PROCEEDINGS, 44th Workshop on Geothermal Reservoir Engineering
Stanford University, Stanford, California, February 11-13, 2019
SGP-TR-214

# High-Enthalpy Geothermal Simulation with Continuous Localization in Physics

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**Keywords:** continuous localization in physics, high-enthalpy geothermal, negative compressibility

## ABSTRACT

Simulation of heat production in high-enthalpy geothermal systems is associated with a complex physical process when the cold water is invading the steam-saturated control volumes. Because of phase transition and the large variation in thermodynamic properties between liquid water and steam, the nonlinear numerical solution of governing equations in fully-implicit approximation can experience difficulties commonly known as 'negative compressibility'. In the process of solution, due to the steam condensation, the reduction in fluid volume reduces the pressure in the control volume. It creates a region in parameter space where the gradient of the residual equation does not point to the direction of the solution. If initial guess of the nonlinear problem is located in this region, the solution based on Newton's update cannot converge and needs to be repeated for a smaller timestep. This problem brings simulation to the stalling behaviour where nonlinear solver wastes a lot of computations and performs at very small timestep. To tackle this problem, we formulate continuous localization of Newton's method based on Operator-Based Linearization (OBL) technique. In OBL approach, the continuous operators in the governing equations, related to different physical mechanisms (e.g. convection or conduction), are translated into multi-dimensional tables. In the course of simulation, only the supporting points evaluated based on the reference physics when points between them are interpolated. This provides a unique mechanism where nonlinear physics can be represented at different scales of accuracy. The coarser is the representation, the more linear operators become. In our continuous localization approach, we start with the coarse approximation of the governing physics in pressure-enthalpy parameter-space. Due to the more linear form of operators, only a few nonlinear iterations reduce residual below the predefined tolerance. Next, the OBL approximation is modified towards the reference nonlinear physics and a few more iterations bring the residual below the tolerance again. With the refinement in physics, the solution will gradually approach the final solution where residual will satisfy the convergence criteria of the reference physics. This continuous localization in physics avoids the 'negative compressibility' phenomena since the problem at the coarser approximation has a unique gradient pointing towards the correct solution and helps to localize the solution for higher resolutions in the region of monotone gradient behaviour. As a result, simulation can perform at larger timesteps in comparison to the traditional nonlinear solution.

## 1. INTRODUCTION

During the development of geothermal reservoirs, the injected cold water will be heated by in-situ fluid/rock and the heat could be carried up to the surface through water reinjection and cycling. For high-enthalpy geothermal systems, either single phase (vapor or liquid) or their two-phase mixture can be present at the reservoir conditions. When developing the high-enthalpy geothermal reservoir with cold water injection, hot steam condensation happens after its contact with cold water. Therefore, multiphase flow and transport with phase changes appear in high-enthalpy geothermal systems.

In geothermal simulation, the mass and energy formulations are often tightly coupled because of the fluid thermodynamic properties (Coats et al., 1974). The fully-coupled fully-implicit approach is generally adopted to solve the system. In a high-enthalpy geothermal simulation, numerical simulators can experience great difficulties, one of which is commonly known as 'negative compressibility' (Coats, 1980). This problem was first described by Coats (1980) with single-cell setup, where cold water is injected at fixed pressure into a cell with saturated steam. Due to the invading of cold water, hot steam will condense, and the cell pressure will drop with steam shrinkage during phase transition. The cell pressure will constantly decrease until the steam is condensed and cell pressure goes up to the injection pressure. To guarantee convergence, the timestep should be severely restricted which is often addressed as 'stalling behaviour', see Pruess (1999) for example.

Pruess et al. (1987) and Falta et al. (1992) discussed the 'negative compressibility' problem. They connect the 'negative compressibility' effect because of the idealization of complete thermodynamic equilibrium within the computational grids. Spurious pressure variation could happen in the cells that contain the two-phase front because of the instantaneous thermodynamic equilibrium assumption, which will enforce severe limitations to the nonlinear convergence. Wang (2015) made an analysis of 'negative compressibility' problem in the fully implicit formulation. In that analysis, to ensure convergence of the fully implicit solution, a stability criterion for the timestep was developed and unnecessary timestep cuts were avoided. However, the derived stability criterion still enforces a severe limitation to the allowable timestep size. Wong et al. (2018) applied a nonlinear preconditioner to the fully coupled, fully implicit solution. The formulations were first solved with a sequential fully implicit approach (SFI) and then the solutions were taken as the initial guess for the fully implicit method (FIM) (Wong et al., 2017). Using this approach, the severe timestep restriction was reduced for some practical scenarios. However, there is still no robust strategy for converging high-enthalpy nonlinear solution at a target timestep in the presence of the 'negative compressibility' phenomena.

