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open Delft Advanced Research Terra Simulator (open-DARTS)

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Summary

Open Delft Advanced Research Terra Simulator (Voskov et al., 2023) is a simulation framework for forward and inverse modelling and uncertainty quantification of multi-physics processes in geo-engineering applications such as geothermal, CO2 sequestration, water pumping, and hydrogen storage. To efficiently achieve high levels of accuracy on complex geometries, it utilizes advanced numerical methods such as fully implicit thermo-hydro-mechanical-chemical (THMC) formulation, a highly flexible finite-volume spatial approximation and operator-based linearization for nonlinear terms. open-DARTS goals are computational efficiency, extensibility, and simplicity of use. For this reason, open-DARTS is based on a hybrid design with an efficient core C++ implementation wrapped around a highly customizable and easy-to-use Python code.

Statement of need

open-DARTS is designed to use Python as its user interface (while other simulators such as GEOS (Settgast et al., 2022) and MRST (Lie, 2019) have C++ and Matlab interfaces, respectively), which makes it easy to use in education and research: 6 graduate courses at TU Delft and 4 external courses, 8 research projects in collaboration with industrial partners and 7 academic projects with various research institutes are considered in 2024. It is a reservoir simulator with advanced capabilities that are not reliant on proprietary nor licensed software, thus significantly reducing the entry barrier for researchers and students interested in energy transition applications for the subsurface. The modules `discretizer` and `darts-flash` allow efficient processing of Corner Point Geometry meshes and advanced multiphase equilibrium evaluation for complex fluids respectively.

The open-DARTS framework is fully validated and benchmarked for geothermal applications showing similar accuracy as state-of-the-art simulators TOUGH2 (O'Sullivan et al., 2001) and AD-GPRS (Garipov et al., 2018) while providing a noticeable reduction in CPU time mainly due to the OBL approach (Wang et al., 2020). While open-DARTS uses the OBL approach to cache evaluation points and calculate derivatives through interpolation, TOUGH2 uses numerical derivatives and AD-GPRS automatic differentiation. In the modelling of CO2 geological storage, open-DARTS was one of the frameworks tested on the FluidFlower validation benchmark study (Flemisch et al., 2023), where it was compared with experiments and other simulators (Ahusborde et al., 2024; Hoop et al., 2024; Wapperom et al., 2023). open-DARTS has been used for studying hydrocarbon production when it was validated against commercial simulator (Lyu et al., 2021). Recently, the modelling of fault reactivation has been supported in open-DARTS (Novikov, 2024) that has been validated against semi-analytical benchmarks and PorePy simulation tool (Keilegavlen et al., 2021).

Open-DARTS' primary advantage over other simulators is its ability to simultaneously provide an OBL implementation, inverse capabilities, and a flexible, modular framework without compromising on performance (Khait & Voskov, 2021). Its versatility is evidenced by its capability to cater to a wide range of applications. Furthermore, advanced inverse capabilities based on adjoint gradients allow open-DARTS to effectively address data assimilation (Tian et al., 2024) and uncertainty quantification (Wang et al., 2023) for energy transition applications.

Key features

Unified thermal-compositional PDE formulation

open-DARTS has a generic PDE formulation for thermal compositional flow in porous media (Khait & Voskov, 2018). This makes it possible to adjust terms in the PDEs to account for various multi-physical phenomena such as darcy flow, gravity, multi-component & multiphase flows, thermal flows, chemical and kinetic reactions, etc.

Geomechanics

open-DARTS is capable of modelling coupled THMC processes in linear thermo-poroelastic media under the assumption of small deformations. Unlike most of simulators, the system of conservation laws is handled by the Finite Volume Method alone that enables support of a wide range of cell topologies. Moreover, the method benefits from the unified formulation of mass, energy and momentum fluxes discretized with multi-point approximations. This formulation allows for calculating displacements and stresses in a single collocated grid for all physics phenomena on complex meshes (Novikov et al., 2022). The framework is suitable for solving multi-scale hydro-mechanical, discrete fracture networks (Hoop et al., 2022), and friction contact mechanics (slip-fault) problems (Novikov et al., 2024).

Discretization

open-DARTS employs the finite volume method for spatial discretization and the fully implicit backward Euler method for time discretization. This approach supports arbitrary star-shaped polyhedral cells, offering high flexibility. Additionally, open-DARTS implements both two-point and multi-point flux approximations.

Different grid types supported by open-DARTS are *a) structured grids* for teaching and basic modelling, *b) radial grids* for near-well and core scale laboratory experiments, *c) corner-point geometries* for industry-related applications, *d) unstructured grids* for modelling of flow with complex geometries and discrete fracture networks.

Operator-Based Linearization

One of the most computationally complex and expensive parts is the calculation of partial derivatives to construct the Jacobian. open-DARTS exploits Operator-Based Linearization (OBL) (Khait & Voskov, 2017; Voskov, 2017), where the terms in the PDEs are separated into space-dependent terms and thermodynamic state-dependent operators. The latter can be parameterized with respect to the nonlinear unknowns using multidimensional tables at different resolutions. The values and derivatives required for the assembly of the linear system can be approximated through multi-linear interpolation in the parameter space using calculated values at the nodes.

Using adaptive parametrization (Khait & Voskov, 2018), derivative computation is performed at nodes of the structured grid in the primary variables space around the required point. Re-using computed values at nodal points can significantly reduce the Jacobian construction stage, especially in the case of ensemble-based simulations.

Inverse modelling

Inverse modelling methods necessitate a substantial number of simulations to accurately calibrate model parameters against observed data. Such algorithms are highly computationally intensive, particularly when employing gradient-based methods. The implementation of the adjoint method in open-DARTS remarkably enhances its efficiency in computing the required gradients for inverse modelling or history-matching processes (Tian & Voskov, 2023). Moreover, the flexibility of open-DARTS's Python interface significantly simplifies the coupling process with various data assimilation algorithms. The inverse modelling module of open-DARTS accommodates various types of observation data such as: well rates, well temperatures, BHP, time-lapse temperature distributions, and any custom outputs definable in the form of operators within open-DARTS.

Software implementation

The most computationally expensive part of open-DARTS is written in C++ with OpenMP parallelization. open-DARTS can be installed as a Python module and it has a Python-based interface, which makes it suitable for teaching and users unfamiliar with C++ language. There are several benefits of this approach compared to a code fully written in C++.

- Easy installation via pip and PyPI.
- No need to install compilers.
- Flexible implementation of simulation framework, physical modelling and grids.
- Easy data visualization, including internal arrays and `vtk`.
- Use popular Python modules within open-DARTS and the user's model for data processing and input/output.
- Coupling with other Python-based numerical modelling software.

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