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Modernization of WIPP PA

Heeho Park

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



Overview



- Introduction to WIPP
 - WIPP and WIPP PA
 - Why Modernize PA?
- Introduction to PFLOTRAN
- Current Progress
 - Integration of WIPP-specific functionality
 - Proof-of-concept 3D two-phase undisturbed scenario
 - Proof-of-concept 3D single-phase human borehole intrusion
- Advantages of Modernization
 - Consolidation into one code and single conceptual model
 - V&V testing suite and documentation

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WIPP





WIPP PA



- The DOE demonstrates compliance with containment requirements by means of performance assessment (PA) calculations conducted by Sandia National Laboratories (SNL) to Environmental Protection Agency (EPA)
- WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure.



PA Modernization



- Why?
 - 3D representation of the waste repository
 - Modifications or expansions
 - No requirement for symmetry
 - More realistic representation
 - More mechanistic process models
 - Anisothermal (heat generating wastes)
 - Miscible multiphase flow
 - Multicomponent transport
 - Radioactive decay and ingrowth, sorption, etc.
 - High-resolution mesh near repository (unstructured grid)
- How?
 - Massively parallel computing capability
 - Simulation size only depends on hardware capability





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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

Application of PFLOTRAN



- Nuclear waste disposal
 - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
 - DOE Used Fuel Disposition Program
 - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos²¹)
- 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
- CO₂ sequestration
- Enhanced geothermal energy
- Radioisotope tracers
- Colloid-facilitated transport



PFLOTRAN Multi-Physics Capability



- Flow
 - Single phase, variablysaturated
 - Multiphase gas-liquid
 - Interchangeable constitutive models and equations of state
- Energy
 - Thermal conduction and convection
- Multi-Component Transport
 - Advection
 - Hydrodynamic dispersion

- Chemical Reaction
 - Aqueous speciation
 - Mineral precipitationdissolution
 - Sorption
 - Microbiological
 - Radioactive decay with daughter products
- Geomechanics
 - Elastic deformation
- Geophysics
 - Coupling to E4D (Tim Johnson, PNNL)

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



PFLOTRAN Developers





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WIPP-Specific Functionality



- Gas generation in two-phase flow
- Change in porosity due to creep closure
- Fractures in marker beds and disturbed rock zones (DRZ)
- Klinkenberg effect
- RKS equation of state for gas density
- Material map change due to creep closure and borehole intrusion
- Direct brine release
- LHS interface with PFLOTRAN
- Preprocessor of PFLOTRAN PrePFLOTRAN

Verification of Functionalities



- WIPP-specific functionalities are implemented to PFLOTRAN
- The functionality is verified by comparing to the current PA code
- Verification on complex problem scenarios not possible due to key differences in process models.



WIPP Underground Structures





VisIT figures

Panels and Rooms



Room 7 Room 6 Room 5 Room 4 Room 3 Room 2 Room 1



Waste Rooms





3D two-phase flow and transport



- 3D single panel model
- Designed for proof of concept
- Flow model
 - Two-phase involving gas-liquid-energy (hydrogen, brine)
 - Initial Conditions
 - Excavated waste panel is unsaturated
 - Disturbed rock zone (DRZ) is 40% saturated due to mechanical opening
 - Rest of the domain is saturated up to the water table
 - Boundary Condition
 - No-flow boundary condition at 2 km away
 - Waste area generates gas (hydrogen) for 10,000 years as a function of saturation
 - Isothermal, Creep Closure, Fracture
- Transport model
 - Tracking tracer; Am-241, Pu-239, Pu-238, U-234, and Th-230;
 - Radioactive decay reactions
 - Pu-238 ($t_{1/2}$ =84yr) → U-234 ($t_{1/2}$ =2.46E5yr) → Th-230
 - Sorption

Single Panel Model Domain



- 97,614 elements
- Domain spans out 2 km from the panel in x and y directions



Geologic Structures at WIPP





VisIT figures

WIPP Surroundings





VisIT figures





BRAGFLO

PFLOTRAN



WIPP Specific Functions





3D two-phase flow and transport





ParaView Figures

3D two-phase flow and transport





ParaView animation

Borehole intrusion to brine pocket



- 3D single room with very large pressurized brine pocket model
- Designed for proof of concept
- Flow model
 - Single-phase with brine only
 - Initial Conditions
 - The domain is fully saturated even in excavated zone
 - Most extreme brine pocket pressure (15 MPa)
 - Boundary Condition
 - No-flow boundary condition at 600 m away from the room
- Transport model
 - Tracking tracer; Am-241, Pu-239, Pu-238, U-234, and Th-230;
 - Radioactive decay reactions
 - Pu-238 ($t_{1/2}$ =84yr) → U-234 ($t_{1/2}$ =2.46E5yr) → Th-230
 - Sorption