During numerical simulation, the governing equations need to be discretized in both space and time to get approximate solutions. Usually, the formulation in discretized form is nonlinear and should be linearized. The Newton-based process is generally adopted to linearize the discretized formulation, which includes the construction of the Jacobian matrix and residuals. The values of fluid properties and their derivatives are involved in Jacobian assembly. When complex physics (i.e. multiphase compositional flow, complex chemical reaction) are present in the model, multiphase flash calculation is often necessary for accurate fluid/rock properties estimation, which requires to solve highly nonlinear local constraints during each Newton iteration for molar formulation (Collins et al., 1997, Voskov and Tchelepi, 2012). Therefore, the Jacobian assembly can take up a large portion of overall simulation time. Voskov (2017) proposed the operator-based linearization (OBL) approach to simplify this process and accelerate the linearization process. Like discretization in space and time, the main idea of OBL is to discretize the physics within the space of nonlinear unknowns.

In OBL, the governing equations are written in form of operators with two categories: state-dependent and space-dependent. The state-dependent operators can be parameterized with respect to nonlinear unknowns in multi-dimension tables with different resolutions. The tables consist of pre-computed supporting points. The values and derivatives of the operators in parameter space can be interpolated and evaluated based on supporting points. For adaptive parameterization technique (Khait and Voskov, 2018b), the supporting points are calculated 'on-fly' and stored for later re-usage, which could largely save time for parameterization in high-dimensional parameter-space (i.e. in multi-component compositional simulation). At the same time, the Jacobian assembly becomes simple and flexible with OBL even for very complex physical problems.

The OBL approach provides an opportunity to control the nonlinearity in physics by changing the resolution of parameter space. In other words, if fewer supporting points are chosen in parameter space, the nonlinear physics will become more linear, which makes it easier for the nonlinear solver to converge (Voskov, 2017). In this work, we follow the hierarchy of physical approximation in parameter space using OBL formalism and construct a continuous solution in physics to solve the 'negative compressibility' problem. We start with general formulations and numerical strategies used in thermal-compositional simulations and briefly introduce the OBL approach. Next, 'negative compressibility' problem in single-cell is described from Newton path, residual distribution and operator surface. Afterward, the continuous localization in physics is adopted to solve the 'negative compressibility'. In the end, an idealized one-dimension test case is used to verify the feasibility of the proposed method.

## 2. METHODOLOGY

Here, we consider the governing equations and nonlinear formulation for two-phase thermal simulation with flow and transport in aqueous reservoir. This problem can be described by mass and energy equations:

$$\frac{\partial}{\partial t}\left(\phi \sum_{j=1}^{n_p} \rho_j s_j\right) - div \sum_{j=1}^{n_p} \rho_j u_j + \sum_{j=1}^{n_p} \rho_j \tilde{q_j} = 0, \tag{1}$$

$$\frac{\partial}{\partial t}(\phi \sum_{j=1}^{n_p} \rho_j s_j U_j + (1-\phi)U_r) - div \sum_{j=1}^{n_p} h_j \rho_j u_j + div(\kappa \nabla T) + \sum_{j=1}^{n_p} h_j \rho_j \tilde{q_j} = 0, \tag{2}$$

where: $\phi$ is porosity, $s_j$ is phase saturation, $\rho_j$ is phase molar density, $U_j$ is phase internal energy, $U_r$ is rock internal energy, $h_j$ is phase enthalpy, $\kappa$ is thermal conduction.

Fluid flow in the reservoir follows Darcy's law,

$$u_j = K \frac{k_{rj}}{\mu_j}\left(\nabla p_j - \gamma_j \nabla D\right), \tag{3}$$

where: $K$ is permeability tensor, $k_{rj}$ is relative permeability, $\mu_j$ is viscosity of phase $j$, $p_j$ is pressure in phase $j$, $\gamma_j$ is gravity vector, $D$ is depth. In addition, to close the system, the summation of phase saturation should be equal to one, $\sum_{j=1}^{n_p} s_j = 1$

Next, Darcy's law is substituted into the governing equation and the resulting nonlinear equations are discretized with finite-volume method in space on a general unstructured mesh and with backward Euler approximation in time:

$$V\left[(\phi \sum_{j=1}^{n_p} \rho_j s_j)^{n+1} - (\phi \sum_{j=1}^{n_p} \rho_j s_j)^{n}\right] - \Delta t \sum_{l}\left(\sum_{j=1}^{n_p} \rho_j^l \Gamma_j^l \Delta\psi^l\right) + \Delta t \sum_{j=1}^{n_p} \rho_j q_j = 0, \tag{4}$$

