SAND2021-8173PE

Exceptional service in the national interest

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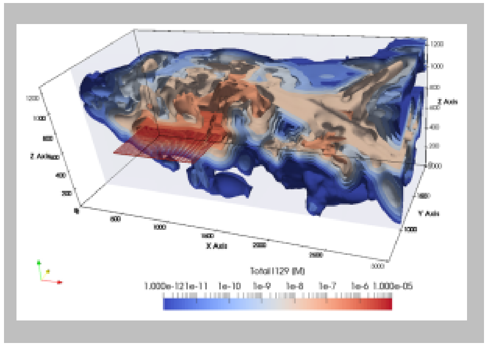
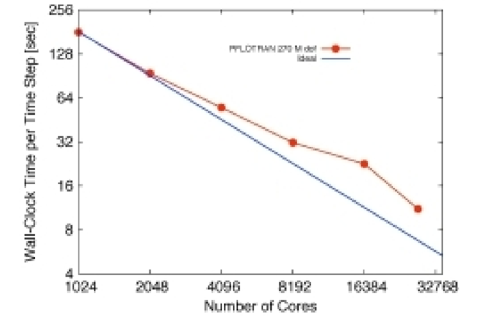
$$\frac{\partial m_a}{\partial t} = -\nabla\cdot\left(\rho_l X_a^l \boldsymbol{q}_l + \rho_g X_a^g \boldsymbol{q}_g + \boldsymbol{J}_a^l + \boldsymbol{J}_a^g\right) + q_a^G,$$

$$\frac{\partial m_w}{\partial t} = -\nabla\cdot\left(\rho_l X_w^l \boldsymbol{q}_l + \rho_g X_w^g \boldsymbol{q}_g + \boldsymbol{J}_w^l + \boldsymbol{J}_w^g\right) + q_w^G,$$

$$\frac{\partial e}{\partial t} = -\nabla\cdot\left(\rho_l H_l \boldsymbol{q}_l + \rho_g H_g \boldsymbol{q}_g - \kappa_{\text{eff}}\nabla T\right) + q_e^G,$$





PFLOTRAN Multiphase Flow

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Immiscible/Miscible

Figure 13: Immisible fluids on the left and miscible fluids on the right [32].

[32] Baldwin Lawrence. *Unit 3 Solutions Chemistry*, Aug 2015. URL `http://slideplayer.com/slide/5941102/release/woothee`.

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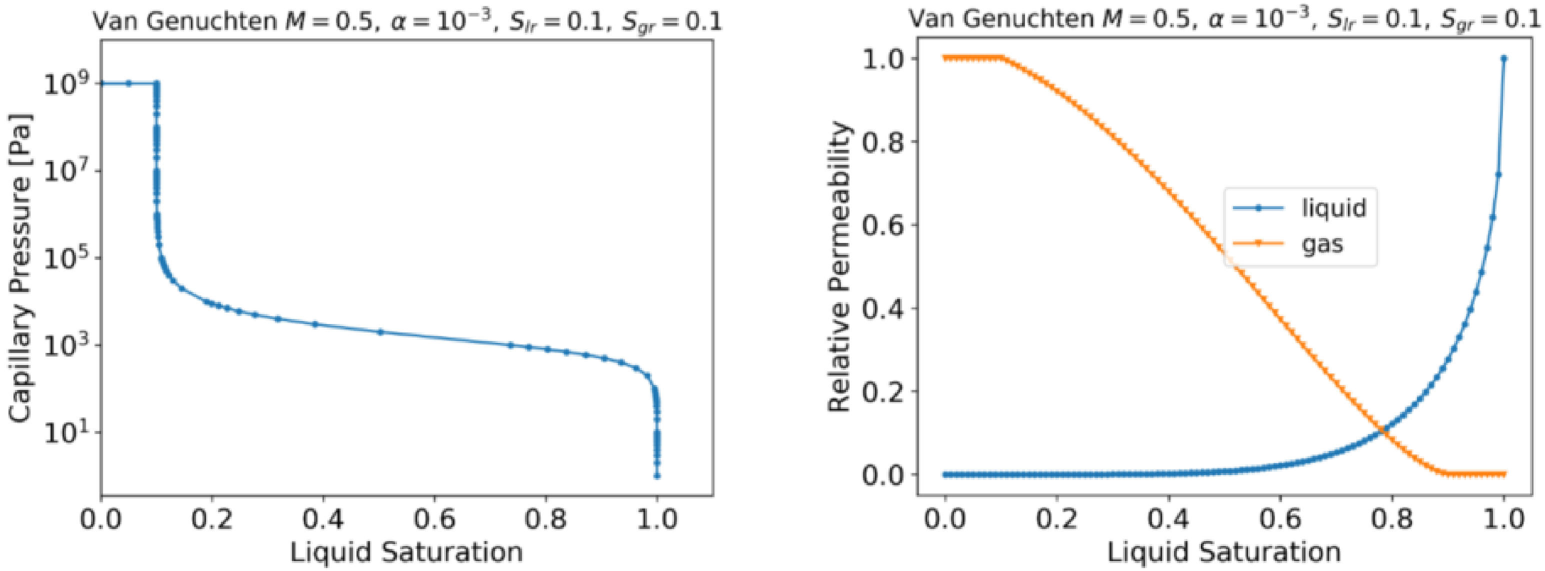
Capillary Pressure Relative Permeability