Borehole intrusion to brine pocket





Borehole intrusion to brine pocket





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 - PrePFLOTRAN "run control" system
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Consolidation into one code







D Unstructured/structured grid Coupled flow and transport Iculations Massively parallel Simulation size only depends on Irdware capability Mechanistic process models and

One conceptual model for Culebra and Halite





PFLOTRAN





Advantages of Modernization



- Offers easier peer review process in support of upgrades
 - A single governing equation for all flow
 - A single governing equation for all transport
 - Peer review of a single code when a new process model is introduced
- In-house code development expertise
- Every code modification is tracked and verified through automated regression, unit, and QA testing
- Easy to change grid if necessary (less bookkeeping required)
- Direct brine release simulation will use the same domain or a subset of the full domain (no need to read and assign artificial initial conditions).

PrePFLOTRAN



- Written in Python (ubiquitous and free)
- Documented with Sphinx
- Provides centralized "run control" for WIPP PA
 - Imports parameters from WIPP PA database
 - Converts parameters to PFLOTRAN-consistent format
 - Exports PFLOTRAN input decks (all files to execute a simulation) for all simulations (i.e. all vectors, scenarios, replicates)

Execution process





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Current file management





New file management





The Input Record File



- A text file which prints out all of the "ingested information" from the input file (parameter values, options, etc.)
- Can help catch mistakes a user makes in the input file
 - Parameters that are commented out or defined multiple times
- Can act as a stand-alone document which describes the specifics of a simulation
 - Anyone should be able to re-create the simulation with this file alone
- More reader-friendly
 - It's a less cryptic description of the simulation

10 transient pressure BC 2nd ki	
PFLOTRAN INPUT RECORD TU	e Aug 30 12:43:24 2016
input file: 1D_transi	ent_pressure_BC_2nd_kind.in
group:	
n processors: 1	
	CHECKPOINTS
specific times:	OFF
DMC:	PMCSubsurface
pmc timestepper:	FLOW
initial timester size:	8.6400000000000006 sec
nm:	flow
mode:	thermo-hvdro
	- Alternative Contraction (
simulation type	subsurface
flow mode:	thermo-hydro
reaw hode.	
:	TIME
max. timestep:	1.0000000E-02 day at time 0.0000000E+00 day
final time:	2.0000000E-01 day
periodic screen	ON
screen increment.	1
output time unit:	dav
······································	snanshot file output
format:	vtk
periodic timesten:	OFF
periodic time:	OFF
specific times:	ON
times (day):	1.0000000E-02 .4.0000000E-02 .9.0000000E-02 1.20000
variable list:	Temperature [C]
	Liquid Pressure [Pa]
	Liquid Saturation []
	Liquid Density [kg/m^3]
	Liquid Energy [k]/mol]
	Liquid Viscosity [Pa.s]
	Liquid Mobility [1/Pa.s]
	Material ID []
print initial time:	OFF
print final time:	ON
	observation file output
format:	tecplot
periodic timestep:	OFF
periodic time:	OFF
specific times:	OFF
variable list:	Temperature
	Liquid Pressure [Pa]





Test problems must remain simple (analytical solutions must exist)!