$$V\left[\left(\phi \sum_{j=1}^{n_p} \rho_j s_j U_j + (1-\phi)U_r\right)^{n+1} - \left(\phi \sum_{j=1}^{n_p} \rho_j s_j U_j + (1-\phi)U_r\right)^{n}\right] - \Delta t \sum_{l}\left(\sum_{j=1}^{n_p} h_j^l \rho_j^l \Gamma_j^l \Delta\psi^l + \Gamma_c^l \Delta T^l\right) + \Delta t \sum_{j=1}^{n_p} h_j \rho_j q_j = 0, \tag{5}$$

where $V$ is the control volume and $q_j = \tilde{q}_j V$ is the source of phase $j$. $\Delta\psi^l$ is the phase pressures difference (including gravity and capillary pressure) between blocks connected via interface $l$, while $\Delta T^l$ is a temperature difference between these neighboring blocks; $\Gamma_j^l = \Gamma^l k_{rj}^l / \mu_j^l$ is a phase transmissibility, where $\Gamma^l$ is the constant geometrical part of transmissibility (which involves permeability and the geometry of the control volume). $\Gamma_c^l = \Gamma^l \kappa = \phi(\sum_{j=1}^{n_p} s_j^l \lambda_j^l - \kappa_r) + \kappa_r$ is the thermal transmissibility.

Molar formulation (Faust and Mercer, 1975; Wong et al., 2015) is taken as the nonlinear formulation, in which pressure and enthalpy are chosen as primary variables. In general, Newton-Raphson method is adopted to solve the linearized system of equations in each nonlinear iteration in the following form:

$$J(\omega^k)(\omega^{k+1} - \omega^k) + r(\omega^k) = 0, \tag{6}$$

where $J$ is the Jacobian defined at the $k_{th}$ nonlinear iteration. In conventional approach, the Jacobian assembly involves calculation of accurate property values and their derivatives with respect to nonlinear unknowns. This may require either various interpolations (for properties such as relative permeabilities) or solution of a highly nonlinear systems (e.g. multiphase flash). As a result, the nonlinear solver takes a lot of time to resolve all small variations in properties, which are sometimes unimportant due to the numerical nature and uncertainties in property evaluation. The Operator-Based Linearization approach, described below, is proposed to resolve this issue.

## 3. OPERATOR-BASED LINEARIZATION (OBL) APPROACH

Based on the OBL approach, the mass and energy governing equations are distinguished into different operators, which are expressed as functions of a physical state $\omega$ and/or a spatial coordinate $\xi$ (Voskov, 2017; Khait and Voskov 2018a). Pressure and enthalpy are taken as the unified state variables for a given control volume. Flux-related fluid properties are defined by the physical state of upstream block $\omega_{up}$, determined at interface $l$. The state-dependent operator is defined as a function of the physical state only; the space-dependent operator is defined by both physical state $\omega$ and spatial coordinate $\xi$.

The discretized mass conservation equation in operator form reads as:

$$a(\xi,\omega)\big(\alpha(\omega) - \alpha(\omega_n)\big) + \sum_l b(\xi,\omega)\beta(\omega) + \theta(\xi,\omega,u) = 0; \tag{7}$$

$$a(\xi,\omega) = \phi V;\ \alpha(\omega) = \sum_{j=1}^{n_p} \rho_j s_j;\ b(\xi,\omega) = \Delta t \Gamma^l (p^b - p^a);\ \beta(\omega) = \sum_{j=1}^{n_p} \rho_j^l \frac{k_{rj}^l}{\mu_j^l}. \tag{8}$$

The discretized energy conservation equation in operator form is as follows:

$$a_e(\xi,\omega)\big(\alpha_e(\omega) - \alpha_e(\omega_n)\big) + \sum_l b_e(\xi,\omega)\beta_e(\omega) + \sum_l c_e(\xi,\omega)\gamma_e(\omega) + \theta_e(\xi,\omega,u) = 0; \tag{9}$$

$$a_e(\xi) = V(\xi);\ \alpha_e(\omega) = \phi\left(\sum_{j=1}^{n_p} \rho_j s_j U_j - U_r\right) + U_r;\ b_e(\xi,\omega) = b(\xi,\omega);\ \beta_e(\omega) = \sum_{j=1}^{n_p} h_j^l \rho_j^l \frac{k_{rj}^l}{\mu_j^l}; \tag{10}$$

$$c_e(\xi) = \Delta t \Gamma^l (T^b - T^a);\ \gamma_e(\omega) = \phi\left(\sum_{j=1}^{n_p} s_j \lambda_j - \kappa_r\right) + \kappa_r. \tag{11}$$

This representation significantly simplifies the general-purpose simulation framework. Instead of performing a complex evaluation of each property and its derivatives during the simulation, we can parameterize the state-dependent operators in the space of unknowns with a limited number of supporting points and use multilinear interpolation to evaluate them (Voskov, 2017). This not only makes the Jacobian assemble simpler but also improves the performance since all expensive property evaluations can be skipped. In addition, due to the piece-wise multilinear approximation of physical operators, the system will become more linear and performance of nonlinear solver can be improved.

