

## Computation frameworks for modelling, migration and inversion

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### Summary

Over the past decade, scientific computing has witnessed significant advancements, including the introduction of new programming languages, pre-built libraries optimized for high-performance computing, and the rise of generative artificial intelligence, which provides innovative approaches to solving computational problems. Traditional methods for developing migration and inversion algorithms—built step-by-step in low-level languages—now face competition from modern frameworks that abstract many computational details, allowing researchers to focus on core challenges. While these frameworks often simplify initial development, their benefits may diminish as projects demand more detailed solutions and optimizations. However, they also introduce fresh ideas and possibilities that extend beyond conventional approaches.

This talk will explore current trends in modelling, migration (RTM), and Full Waveform Inversion (FWI) across diverse programming environments. We will discuss traditional frameworks, such as open-source compiled languages, for acoustic and elastic modelling, RTM and FWI from topography. Additionally, we will examine modern approaches, including Devito, Python-based methods with and without machine learning, physics-informed neural networks (PINNs), neural operators, generative artificial intelligence for programming and ongoing efforts to advance 3D modelling and FWI.

### Theory / Method / Workflow

Full Waveform Inversion (FWI) (Tarantola, 1984; Virieux and Operto, 2009) has emerged as one of the most prominent and widely researched methodologies in both industry and academia for seismic exploration and subsurface monitoring. Its broad appeal is driven by the complexity and depth of the challenges it presents. On one hand, FWI requires a robust understanding of wave propagation, imaging, and optimization. On the other hand, it demands high-performance computing expertise due to the intensive computational resources required. A key challenge in FWI lies in the implementation of realistic large-scale tests, which are often limited by computational costs, consequently constraining the reliability and applicability of the results.

Recent advancements in software and hardware, particularly in programming for graphic processing units (GPUs) (Lindholm et al., 2008) and cloud computing (Armbrust et al., 2010) have significantly expanded the possibilities for high-performance scientific computing. As researchers, we are only beginning to explore the potential of these technologies to overcome computational bottlenecks, which have historically limited the scope and efficiency of FWI. Traditional FWI implementations rely heavily on low-level programming languages that interface directly with hardware to optimize performance. While this approach effectively addresses the computational demands of FWI, it comes at the cost of substantial programming effort, often slowing the pace of scientific progress. Despite these challenges, we have consistently employed such approaches to ensure methodical and reliable research outcomes. However, the rapid evolution of programming paradigms has opened new possibilities that we are eager to explore.

High-level scientific computing frameworks, equipped with libraries like Devito (Louboutin et al., 2019) and JAX (Bradbury et al., 2018), now offer an alternative that simplifies coding complexity without sacrificing computational efficiency. These advances, supported by techniques such as Just-In-Time (JIT) and Ahead-Of-Time (AOT) compilation, have narrowed the performance gap between high-level and traditional low-level programming. Nevertheless, the trade-off often involves reduced flexibility in the customization of algorithms, as high-level tools abstract many underlying details. These tools, however, enable researchers to focus on broader scientific questions rather than low-level implementation specifics.

In recent years, artificial intelligence (AI) has revolutionized not only seismic exploration but also the broader landscape of scientific programming. Generative AI tools have streamlined the process of code generation (Phung et al., 2023), enabling researchers to develop algorithms with unprecedented efficiency. Furthermore, the incorporation of deep learning, particularly through transformer architectures, has significantly altered traditional approaches to geophysical algorithms like FWI.

The classical approach, rooted in detailed physical laws and differential equations, is increasingly being augmented—or even replaced—by machine learning techniques. These approaches offer a flexible template for solving complex physical problems by relying on neural networks, wherein the computational workload shifts to an automatic optimization process (e.g., backpropagation). While this shift offers the potential for faster and more adaptive solutions, it also brings increased computational demands and the need for vast amounts of training data. However, the use of self-supervised learning, which generates training examples automatically, offers a potential path to mitigate these challenges.