Software Verification Testing Suite



- Example test:
 - 3D domain
 - steady fluid flow/pressure field (steady-state solution)
 - dirichlet pressure boundary conditions



PFLOTRAN Documentation Overhaul

SPHINX

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- Overhaul approach:
 - Use a documentation generator program, such as Sphinx, to generate both the website and the PDF versions of the documentation:

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yThe 141	The PETROTEN Income Fill Flow OA Tests 110	compiler binaries (gou'glottran 4.9 at the > User's Guide 43	2 CONTENTS	
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Flo 213	Section 2.1.2, pg.15, "A 1 1D Transient T 160	HDH5 (pasilet output) 10 Steady The 120		
Flo 225	The domain is a 100x10x1	METIS/ParMETIS (southertand pids) 2D Steady The 130	Brooks-Corey Saturation Function	zero slope at the fully saturated end point and matching the derivative at a chosen variably saturated point that is close to fully saturated. The resulting equations for coefficients $a_{in} i = 0 - 3$, are given by
/Flo 239	ing properties: themal of the Television T	PELITRAN D Steady The 141	The Brooks-Corey saturation function is a limiting form of the van Genuchten relation for $p_1/p_1^2 \gg 1$, with the form	$a_1 + a_1x_1 + a_2x_2^2 + a_3x_1^2 - f_1$
/Flo 248	specific heat capacity Cp-1 TO Transferite T 190	2.2.2 Installing PFLOTRAN 3D Steady The 153	$n = \left(\frac{p_0}{p_1}\right)^{-1}$	$a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_3^2 = f_q,$
y Flo 260	heat flaxq(x=L)==15 W/ arp research (Fig. 200	10 Transient T 169	- (e)	$a_1x_1 + 2a_2x_1 + 3a_3x_1^2 = f_1^2$.
Flo 272	temperature distribution d 1D Stready Fig. 215	The first stars is in developed the developer stars. 10 Transferst T 179	with $\lambda = containd interverse relation$	$a_1x_2 + 2a_2x_3 + 3a_4x_4^4 = f_4,$
nt F 288	The LaPlace equation gov 10 Steerdor Fig. 225	Developer web site. The recommended approad the Transferrer T 192	$p_{ii} = p_i^0 s_i^{-1/3}$.	for chosen points x_1 and x_2 . In matrix form these equations become
nt F 298	10 Steady Flo 239	To compile PETSc it is first necessary to cost 2D Transland T 200	Relative Research The	$\begin{bmatrix} 1 & x_1 & x_1^* & x_1^* & x_2^* \\ 1 & x_2 & x_1^* & x_2^* & x_1^* & x_2^* \end{bmatrix} \begin{bmatrix} x_1 \\ x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \begin{bmatrix} x_1 $
	ZD Steady Flo 248 The solution is given by 20 Steady Flo 248	the installation, respectively. Eg., if using the 14	Landstee Landsteell	$\begin{vmatrix} 0 & 1 & 2x_1 & 3x_2' \\ 0 & 1 & 2x_2 & 3x_1' \\ \end{vmatrix} = \begin{vmatrix} x_1 \\ x_2 \end{vmatrix}$
	2D Steady Flo 200	seterr PETEC_DIA "path to petat-dev" 10 Steady Flo. 275	Two forms of the relative permeability function are implemented based on the Muslem and Bodine formulations. The quantity is is related to so by the expression.	
	SD Steady Flo 272	and 10 Steady Fig. 230		$f_1 = (s_1)_1, f_2 = 1, f'_1 = (s'_1)_1, f'_2 = 0.$ For minibut primetability $f = h_1(s_1), s_1 = 1, s_2 = 0.90, f_1 = 1.$
	When the boundary condi ID Transfort F 200	setery PETIC_ACE NecOIX-10.10.x-gct 30 Steady Flo. 340	$m = 1 - \frac{1}{n}, n = \frac{1}{1 - m},$ (12)	$f_2 = (k_r)_3, f_1^r = 0, f_2^r = (k_r^r)_3.$
	10 transience 290	Finally set the environmental variable VD 1 IV/1 2D Stearby Flo 240	for the Muslem Introduction and by	1.1.3 Mode: MPHASE
		autory W1 KWK CUPTER DIBU/CUPTER 3D Steady Flo. 272	$m = 1 - \frac{2}{n}, n = \frac{2}{1 - m},$ (13)	The mode MEMATE where the two-share content of water and unservitical CO. It may also be counted to chemistry
		setenv PATH SUPI_HOME/biniSPATH 1D Transleet E 300	for the Burdine formulation.	using the CHEMISTRY keyword and its various associated optional and required keywords for selecting the primary