## 4. SINGLE CELL PROBLEM

### 4.1 Formulations

The 'negative compressibility' problem can be described using a single-cell model with a cold-water injection at the fixed pressure (Coats, 1980; Wong et al., 2018). To facilitate the description, the following assumptions are made: (1) neglect the rock energy; (2) heat conduction is ignored; and (3) rock is incompressible. Therefore, we get the following mass and energy conservation equation for a single cell problem:

$$\mathrm{V}\frac{\partial \rho_t}{\partial t} - \Upsilon(p_{in} - p) = 0, \tag{12}$$

$$\mathrm{V}\frac{\partial \rho_t h}{\partial t} - H_{in}\Upsilon(p_{in} - p) = 0, \tag{13}$$

$$\rho_t = \rho_w s_w + \rho_s s_s, \tag{14}$$

where: $\Upsilon$ is the flow transmissibility at the injection boundary, $p_{in}$ is the fixed pressure of the injection boundary, $p$ is the cell pressure, $h$ is the cell enthalpy, $\rho_t$ is the fluid density, $\rho_w$, $\rho_s$ are the density of water and steam, $s_w$, $s_s$ are the enthalpy of water and steam. Below, we take an example to illustrate this problem with $p = 50$ bar, $h = 2000$ kJ/kg, $s_s = 0.97$ and $p_{in} = 90$ bar, $H_{in} = 345$ kJ/kg.

### 4.2 Newton path

Wong et al. (2018) derived and distinguished the timestep based on the pressure solution of Newton update. Here, we take the timestep that force Newton solution to diverge. Figure 1 shows the Newton path with an initial guess chosen at the initial conditions. Because of the large variations in thermodynamic properties between water and steam phase, the residual equation becomes highly nonlinear. In Figure 1, one can recognize two minima in the residual map: one (at the upper right part) is the local minimum which does not correspond with the solution (here residual is not equal to zero); the other one (at the lower middle part) is the real solution of the problem. If the Newton update follows the gradient of the residual equation starting with the proposed initial guess, it will converge to the wrong local minimum. Notice that in conventional nonlinear solvers, the solution at previous timestep is taken as the initial guess for Newton method which can be any point in parameter space. To check how convergence for a given set of parameters depends on the initial guess, we choose uniformly distributed points within pressure-enthalpy space and check convergence for all of them respectively. The convergence map is shown in Figure 2.

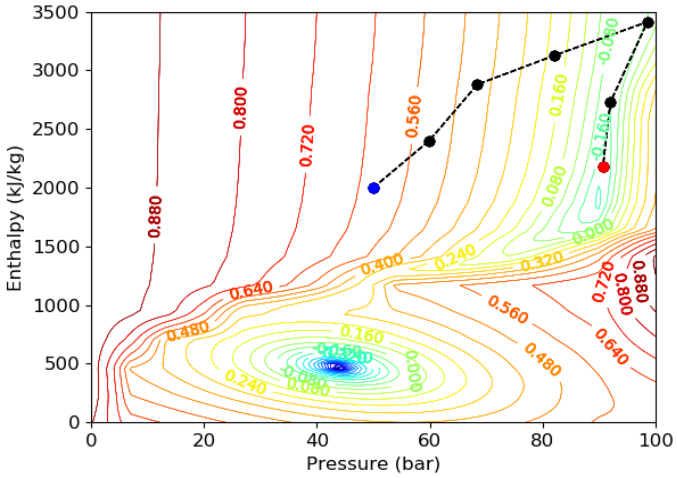


**Figure 1: Newton path (dash line) starts from the initial condition; the contours (in $l_2$-norm) show the residuals, blue dot represents the initial condition of the cell, black dots are the Newton updates, red dot shows the solution for a current timestep.**

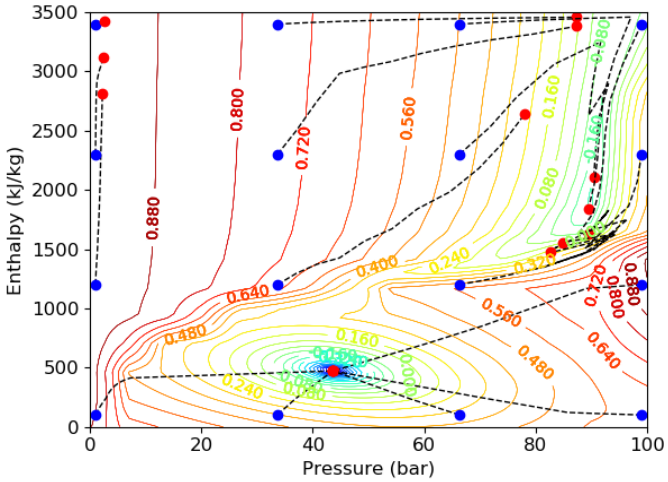


**Figure 2: Newton paths (dash line) starts from various points in pressure-enthalpy space; the contours (in $l_2$-norm) show the residuals, blue dots represent the initial guess, red dots show the solution for a current timestep.**