(a) (b)

Figure 2: This is an example of van Genuchten analytical formulation with $s_{rg} = 0.1$, $s_{rl} = 0.1$, $\alpha = 10^{-3}$, and $m = 0.5$: (a) capillary pressure as a function of saturation is in Eq. 10 and (b) liquid and gas relative permeability as a function of a liquid saturation in Eq. 13 and Eq. 14, respectively.

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Governing Equations

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]

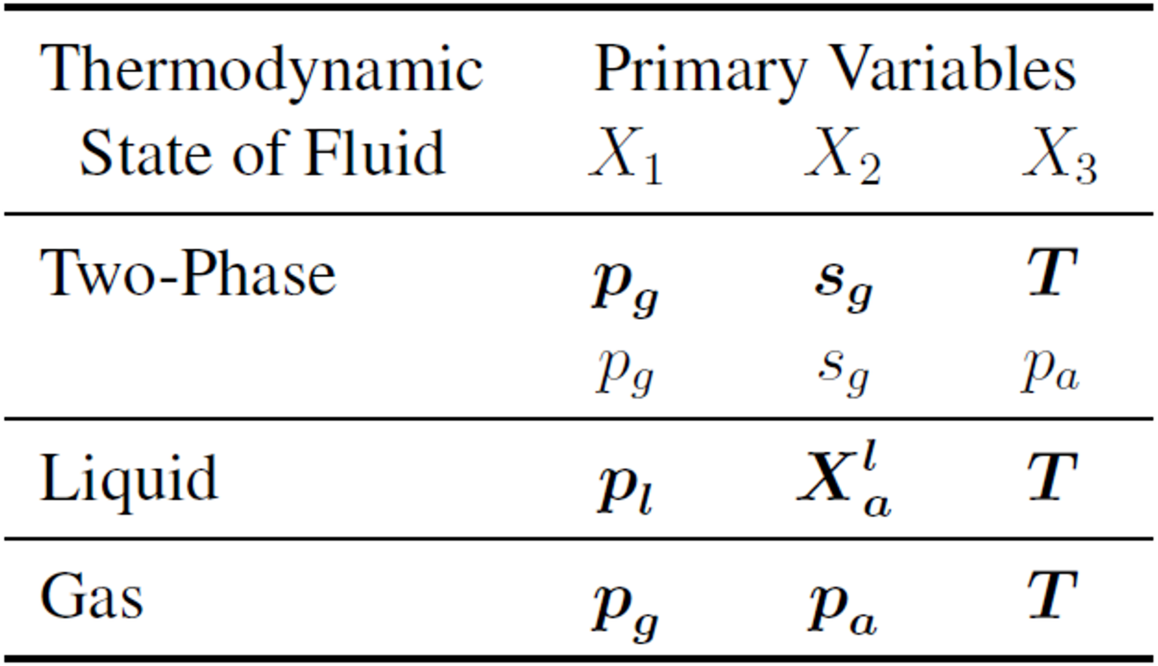
$\boldsymbol{J}_a^g$ = diffusive flux of air in gas phase [kmol/m^2-s]

