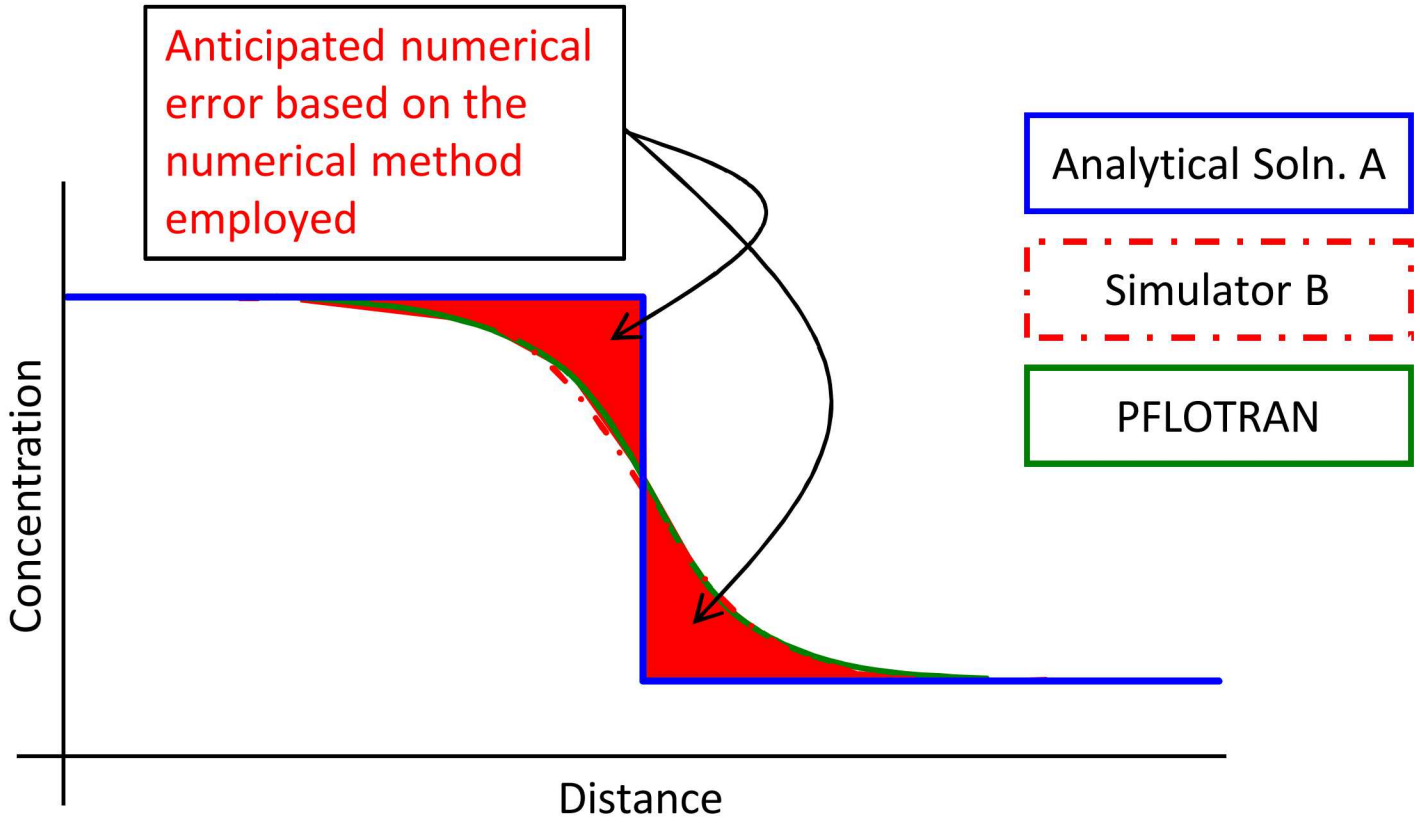
Object-Oriented QA Test Suite



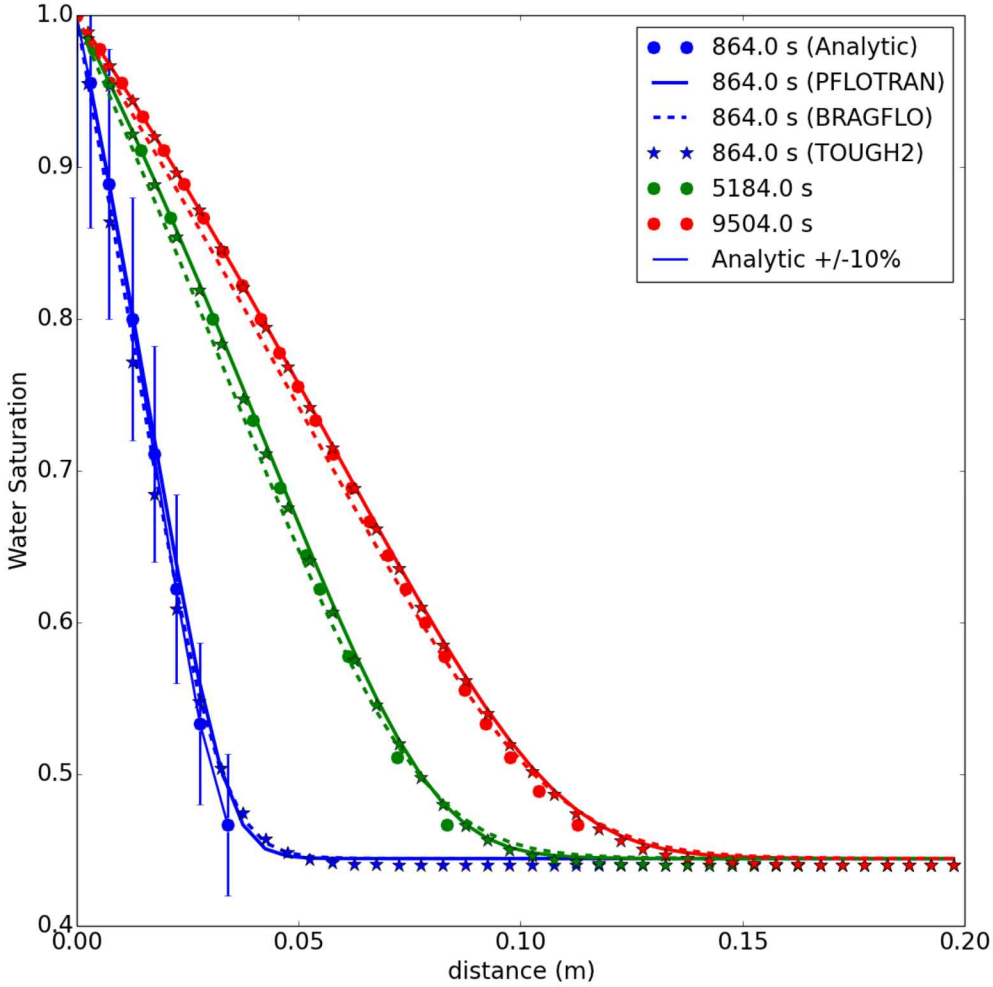
Hammond and Park

Verification Against Alternate Simulators

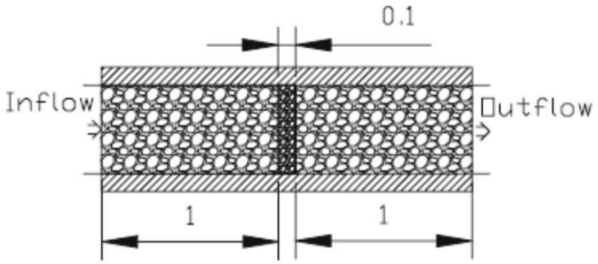
Concentration Profile for Solute Advection with No Diffusion