It is clear from Figure 2 that the Newton path starting with points in the two-phase region (upper part of the residual map) will either diverge or converge to the local minimum; while for the points in the single-phase region, the Newton iterations will converge to the real answer. As the results, if the initial guess is in the two-phase region, the simulation at this timestep will waste several nonlinear iterations and finally cut the current timestep (and, possible, few more after). This indicates that finding a suitable initial guess for Newton iterations is essential to guarantee the performance at a targeted timestep in a geothermal simulation with steam condensation.

### 4.3 Operators

In Figure 3, the operators for mass and energy conservation equations are plotted with fine resolution tables. Here, α_m and β_m correspond to the accumulation and flux term in mass equation (7), α_e and β_e correspond to the accumulation and flux term in energy equation (9). As you can see, all operators are highly nonlinear in pressure-enthalpy parameter space. If the initial guess is in the two-phase region, for the Newton process cannot jump across the phase boundary and stay on the wrong side. This gives another evidence to the fact that nonlinear solver struggles in the high-enthalpy geothermal simulation.

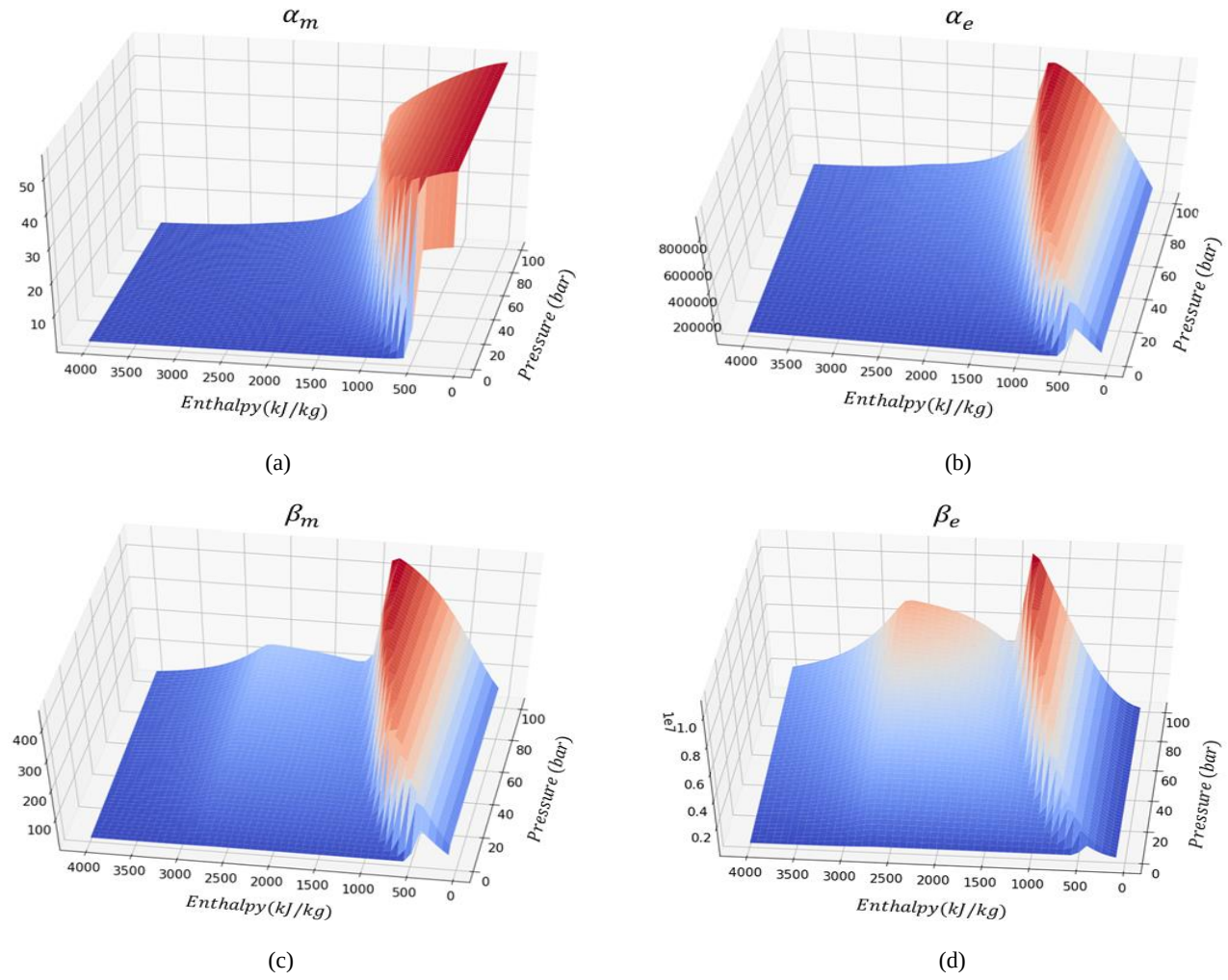


**Figure 3: Operators in mass and energy conservation equations for single cell problem. (a) mass accumulation, (b) energy accumulation, (c) mass flux, (d) energy flux.**

## 5. CONTINUOUS LOCALIZATION IN PHYSICS

Through the analysis above, we notice the high nonlinearity in physics causes difficulties for the gradient-based nonlinear solver and force it updating in the wrong direction. This inspires our approach with a multi-level physics parameterization.

### 5.1 Continuous localization

- Instead of solving the system with reference (fine) physics, we start the simulation for a targeted timestep with the coarse OBL parameterization. Because of the coarse resolution of parameter space, the residual map will change and becomes almost linear with a monotonically behaving residual (see Figure 4(a) as an illustration). This means that only a few iterations are needed to reach the solution at this coarse physics resolution. Notice that even though the solution at this stage is different from the final solution, this solution still belongs to its close neighbourhood.

- Next, the physical space is refined and the previous (coarse) solution is taken as an initial guess. The solution at this finer resolution will be located closer to the real (reference) solution. This will help to localize the Newton update and move in the right direction. Notice in Figure 4(b) that the full residual already behaving non-monotonically and there is a region in parameter-space with a wrong gradient (in the upper-right part). However, the localization stage at a coarser level helps to safeguard the Newton update towards the true solution.

- Finally, we refine the physical space to the reference resolution. Similar to the previous stage, the solution at previous OBL resolution is taken as an initial guess for the reference physical resolution. Even though the residual is non-monotone at the reference resolution and a large region of the parameter-space has the wrong gradient (see Figure 4(c)), the localization near the solution at previous OBL resolutions helps to safeguard the Newton update into the direction of a true solution.