D_g^0 = gas diffusivity [m^2/s]

p_0 = reference pressure [Pa]

Primary Variables

General Mode



Thermodynamic State of Fluid	Primary Variables		
	X_1	X_2	X_3
Two-Phase	$\boldsymbol{p_g}$	$\boldsymbol{s_g}$	$\boldsymbol{T}$
	p_g	s_g	p_a
Liquid	$\boldsymbol{p_l}$	$\boldsymbol{X_a^l}$	$\boldsymbol{T}$
Gas	$\boldsymbol{p_g}$	$\boldsymbol{p_a}$	$\boldsymbol{T}$

Linearized System

General Mode

$$\begin{bmatrix} \frac{\partial F_{p_l}}{\partial p_l} & \frac{\partial F_{p_l}}{\partial x_a^l} & \frac{\partial F_{p_l}}{\partial T} \\ \frac{\partial F_{x_a^l}}{\partial p_l} & \frac{\partial F_{x_a^l}}{\partial x_a^l} & \frac{\partial F_{x_a^l}}{\partial T} \\ \frac{\partial F_T}{\partial p_l} & \frac{\partial F_T}{\partial x_a^l} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_l \\ \delta x_a^l \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_l} \\ F_{x_a^l} \\ F_T \end{bmatrix}_n$$

Single-phase liquid state

$$\begin{bmatrix} \frac{\partial F_{p_g}}{\partial p_g} & \frac{\partial F_{p_g}}{\partial x_w^g} & \frac{\partial F_{p_g}}{\partial T} \\ \frac{\partial F_{x_w^g}}{\partial p_g} & \frac{\partial F_{x_w^g}}{\partial x_w^g} & \frac{\partial F_{x_w^g}}{\partial T} \\ \frac{\partial F_T}{\partial p_g} & \frac{\partial F_T}{\partial x_w^g} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_g \\ \delta x_w^g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_g} \\ F_{x_w^g} \\ F_T \end{bmatrix}_n .$$