A major innovation in applied computational science has been the rise of Physics-Informed Neural Networks (PINNs) (Raissi et al., 2019). These networks integrate deep learning with physical laws, enforcing that the derivatives computed during backpropagation satisfy the governing differential equations. This approach not only enhances the flexibility of optimization algorithms but also ensures that solutions remain grounded in the fundamental physics of the problem.

In addition, Neural Operators have introduced a new paradigm for solving differential equations. Unlike traditional grid-based methods, Neural Operators represent the problem using network graphs, allowing for scalable solutions that can adapt to various problem sizes. This novel approach opens up new avenues for addressing challenges in FWI, particularly in large-scale 3D scenarios.

The intersection of generative AI, computer vision, and PINNs has further expanded the frontier of scientific computing. While generative AI offers creative approaches to generating synthetic data and models, computer vision techniques enhance image-based analysis, facilitating the development of initial velocity models for FWI. Together, these tools provide a transformative framework for tackling longstanding challenges in seismic exploration.

Looking forward, the advent of quantum computing promises another paradigm shift. Though AI currently dominates the scientific landscape, the unique properties of quantum algorithms—such as entanglement and superposition—suggest that quantum computing may offer breakthroughs in areas like FWI, where traditional and AI-based methods still face significant limitations.

In this abstract, we aim to discuss these emerging computational methodologies—ranging from traditional high-performance computing approaches to AI-driven frameworks—for their application in FWI and related seismic imaging techniques. While in CREWES we have successfully developed and tested these methods on synthetic 2D data, extending these solutions to real-world 3D data presents new challenges. Overcoming these obstacles will require re-

engineering existing solutions and further investigation into the strengths and limitations of these cutting-edge technologies.

By leveraging the power of modern computational tools and methodologies, we seek to contribute to the next generation of seismic exploration technologies, pushing the boundaries of what is achievable with FWI in complex, real-world scenarios.

### Examples: elastic FWI using traditional and new ML-based techniques.

During the presentation we will illustrate different ways to calculate FWI using modern computational frameworks. In this part we just will show some examples of elastic modeling RTM and FWI using industry-type implementation with CUDA-C++ but implemented in the open-source framework Madagascar (Fomel et al., 2012). In Figure 1 we see a 2D slice of the 3D model SEAM 2. The model contains the P, S and density model parameters. By using an approach of elastic finite different modelling from topography, we generate several shot gathers that contain all the characteristic of near surface noise (ground roll and scattered waves) (Sanchez, 2023, Trad and Sanchez, 2024). In Figure 2 we see the PP and SS migration results using RTM from topography. Figure 3, shows the results of FWI from topography for these synthetic data. Finally Figure 4, shows an original shot, a predicted shot, the cost function as a function of iterations and the illumination when working directly from topography. This type of implementation, although highly efficient once is finished, requires carefully debugging during the implementation because of the complexities of CUDA development. Many intermediate plots of wavefields and gradients are required to get a working version. Much of the difficulties during the optimization come from data fitting information from the near-surface that requires a very detailed modelling obeying all physical boundary conditions.