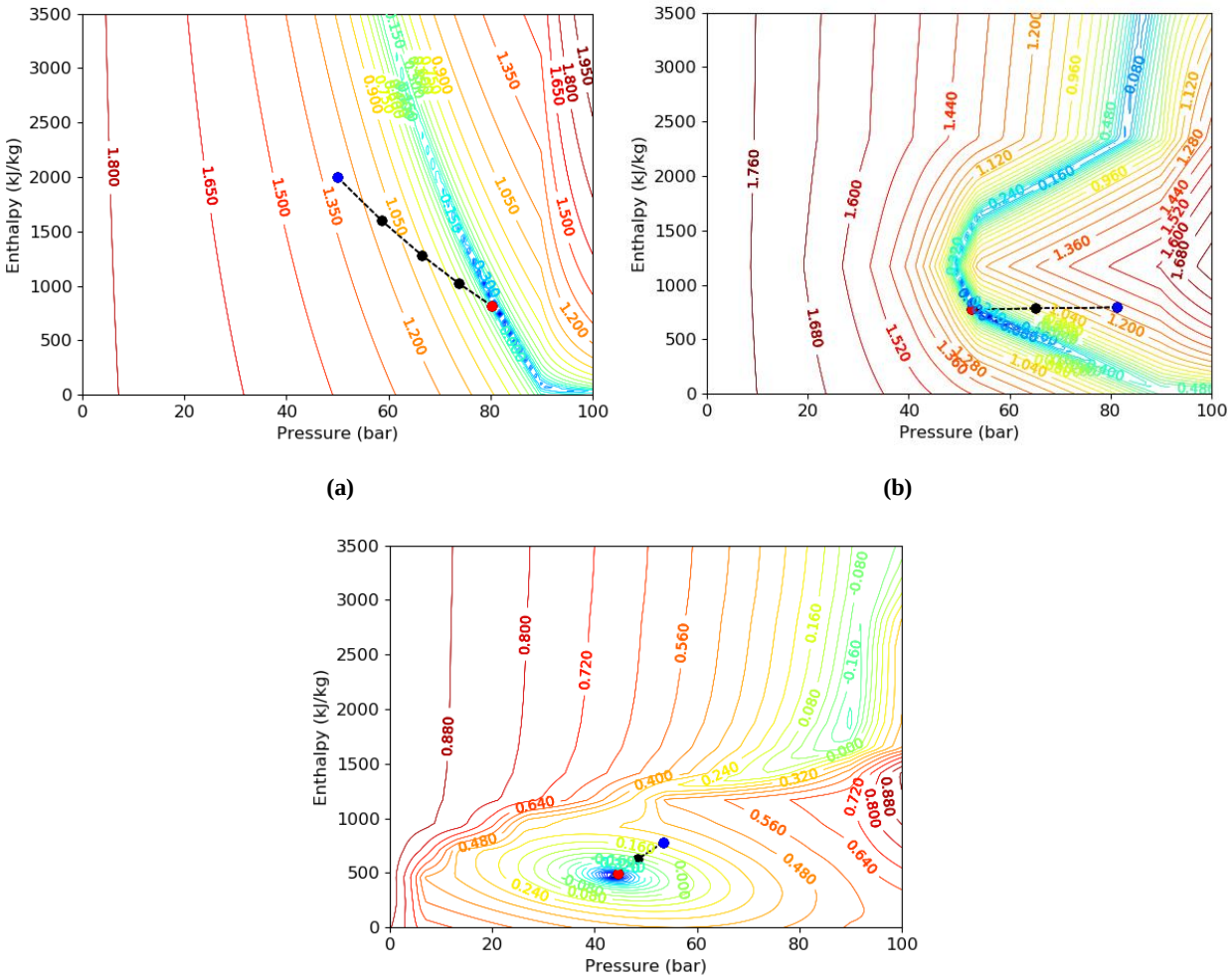


**Figure 4: Newton path and residual contours (in $l_2$-norm) with continuation parameterization in physics: (a) Newton path for a coarse resolution; (b) Newton path for an intermediate resolution; (c) Newton path for fine (reference) resolution; blue dot represents the initial guess, black dot is the Newton update, red dot shows the solution.**

### 5.2 Convergence analysis

To verify the feasibility of our approach for different initial guesses, we choose various points uniformly distributed in the parameter space and the results of Newton convergence are shown in Figure 5. It is obvious that any initial guess in parameter-space will first converge to the unique solution for the coarsest representation, see Figure 4(a). In Figure 5 we show that the approach can converge to the true solutions for different lengths of the timestep. Notice that the nonlinearity of the coarsest representation is low, and the convergence rate for this resolution is fast. With the refinement, the nonlinearity is growing, but localization helps to keep a high convergence rate. As the result, independent from the initial guess, the nonlinear solver based on continuous localization in physics remains fast and unconditionally stable.

