



EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling



Preconditioning for Thermal Reservoir Simulation

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1 Introduction

Background

Models of fluid flow in porous media are used in the simulation of applications such as petroleum reservoirs, carbon storage, hydrogeology, and geothermal energy. In some cases, fluid flow must be coupled with heat flow to capture thermal effects. For example, heat from the Earth's core (geothermal energy) flows upward, heating water reservoirs in the crust. These reservoirs can be tapped to generate electricity or heat buildings. This process involves the flow of water, steam, and heat through porous rock.

Oil and gas recovery from petroleum reservoirs is the main application of interest for this project. A petroleum reservoir is a subsurface pool where hydrocarbons and water sit deep underground in porous rock trapped under a layer of impermeable rock. This is illustrated in Figure 1. The drilling of wells creates a pressure gradient that causes the fluids to flow up to the surface, allowing for the extraction of hydrocarbons. This is known as the Primary Oil Recovery. Once they stop naturally lifting to the surface, water can be injected inside the reservoir to displace some of the remaining hydrocarbons and maintain the pressure difference.



Figure 1 – A typical oil and gas reservoir.

To increase recovery, "Enhanced Oil Recovery" (EOR) techniques are then used. This is especially important for heavy viscous oils. EOR techniques include CO_2 injection, chemical injection, and thermal recovery. The recovery of heavy oils can be facilitated by reducing their viscosity. A variety of thermal recovery techniques are used to achieve that goal.

Steam Injection Cyclic Steam Stimulation is a thermal recovery technique consisting of three stages: injection of steam to increase temperature, a resting period to let the heat diffuse, followed by oil production from that same well. Other techniques — Steam or Hot Water Flooding — use steam or hot water injection wells in conjunction with production wells. These methods combine the viscosity-decreasing effects of heat with the physical displacement of oil being pushed by the water. Steam-Assisted Gravity Drainage (SAGD) is an example of Steam Flooding where a horizontal injection well is drilled above a production well allowing gravity to help with the oil displacement. This process is illustrated in Figure 2.

In-Situ Combustion is a thermal recovery technique in which heat is generated through the combustion of the hydrocarbons inside a reservoir by injecting air or oxygen. While less stable, this process is generally cheaper than steam injection. When In-Situ Combustion is successfully applied, distillation and cracking of hydrocarbons can result in the production of lighter and more valuable oil.

A less standard thermal recovery technique is Electromagnetic Heating. An electrical current can be used to increase the temperature of the reservoir, which can be combined with steam injection techniques. Various frequencies are being considered; from low frequency electric resistive heating to high-frequency microwave heating. Such methods could minimise heat losses that occur during steam injection.

Thermal recovery techniques are used to reduce the viscosity of heavy oils.



Figure 2 - Steam-assisted gravity drainage (SAGD).

Reservoir simulation is the use of mathematical models to predict the flow of fluids through porous media. Petroleum engineers use reservoir simulation to optimise oil recovery processes. For example, history matching uses observed behaviour from the actual reservoir to update the reservoir model. This type of inverse problem, as well as other predictive techniques, require the rapid solution of the forward model. This explains the need for fast and robust commercial reservoir simulators. The simulation of geothermal energy problems is also very similar to petroleum reservoir simulation.

Mathematical model

Mathematical models for oil reservoirs describe flow through porous media. For single-phase flow, the model comprises of a conservation of mass equation, where the velocity of the fluid is usually described using Darcy's law, relating the velocity to the pressure gradient. This can easily be generalised for multiphase flow, in which mass transfer between phases is allowed. The presence of different fluids and hydrocarbons are described by saturation or concentration variables. Black-oil systems are a special case of these models in which we assume that there is a water phase, an oil component which can form its own phase or get dissolved in the water, and a gas component which can form its own phase or get dissolved in the oil. This model may be written as a system of coupled partial differential equations (PDEs). In order to solve the systems numerically, we discretise and apply an iterative nonlinear solver (e.g. the Newton-Raphson method) to the resulting nonlinear system. At each iteration of the nonlinear solver, a sparse linearised system must be solved. In the case of reservoir simulation, the linearised system is of the block form

$$Ax = \begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix} \begin{bmatrix} x_p \\ x_s \end{bmatrix} = \begin{bmatrix} b_p \\ b_s \end{bmatrix} = b,$$
(1)