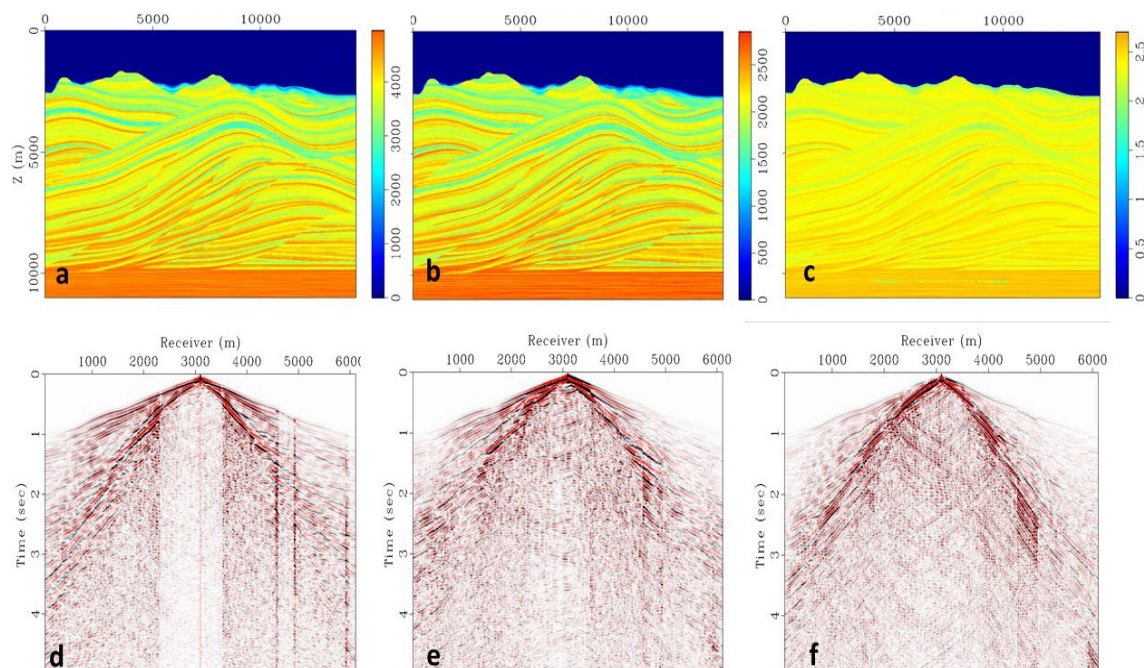


Figure 1 The elastic SEAM II model and the results of elastic modeling from Topography.

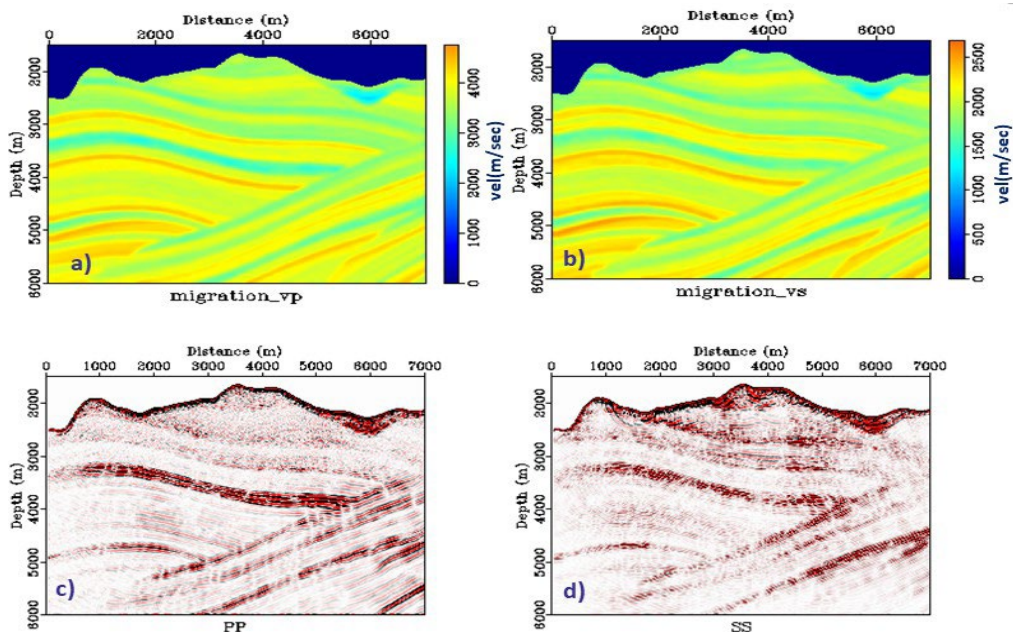


Figure 2 RTM for the SEAM 2 model: a) P velocity, b) S velocity, d) PP RTM, e) SS RTM.