		Decide which options are needed for running PF 4D Translook E 200	For the Mualem relative permeability function based on the van Genuchten saturation function is given by the expres-	and secondary aqueous species and setting up initial and boundary conditions and source/sinks. 10713/EE requires that the species CO2(aq) be used as primary species. In addition, for pure aqueous and supercritical CO2 phases, the
	3.5.2 The PFLOTR	needed then install METIS and ParMETIS. See 10 11 artisteric P 250	sion	input to 30 RASE requires specifying the mole fraction of CO ₂ . When coupled to chemistry, the CO ₂ mole fraction is calculated internally directly from the assesses concentrations specified in the COMPTRATIVE beyond.
	The Control Made 181 (C	For example, to configure PETSC to run in produ	$k_{\pi} = \sqrt{s_{\pi}} \left\{ 1 - \left[1 - (s_{\pi})^{1/m} \right]^m \right\}^{\pi}$. (1.4)	Local equilibrium is assumed between phases for modeling multiphase systems with PFLOTRAN. The multiphase
	CIMILATION	cd ./petac-dev	The Mualem relative permeability function based on the Brooks-Corey saturation function is defined by	partial differential equations for mass and energy conservation solved by PFLOTRAN have the general form:
	SIMULATION_TYPE SI	./config/configure.py -= with -debuggi download-opennpi≈1download-hdf5	$k_r = (s_r)^{3/2+2/\lambda}$	$\frac{\partial}{\partial u}\left(\psi \sum s_{\alpha}\eta_{\mu}x_{i}^{\alpha}\right) + \nabla \cdot \sum F_{i}^{\alpha} = Q_{i},$ (1.6)
	SUBSURFACE_FLOW	Oreck to make some no loce and no 1000 server	$= (p_c/p_c^0)^{-(0\lambda/2+b)}$,	
	HODE GENERAL	e.g. GNU gfortran version 4.7.a, Intel version 12	For the Burdine relative permeability function based on the van Genuchten saturation function is given by the expres-	for the <i>i</i> th component where the flux F_i^n is given by
	120		sion	$F^{lpha}_i = q_{lpha} a_{lpha} x^{lpha}_i - arphi s_{lpha} D_{lpha} q_{lpha} abla x^{lpha}_i,$
			$k_{c} = s_{c}^{2} \left\{1 - \left[1 - (s_{c})^{1/m}\right]^{m}\right\}.$ (1.5)	ad
			The Burdine relative permeability function based on the Brooks-Corry saturation function has the form	$\frac{\partial}{\partial t}\left(\varphi \sum s_{\alpha}\eta_{\alpha}U_{\alpha} + (1 - \varphi)\rho_{c}c_{c}T\right) + \nabla \cdot \sum \left[q_{\alpha}\eta_{\alpha}H_{\alpha} - \kappa\nabla T\right] = Q_{c},$ (1.7)
		44	$k_{-} = (s_{+})^{2+3/\lambda}$	for more in these constitutes of definitions of the latter ($\alpha = 1$ and at immediate T and account B with the same
			$n_{e} = (n_{e})$ $(p_{e})^{-(\theta+bb)}$	we energy, so setse equations α designates a must phase ($\alpha = i$, sc) at temperature I and pressure P_{α} with the same over all fluid phases present in the system, and source/sink terms Q_i and Q_i described in more detail below. Species
			$= \begin{pmatrix} t_{ij} \\ p_{ij}^{aj} \end{pmatrix}$.	are designated by the subscript $i \ (i = H_2O, CO_2)$; φ denotes the porosity of the porosis medium; s_α denotes the phase saturation state; x_α^α denotes the mole fraction of species <i>i</i> satisfying
			Smoothing	$\sum x_i^n = 1$.
		PFLOTRAN Documentation, Release 1.1	At the end points of the saturation and relative permeability functions it is sometimes necessary to arough the func-	the countries on H. H. reflects the maker density and denses of a stability dense of a stability dense of a stability of the
			tions in order for the Newton-Raphson equations to converge. This is accomplished using a third order polynomial	and q_{α} denotes the Datcy flow rate for phase α defined by
			incorporation of manching the values of the function to be in (capitally pressure or netative permeability), and imposing	$q_{\perp} = -\frac{k k_{\perp}}{2} \nabla (P_{\perp} - r_{\perp} \pi \pi),$
				μ. μ
			4 Chanter 1 Theory Guide	11. Annexedix A: Generations 5

Questions?



 Thanks to Glenn Hammond for Introduction to PFLOTRAN slides, and Jennifer Frederick for V&V suite and documentation slides