BRAGFLO Test Case #2 & #3
Horizontal one-dimensional infiltration

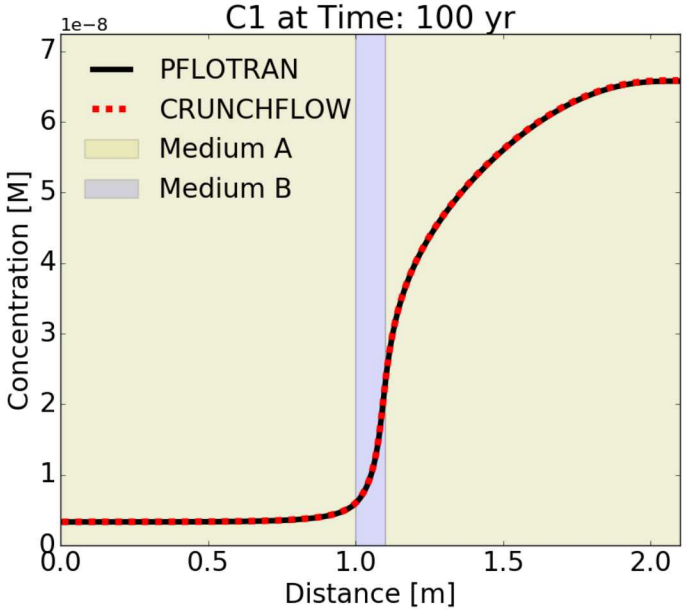


MoMaS Benchmark Carrayrou et al., 2010

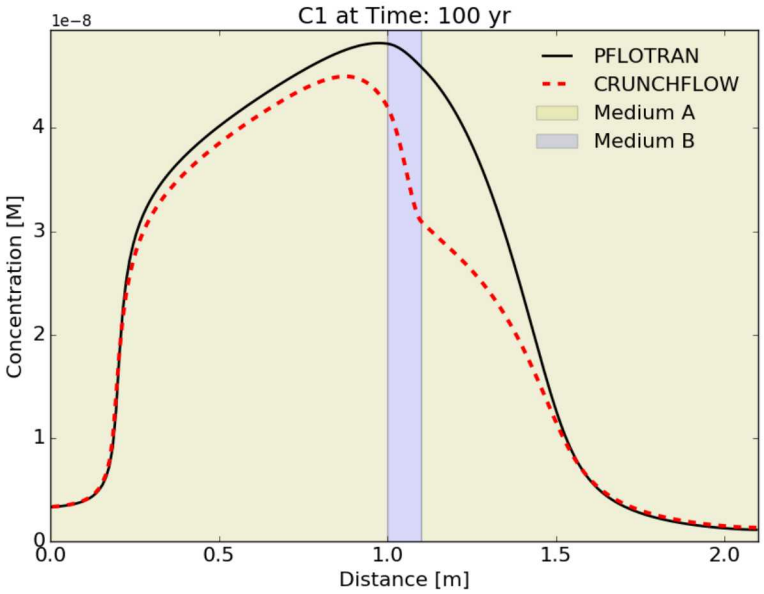


Heeho Park

Monodentate



Bidentate



PFLOTRAN's surface site density considers bulk instead of pore volume requiring porosity dependent log Keqs, which are not implemented in PFLOTRAN.

Example CrunchFlow and PFLOTRAN Template Files

Heeho Park

PFLOTRAN

```
GRID
  TYPE structured
  NXYZ swap{nx,300} 1 1
  DXYZ
    swap{nx1,100}@swap{dx1,0.01} swap{nx2,100}@swap{dx2,0.001} \
    swap{nx3,100}@swap{dx3,0.01}
    0.4
    0.6
  /
/
```

CrunchFlow

```
DISCRETIZATION
space_units meters
xzones swap{nx1,100} swap{dx1,0.01} swap{nx2,100} swap{dx2,0.001} \
       swap{nx3,100} swap{dx3,0.01}
END
```

Questions?

SFWD

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