where A_{pp} is a block matrix representing the "pressure coefficients", A_{ss} is a block matrix representing the coefficients of the "secondary variables" (typically concentrations/saturations), and A_{sp} and A_{sp} represent the respective coupling coefficients. The solution of the system is the vector x, where x_p is the pressure variable and x_s represents the secondary variables. The vector b is the residual of the system, where b_p is the residual of the pressure equation and b_s represents the residuals of the secondary equations. The pressure equation is represented by the first row of this system, and the second row represents the equations for the secondary variables, in that it is elliptic, and the other equations are not. The ellipticity of the pressure equation means that the effect of the pressure is global, i.e. a change in pressure in one part of the reservoir influences the flow everywhere in the reservoir. In contrast, the secondary variables are local in nature.

Since the linear system (1) can be very large, solving it directly may simply require too much time or memory. Instead, iterative methods, generally Krylov subspace methods, are used to generate a sequence of improving approximate solutions. These linear solvers benefit from the sparsity of the linearised system. The convergence of iterative methods can be accelerated by the use of preconditioners (transformations applied to the linear system). Earlier preconditioners were mostly designed for general linear systems, and

The ellipticity of the pressure equation means that the pressure variable has an influence over the whole reservoir.

A preconditioner makes a linear system easier to solve by iterative methods. can be very successful for simple scalar PDEs (e.g. Incomplete LU factorisation (ILU)). However, the simulation of coupled multiphysics problems involves solving systems of highly coupled PDEs.

The linearisation of a system of PDEs results in a linear system with a block structure like (1). The different blocks represent the different "physics" of the problem acting on the different variables. This justifies the use of block preconditioners which allow the treatment of the different "physics" within the preconditioner, whilst a Krylov subspace method is applied to the complete coupled problem. These problem-specific preconditioners usually perform much better than their generic counterparts.

An important part of block preconditioning is the design of efficient Schur complement approximations. The Schur complement appears when factorising the system matrix as a product of block matrices. Approximating the Schur complement is needed to maintain the sparsity of the preconditioning operator for a fast solution.

The global nature of the pressure variable requires a more precise global preconditioning than saturation variables for which local preconditioning is sufficient. This justifies the use of two-stage preconditioners where we first solve for the pressure approximately (using Algebraic Multigrid for example) and then solve the full system (using ILU for example). This preconditioner is known as constrained pressure residual (CPR) [1].

Multigrid methods combine successively coarser grids and a basic iterative method (relaxation) to reduce all error components. This strategy is "global" and thus effective for elliptic differential operators. Instead of needing a coarse grid hierarchy, Algebraic Multigrid (AMG) constructs the coarse problems solely with information from the system matrix. The elliptic-like nature of the pressure system solved in the first stage of CPR makes it an ideal candidate for the use of multigrid methods. AMG typically requires less work from the user than geometric variants (for example, a mesh hierarchy is not required for AMG). Therefore, it is often preferred in industrial code.

Glossary of terms

- <u>Diffusion</u>: The movement of something from a region of higher concentration to a region of lower concentration.
- **Advection:** The transfer of something by the flow of a fluid.
- **Sparse:** A linear system is *sparse* if the system matrix has mostly zero entries.
- <u>Algebraic Multigrid (AMG)</u>: Numerical method effective at solving elliptic problems.
- Incomplete LU factorisation (ILU): Simple numerical method effective at solving transport problems.
- **Schur complement:** A dense block that appears when factorising the system matrix as a product of block matrices.

Challenges of thermal reservoir simulation

In non-isothermal models, an energy conservation equation is added to the system along with a temperature (or enthalpy) variable. For fully implicit formulations, the industry-standard preconditioner is CPR where temperature variables are grouped with the secondary variables (as denotes by s in (1)). This is often appropriate since heat is being advected similarly to the saturations. However, heat is also diffused through rock and fluids. Diffusion can dominate in cases where the fluid flow is slow, for instance before viscous oils are properly heated, but also numerically due to mesh refinements. In those cases, the second stage of CPR struggles to capture the heat diffusion, and so incomplete factorisations with additional fill are needed. This remedy is not ideal in terms of scalability and memory requirements. Additionally, AMG can struggle in the first stage of CPR for thermal simulations.