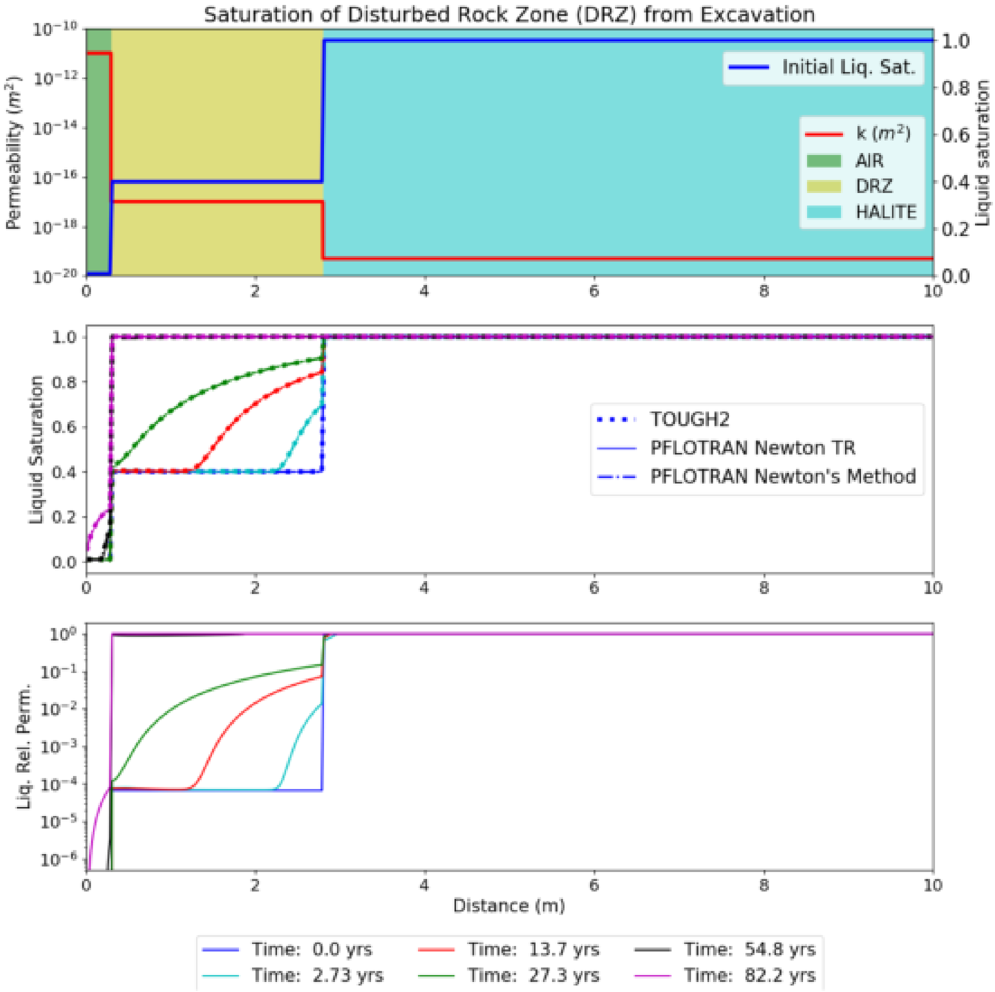
Single-phase gas state

$$\begin{bmatrix} \frac{\partial F_{p_g}}{\partial p_g} & \frac{\partial F_{p_g}}{\partial s_g} & \frac{\partial F_{p_g}}{\partial T} \\ \frac{\partial F_{s_g}}{\partial p_g} & \frac{\partial F_{s_g}}{\partial s_g} & \frac{\partial F_{s_g}}{\partial T} \\ \frac{\partial F_T}{\partial p_g} & \frac{\partial F_T}{\partial s_g} & \frac{\partial F_T}{\partial T} \end{bmatrix}_n \begin{bmatrix} \delta p_g \\ \delta s_g \\ \delta T \end{bmatrix} = - \begin{bmatrix} F_{p_g} \\ F_{s_g} \\ F_T \end{bmatrix}_n$$

Two-phase state

Phase transition	Criteria
Liquid phase → two-phase	$p_v \leq p_{sat}(T)$
Liquid phase ← two-phase	$S_g < 0.0$
Gas phase → two-phase	$p_v \geq p_{sat}(T)$
Gas phase ← two-phase	$S_g > 1.0$