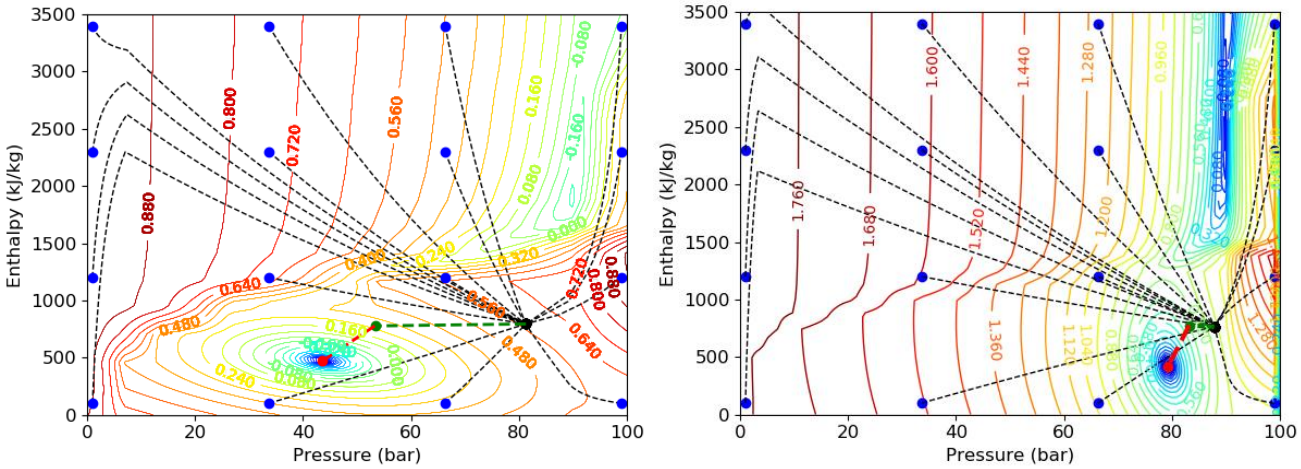


**Figure 5: Newton path (dash line) starting from various points in pressure-enthalpy space with (a) moderate and (b) large timestep; blue dots represent the initial guess, black dot is the solution of coarsest resolution, green dot is the intermediate solution and red dot is the true solution; dash lines in black, green and red represent the Newton path in the coarse, intermediate and fine (reference) physics resolution respectively; residual contours (in $l_2$-norm) are plotted for the reference physics.**

### 5.3 One-dimensional test case

To support the proposed strategy with simulation results, we present a simple synthetic 1D model. Here we assume that the cold water is injected at a fixed pressure into a water reservoir at two-phase (water-steam) conditions, see Figure 6 as an illustration. We compare conventional Newton-based nonlinear solver with the proposed continuous-localization strategy in this model. The simulation results are shown in Figure 7.