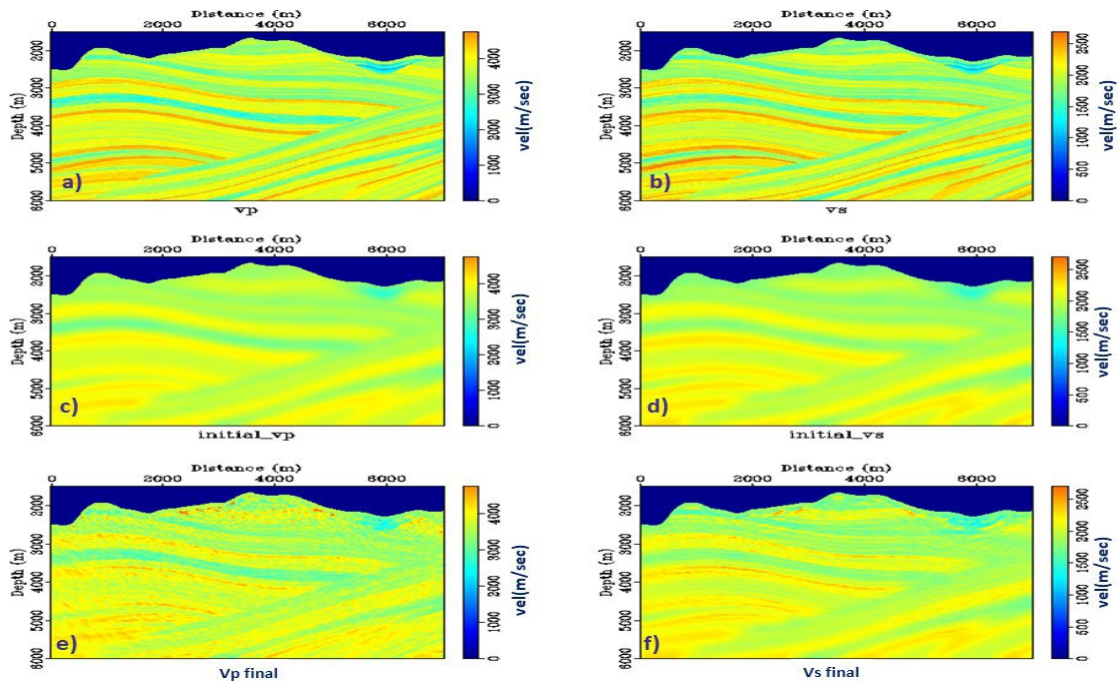


Figure 3Elastic FWI from topography for the SEAM 2 model after 20 iterations: a) True P velocity, b) True Vs velocity, c) initial VP velocity, d) Initial Vs velocity, e) FWI VP from topography using the complete data set (including near-surface noise). F) same for FWI -Vs