Benchmark



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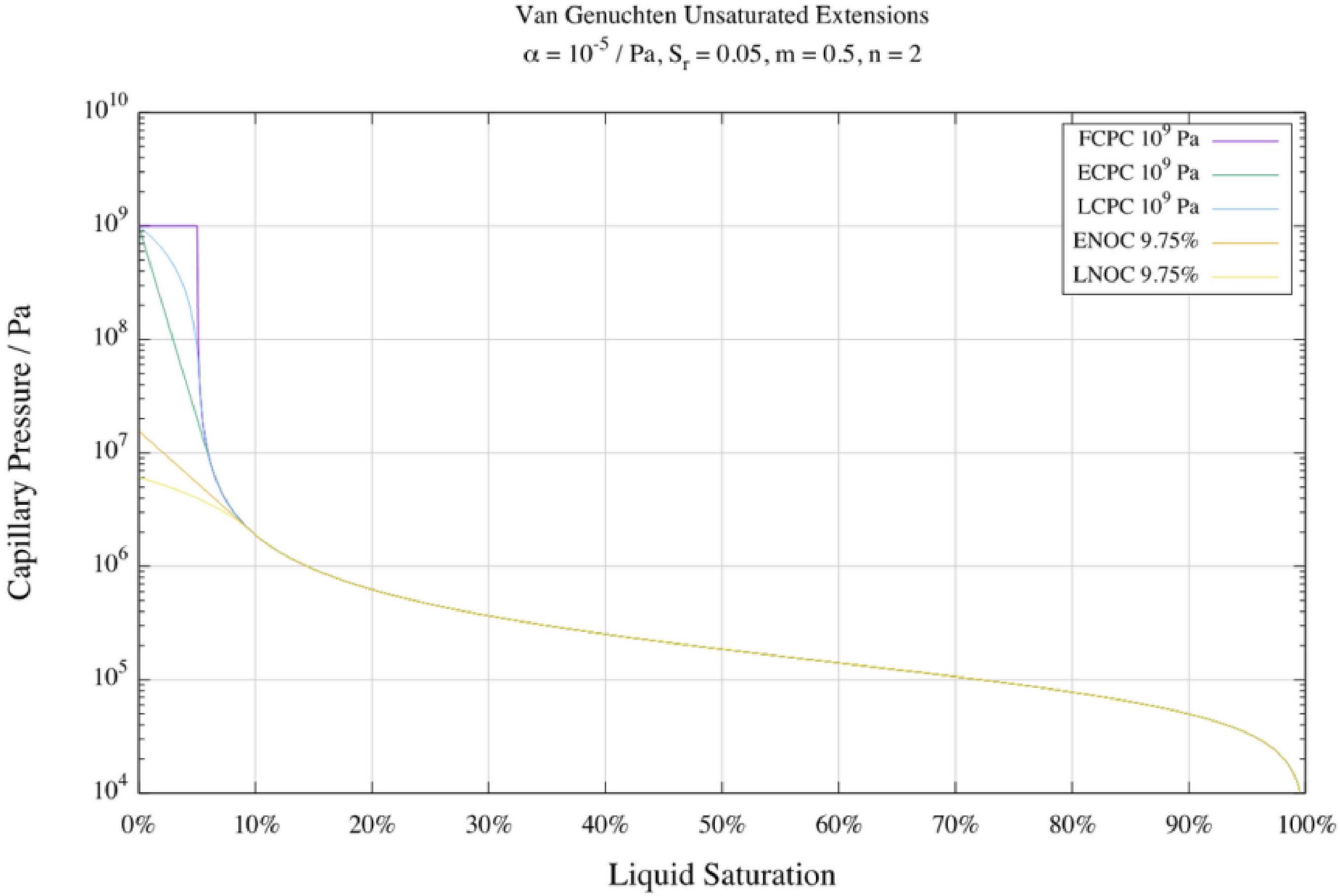
van Genuchten extension