How to precondition linear systems resulting from thermal cases is still an open question. Efforts to find an answer are limited in the reservoir engineering community.

The global nature of the pressure variable requires a global preconditioning strategy. CPTR is an extension of CPR for the thermal case. In this project, we develop an extension of CPR for non-isothermal flow. Instead of solving a restricted pressure system in the first stage of CPR, we solve a restricted pressure-temperature system, resulting in a Constrained Pressure-Temperature Residual method (CPTR). The choice of solver for the first stage of CPTR is a major challenge for this approach. To investigate pressure-temperature solvers, we first consider single-phase non-isothermal flow. The single-phase model results in a pressure-temperature system of similar properties to the one considered in the first stage of CPTR. On its own, the single-phase case is relevant for simple geothermal energy and reservoir simulation examples but is also similar to miscible displacement problems (where a concentration plays a similar role to temperature, and molecular diffusion is analogous to heat diffusion).

For the single-phase case, we created a Schur complement approximation for the pressuretemperature system. Such an approximation leads to an effective block preconditioner. Then, we propose an extension of that method to the multiphase flow situation and use it for the pressure-temperature subsystem in the first stage of CPTR. As an alternative, we also consider applying an unknown-based AMG method to the pressure-temperature subsystem.

2 Two-stage preconditioning

The methods described in this section are multiplicative two-stage preconditioners, and so we first provide here a generic definition for a linear system Ax = b. Let M_1 and M_2 be two preconditioners approximating the system matrix A, for which we know a way of applying their (generally approximate) inverses M_1^{-1} , and M_2^{-1} . Applying the resulting two-stage preconditioner for the system Ax = b can be done as follows:

- 1. Apply the first preconditioner: $x_1 = M_1^{-1}b$;
- 2. Compute the new residual: $b_1 = b Ax_1$;
- 3. Apply the second preconditioner: $x = M_2^{-1}b_1 + x_1$.

The action of the two-stage preconditioner can also be written in the explicit form

$$M^{-1} = M_2^{-1}(I - AM_1^{-1}) + M_1^{-1}.$$
 (2)

Constrained Pressure Residual (CPR)

The CPR preconditioner is a two-stage preconditioner where the preconditioner M_1 solves a restricted system for the pressure

$$M_1^{-1} \approx \begin{bmatrix} A_{pp}^{-1} & 0\\ 0 & 0 \end{bmatrix},$$
 (3)

where A_{pp}^{-1} is generally approximated using an AMG.

If the pressure solution given in the first stage is accurate, only transport problems for the saturations and temperature remain (assuming that heat diffusion is not significant). Therefore, a simple method such as ILU is adequate for the second stage preconditioner M_2 .

Constrained Pressure-Temperature Residual (CPTR)

The addition of an energy conservation equation introduces cases where the pressure preconditioner fails to fully capture the behaviour of the flow. Indeed, in thermal simulations, temperature also has a large influence over the flow and should be treated differently from the saturation variables. We are interested in developing preconditioners which consider the effect that temperature has on fluid flow and heat flow.

Consider temperature-related blocks differently from the saturation blocks. We rewrite (1) as

$$Ax = \begin{bmatrix} A_{pp} & A_{pT} & A_{ps} \\ A_{Tp} & A_{TT} & A_{Ts} \\ A_{sp} & A_{sT} & A_{ss} \end{bmatrix} \begin{bmatrix} x_p \\ x_T \\ x_s \end{bmatrix} = \begin{bmatrix} b_p \\ b_T \\ b_s \end{bmatrix} = b,$$
(4)

where the entries with subscript T now denote the energy/temperature-related entries. Let the pressure-temperature submatrix

$$A_{00} = \begin{bmatrix} A_{pp} & A_{pT} \\ A_{Tp} & A_{TT} \end{bmatrix}, \text{ so that } A = \begin{bmatrix} A_{00} & A_{0s} \\ A_{s0} & A_{ss} \end{bmatrix}.$$
 (5)

For CPTR, The first stage preconditioner M_1 is given by

$$M_1^{-1} = \begin{bmatrix} A_{00}^{-1} & 0\\ 0 & 0 \end{bmatrix},$$
 (6)

where A_{00}^{-1} is an approximation of the action of the inverse of A_{00} . An important challenge for CPTR is to determine an efficient pressure-temperature solver A_{00}^{-1} .