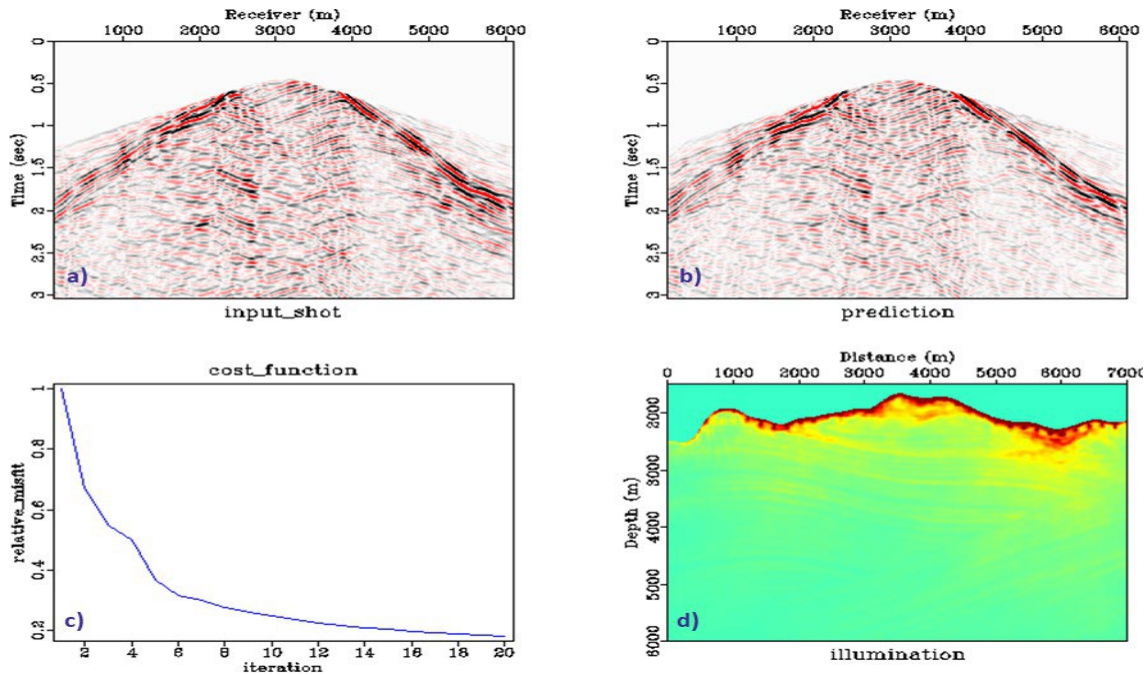


Figure 4 Elastic FWI from topography for the SEAM 2: a) One input shot, horizontal particle velocity, b) corresponding prediction, c) Cost function (sum of vertical and horizontal particle velocity misfits, d) illumination (average of vertical and horizontal).

An alternative, is the development of methods based on machine learning, which use automatic calculation for the elastic gradients and optimization techniques without line search (Sun et al 2020, Zhang et al, 2024). An example of that can be seen in Figure 5.

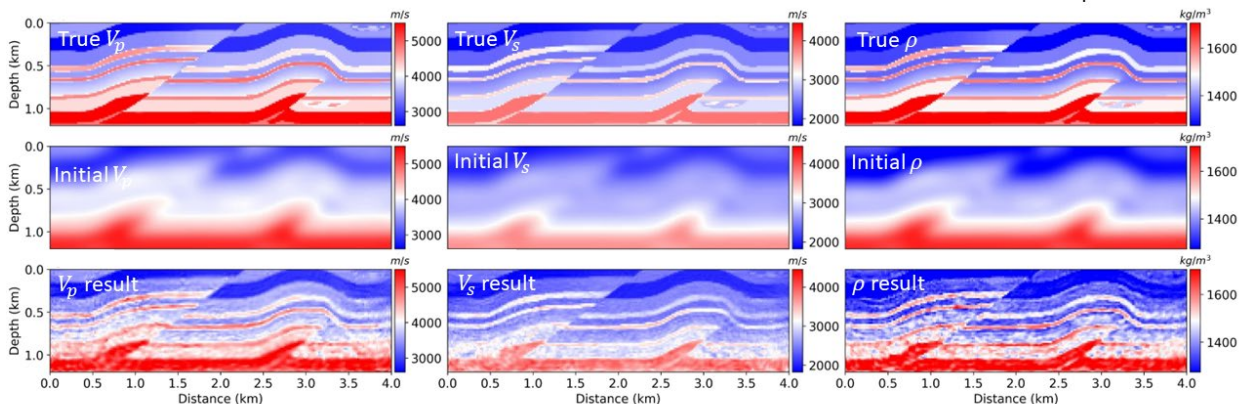


Figure 5. Example for elastic FWI using a machine learning framework.

## Conclusions

In this abstract we discussed some of the different frameworks available to implement advanced and computationally expensive algorithms like full waveform inversion. We illustrate some of the

traditional, difficult but efficient in memory and calculation and more modern techniques that permits to by-pass some of the complications involved in the implementation.

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