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Performance

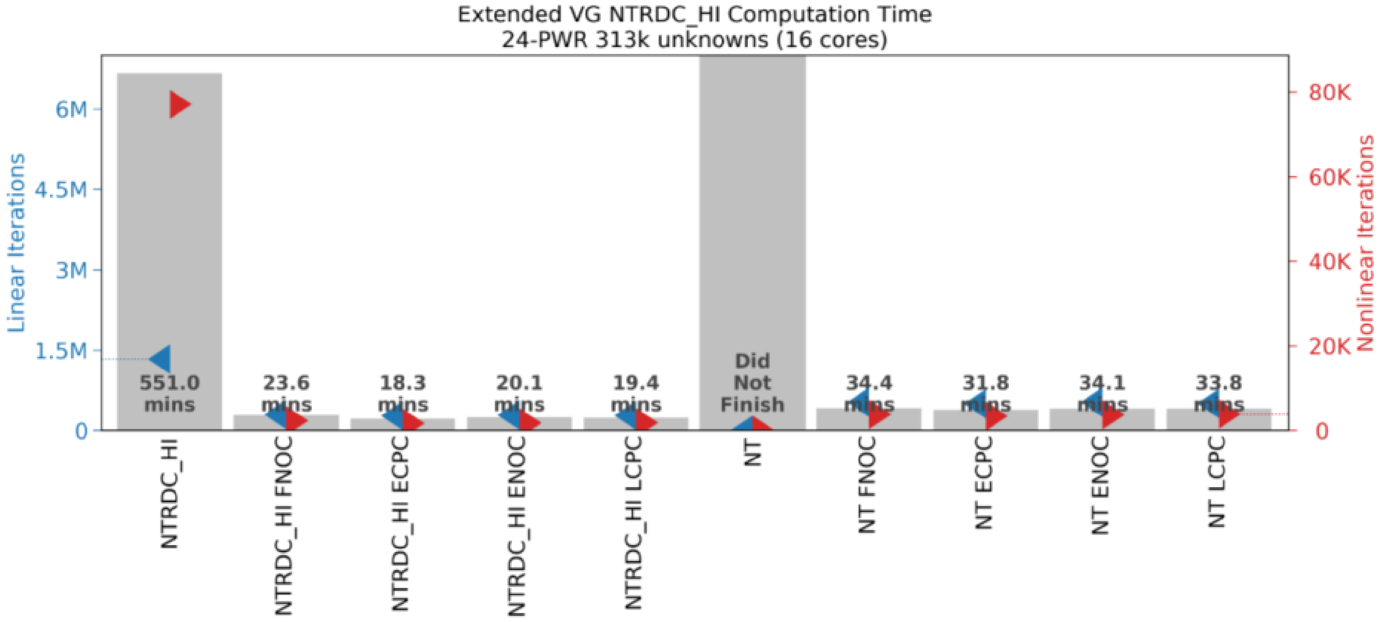

Figure 11: The plot shows the coarsened model 24-PWR case (boiling) computation wall clock time. VG1 is the original van Genuchten curve, VG2 is FNOC, VG3 is ECPC, VG4 is ENOC, and VG5 is LCPC in Figure [VG curve variance added by Matt]. The extended curve at the liquid residual saturation improves the nonlinear solver performance.

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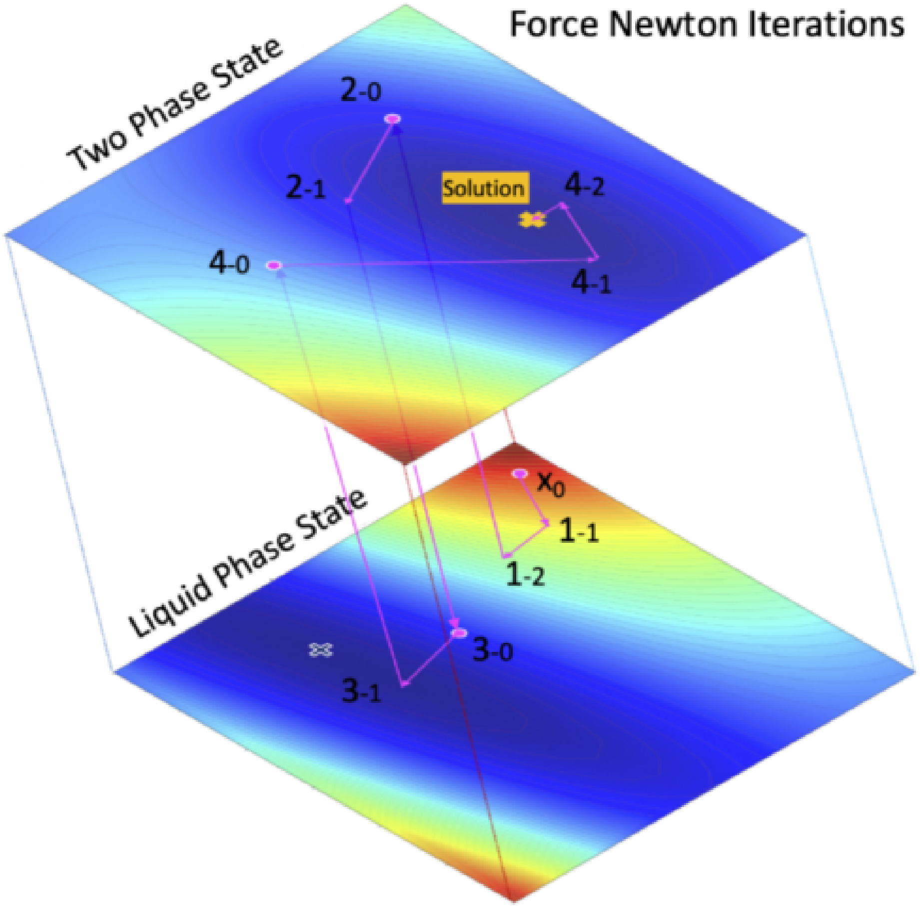
Residual Space Change for State Changes