Similarly to CPR, we use ILU for the second stage preconditioner M_2 .

Pressure-temperature solver

In order to study the effects of both pressure and temperature on fluid and heat flow, we first consider a model of non-isothermal single-phase flow through porous media. By focusing on single-phase flow, we are able to isolate the properties of the pressure-temperature subsystem.

Our studied system is nonlinear since both the density and viscosity of the fluid are functions of pressure and temperature. The fluid velocity depends on the viscosity and so it is coupled with temperature. Additionally, the heat flow depends both on advection (and so pressure dependent) and diffusion (or conduction). This cross-coupling must be considered when preconditioning. We consider new preconditioning strategies that include variants of Algebraic Multigrid.

The single-phase problem requires the solution of a linearised system for pressure and temperature, which can be written as a 2x2 block system. For the pressure-temperature system, we develop a block preconditioner for which we need an efficient Schur complement approximation.

For our approximation, we considered the similarities between the advective terms of the mass and energy equations to argue that some differential operators in the Schur complement can cancel under reasonable assumptions. In the end, our Schur complement approximation is the temperature block without the terms resulting from linearisation. The resulting block preconditioner provides a treatment of the temperature block using an Algebraic Multigrid method. This results in the preconditioner capturing the heat diffusion appropriately.

We then extended the block preconditioner developed for the pressure-temperature system in the single-phase case to the multiphase case for the first stage of CPTR.

An alternative to the block preconditioner is the unknown-based AMG method. The strategy is to treat the variables corresponding to the same unknown separately. For a block matrix, classical AMG coarsening and interpolation are applied to the individual diagonal blocks. Computationally cheap and easy to implement, the unknown-based approach will perform well if the cross-coupling between unknowns is not too strong and the diagonal blocks are amenable for the application of classical AMG.

3 Outcomes

To have easy access to the different preconditioners provided by the PETSc library, we use the open-source Finite Element software Firedrake to handle spatial discretisation. Using Firedrake, we implemented a fully implicit parallel non-isothermal multiphase flow in porous media simulator. This implementation includes all the methods described above. The code used for our experiments can be found on GitHub¹.



(a) Permeability in *x* and *y* directions.

(b) Permeability in *z* direction

Figure 3 – Log of permeability of the SPE10 test case (mm²).

We consider the two-phase flow of highly viscous oil and water. We perform mesh refinement studies on homogeneous (isotropic and anisotropic) porous media. We also investigate the parallel scalability of the different methods for these cases as well as the heterogeneous SPE10 case illustrated in Figure 3.

For the single-phase case with only oil, we evaluate the performance of CPR and the block preconditioner on the pressure-temperature system. We compare different Schur complement approximations. Then, for the multiphase case, we compare CPR to CPTR. For the first stage of CPTR, we compare unknown-based AMG with the block preconditioner with our own Schur complement approximation.

For the single-phase block preconditioner, our Schur complement approximation performs better than the simple ones, especially in cases with heterogeneous or anisotropic permeability. As we refine the mesh, the number of iterations has a very small increase for the block preconditioner, but a large increase for CPR. The heat diffusion is much more noticeable on fine meshes, which CPR does not treat appropriately. Note that the success of the block preconditioner is also due to the linear scalability of AMG for elliptic problems. By removing the need for ILU, we get a nearly mesh-independent preconditioner.

While the block preconditioner performs well for diffusion-dominated cases, CPR is still the method of choice for advection-dominated (manufactured) cases, at least in serial. However, the block preconditioner scales nearly optimally with the problem size while CPR does not do well under mesh refinement. Additionally, the block preconditioner remains efficient in parallel, while the CPR iteration count increases gradually as we increase the number of processors.

For CPR in the multiphase case, temperature-related effects are only treated in the second stage by ILU. On the other hand, the CPTR strategy tackles these effects in the first stage using some type of AMG method, which captures diffusive effects. As the mesh is refined, heat diffusion becomes more significant, resulting in the poor scaling of CPR, while CPTR exhibits near mesh independence in most cases.

In terms of computational time, CPTR becomes competitive when diffusion is dominant, which in our experiments is when the mesh is sufficiently refined.