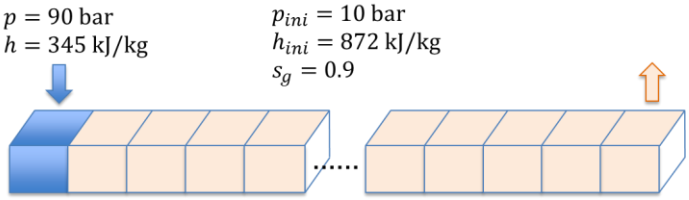


**Figure 6: Schematics of 1D test case**

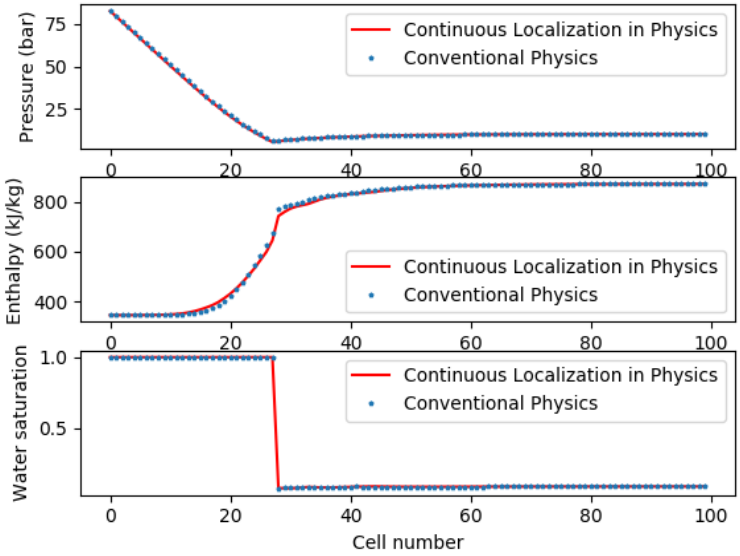


**Figure 7: Simulation results with continuous localization in physics with a large timestep (red line) and conventional Newton-based approach with the reduced timestep (blue dots)**

Due to the 'negative compressibility' phenomena, the conventional nonlinear solver cannot converge at targeted timestep and keep cutting timesteps. When we run the conventional simulation at timestep 10 times lower, the simulation successfully converged, see results in Figure 7 as blue points. At the same time, the continuous localization approach helps to converge nonlinear iterations at the target timestep. The total number of nonlinear iterations in continuous localization is 1350 versus 8556 in the conventional simulation with reduced timestep. Notice that the number of nonlinear iterations is directly proportional to the simulation const.

## CONCLUSION

Since mass and energy conservation equations are tightly coupled through the fluid thermodynamics in high-enthalpy geothermal processes, they usually solved in a fully-implicit manner. The 'negative compressibility' phenomena can significantly struggle the convergence of the nonlinear solver. Because of the large variation of thermodynamic properties between water and steam, the governing equations show high nonlinearity with phase transition. We analyse the problem in a single cell setup with a cold water injection at fixed pressure. The analysis of residual map demonstrates that two different minima can be present in the parameter space when simulator is performing at sufficiently large timesteps, which brings challenges for gradient-based nonlinear solver. Suitable initial guess is essential for the Newton-based nonlinear strategy.

Applying the Operator-Base Linearization (OBL) approach, we propose the continuous localization in physics to solve the governing system of equations. With parametrization in physics changing from a coarse to fine resolution, the state-dependent operators and resulting residual is changing from almost linear and monotone behaviour to a highly nonlinear and non-monotone shape. In the proposed nonlinear strategy, the solution at a coarser parametrization in physics is taken as an initial guess for the solution at a finer physics resolution. This continuous localization approach makes the nonlinear convergence process more robust in the presence of the 'negative compressibility' phenomena. To verify the feasibility of this approach, we prepare a synthetic one-dimensional test case and make a comparison between the conventional and proposed approaches. The results demonstrate that the simulation of high-enthalpy geothermal applications can benefit from the continuous localization by running the model at sufficiently large timesteps with a limited number of nonlinear iterations.

## ACKNOWLEDGEMENT

We acknowledge Yang Wong and Mark Khait for their technical help and useful discussions.

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