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Absolute Strong Scaling

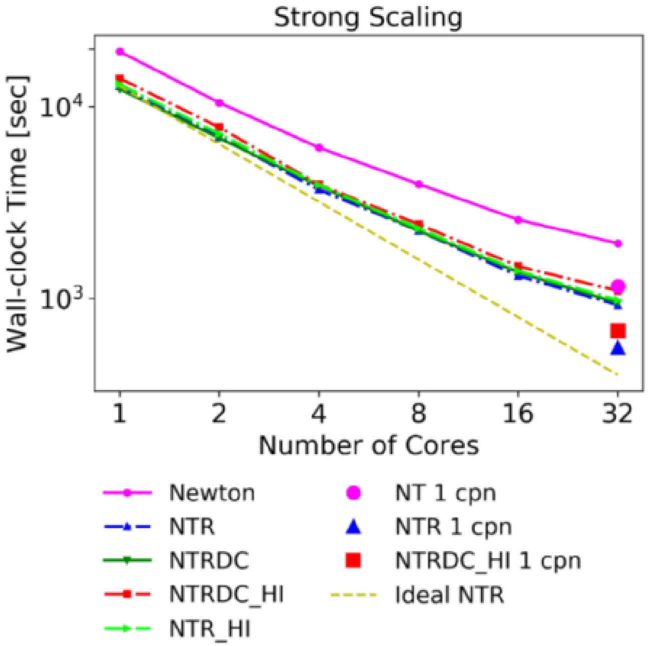

Figure 16: Wall clock time in seconds is plotted against the number of cores involved in the simulation which represents true strong scaling (a single core base case) of Newton (NT), NTR, NTRDC, NTR_HI, and NTRDC_HI. The new nonlinear solvers shows as good of scalability as Newton and follows the trend of ideal strong scaling plot, and it follows the ideal line even closer when node packing defect is reduced by running on 1 core per node on 32 nodes.

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Relative Strong Scaling

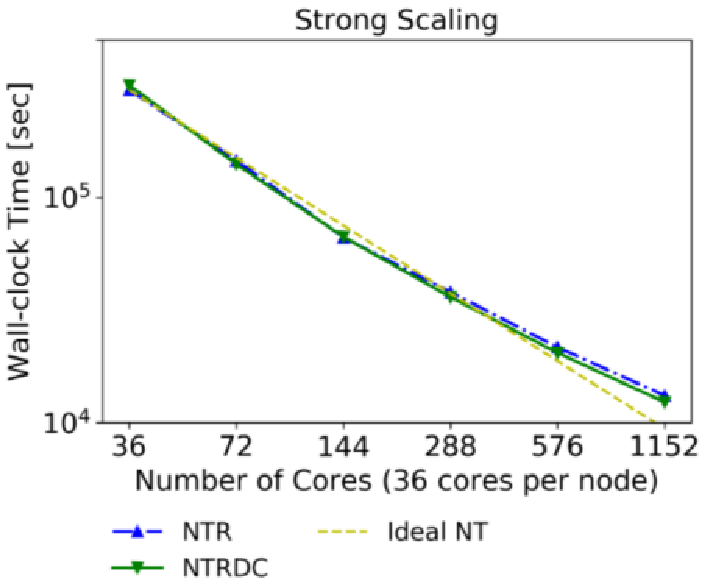

Figure 17: The plot shows the relative strong scaling where the base case is running 1 node with 36 cores, a fully packed node. The strong scalability is right on top of the ideal line.

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