In parallel, ILU is applied to the different blocks of the parallel decomposition. This means that ILU becomes a weaker, albeit cheaper, method as the number of processors increase. Since CPTR does not depend on ILU for the treatment of temperature, it is more robust to a weaker second stage. There are challenging industrial cases where a strong second stage is needed for CPR's convergence.

In brief, CPTR is preferable when the second stage is too weak for CPR, notably for diffusion-dominated flows or when many processors are available.

If the coupling between the pressure and energy equation of the pressure-temperature subsystem is weak, one could consider applying AMG to the pressure and temperature blocks individually (a block diagonal preconditioner on A_{pp} and A_{TT} in (4)). This does not

¹https://github.com/tlroy/thermalporous

Our Schur complement approximation outperforms simpler ones.

CPTR exhibits near mesh independent performance. perform nearly as well as applying unknown-based AMG on the pressure-temperature system or the block preconditioner. This indicates the strong coupling of the pressure-temperature subsystem. In other experiments where the pressure-temperature cross-coupling is artificially increased, our block preconditioner appears more robust than unknown-based AMG for CPTR.

4 Conclusion

In this project, we have considered preconditioning strategies for the solution of non-isothermal flow in porous media. Our main focus has been to develop a two-stage preconditioner, the Constrained Pressure-Temperature Residual method (CPTR). To do so, we first needed an efficient pressure-temperature solver. By first considering single-phase flow, we designed a block preconditioner for the pressure-temperature system.

In [2], we considered different preconditioners for the single-phase case. We sought to design a good Schur complement approximation for an effective block preconditioner. By considering the differential operators associated with the different blocks of the system matrix, we constructed an approximation using heuristical arguments. Our Schur complement approximation performs significantly better than simple ones obtained algebraically. In terms of scalability with the problem size and parallelization, the block preconditioner uses AMG to treat the heat diffusion and thus captures it appropriately. For advection-dominated cases, notably on very coarse grids, CPR is still very competitive.

In [3], we investigated preconditioning approaches for the multiphase case and performed numerical tests for a two-phase model. The CPTR method is a CPR-like method where a restricted pressure-temperature system is approximately solved in the first stage. The Schur complement approximation designed for the single-phase case is easily extended to the multiphase case. This leads to an effective block preconditioner for the first stage of CPTR. In most cases, CPTR exhibits good scaling properties like the block preconditioner for the single-phase case. We also performed an investigation where a strong pressure-temperature cross-coupling is created artificially. CPR performed well under a strong coupling, which indicates that the coupling of the pressure equation with the temperature is not as important. For CPTR, our block preconditioner gave an appropriate solution of the pressure-temperature system, as opposed to less coupled methods which fail to do so.

A major issue with CPR in thermal reservoir simulation is its lack of treatment of heat diffusion. CPTR offers an alternative where heat diffusion is treated using AMG. Diffusion-dominated flows notably appear on fine meshes. Furthermore, since CPTR does not rely on ILU for the energy equation, it is often observed that CPTR has parallel scalability independent of ILU. However, when heat diffusion is not problematic for CPR, CPTR appears to offer little advantage.

We have briefly investigated strong pressure-temperature cross-couplings. For our limited test cases, we do not have systems where the coupling of the pressure equation with temperature is problematic. Such a scenario could be advantageous for CPTR with our block preconditioner since CPR ignores that coupling.

While the models considered in this project are complex enough that they require advanced preconditioners, they do not include many of the features of the models in commercial reservoir simulators. Some of these features could be added to our models for further testing of CPTR with few modifications. More advanced models that include features such as poromechanics, electromagnetics (for heaters), or multiscale behaviour would require substantial effort and a different preconditioning approach.

Christopher Lemon, Software engineer, Schlumberger said: "The InfoMM collaboration with Oxford University has provided us with much greater insight into the challenge of building more robust linear solvers for thermal simulation. The project demonstrates how to implement a separate preconditioning step specifically designed for the temperature variable, and shows how this can have a significant impact on the convergence and scalability of the resulting algorithm. This work has also produced a versatile implementation of a multiphase thermal simulator in Firedrake. This has

the potential to provide a framework for rapid prototyping of new physics and numerical methods, which will help us to remain at the forefront of reservoir simulation technology."

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