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Review of saturated groundwater model codes for Hydro-JULES

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Review of saturated groundwater model codes for Hydro-JULES

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Summary

This report reviews saturated groundwater model codes, one to be implemented into the Hydro-JULES modelling framework. First, the criteria for the code evaluation is described, and then commercial groundwater modelling codes, codes for thermo-hydro-chemical modelling and finally open source groundwater modelling codes are evaluated using the aforementioned criteria. Considering a groundwater code for the simulation of groundwater flooding or drought, we recommend either MODFLOW-2005, or the newly developed MODFLOW 6, the latter will need to be tested. Alternatively, BGS could develop a custom code that can solve the groundwater flow equation using moving grids, allowing a dynamic representation of the model grid for a moving water table. If also thermo and chemical processes are of interest, then codes such as OpenGeoSys, Dumux, and PFLOTRAN could be good choices, however they will need benchmarking to evaluate their ease of use.

1 Introduction and background

This report is part of the Hydro-JULES research programme supported by NERC National Capability funding (Grant number: NE/S017380/1) to the Centre for Ecology & Hydrology (CEH), British Geological Survey (BGS) and National Centre for Atmospheric Science (NCAS). The five year programme (April 2019-March 2024) will develop a new generation of terrestrial hydrological models linked to, and in collaboration with, the Joint UK Land Environment Simulator (JULES) model. A primary objective of Hydro-JULES will be to generate a 3-dimensional model of the complete terrestrial water cycle in such a way as to ensure consistency across space and timescales. Through the development of new models that better simulate the movement of water, both vertically and laterally, advances in land surface-boundary layer science will be made. Two scales will be considered for the application of the modelling approach: The British mainland (England, Scotland and Wales including major islands) and global scale.

At the British mainland scale the following questions are to be considered:

1. How can an integrated approach improve the simulation of major flooding events such as the 2013/4 floods?
2. How can a holistic approach be undertaken to assess water resources under drought conditions?

Any outputs from the Hydro-JULES programme are open as well as freely and easily available to ensure transparency and auditability in the development of the scientific approach.

BGS' role is to deliver the sub-surface part of the Hydro-JULES programme by contributing the geological and hydrogeological understanding to inform the appropriate parameterisation to be encapsulated in the groundwater modelling. The aim is to develop a flow, heat and solute transport modelling approach for the British mainland and to incorporate groundwater flow in the JULES model at the global scale.

1.1 RESEARCH QUESTIONS CONSIDERED FOR THIS WORK

Leading on from the two main questions described above, the research questions that ideally would be addressed using the final linked model include:

For groundwater flow:

- How will climate change affect groundwater drought frequency for the British Mainland?
- Can the extent of groundwater flooding be simulated using the linked model for the British Mainland?

- Does using a land surface model linked to a groundwater model improve the understanding of how climate change affects recharge at a national scale?

Of secondary importance are the inclusion of solute and heat transport.

For Nitrate transport:

- How does land use and climate change affect nitrate concentration in the saturated zone at a national scale?

For heat flow:

- How can shallow geothermal be applied at the scale of the British Mainland?
- How does climate change affect groundwater temperature and in particular affect heat flow to rivers?

1.2 STRUCTURE OF THE REPORT

This report describes different criteria for the evaluation of saturated codes in Section 2 and reviews ten saturated groundwater model codes using these criteria in Section 3. This section is divided into commercial groundwater modelling codes, codes for thermo-hydro-chemical modelling, and open-source groundwater modelling codes. Section 4 summarises the results and makes recommendations for further work.

2 Description of methodology and criteria used

The saturated groundwater codes were evaluated using a list of weighted criteria outlined in Table 1. They were developed in conjunction with modelling colleagues at BGS. Further, the criteria to evaluate the saturated codes are grouped into three priorities:

First priority:

- Full 3D solution of the time variant groundwater flow equation. Can the model deal with vertical flows properly by using a variable discretisation in the vertical dimension?
- Open source of the code. The code will be shared within the Hydro-JULES framework, therefore it will need to be open source.
- Cost. Is the code freely available?
- Linkability. Has the code been linked with another codes at run-time?
- Ease of use. How easy is it to set up the input files and run the code, and can the model be incorporated into the JULES Rose suites, which is a container for the Jules apps fcm_make and Jules.

Second priority:

- Full 3D solution of the solute transport equation.
- Unstructured grids: beneficial to represent flow to boreholes or adits.
- Capable of parallelisation. Has the code already been parallelised or would it be possible?
- Is the code written in an object oriented approach?
- Manual. Does it exist and is it well documented?
- Code guardian. Who is the owner of the code?

Third priority:

- Full 3D solution of heat transport.
- Frequency of use.

These priorities are born in mind in reviewing the codes. The codes are then ranked according to their priorities from Table 1, whereas the criteria from priority one receive three points, criteria from priority two two points and priority three one point.

Table 1. Criteria for saturated code evaluation for Hydro-JULES

Criteria	Description	Priority (1,2 or 3).1 being highest	Comments
Full 3D solution to the GW flow equation	Can the model deal with vertical flows "properly"? Is it a full numerical solution to the GW flow equation?	1	Obtaining a fully 3D time variant model is the priority. Note: this is related to vertical gridding to ensure variable gridding in the vertical direction. Alongside this, a simple 2D solution will be required to test the implementation within the Hydro-JULES framework.
Full 3D solution to the GW solute transport equation	Can solute transport be simulated?	2	Again, start simple and increase complexity as for flow.
Full 3D solution to the GW heat transport equation	Can heat flow be simulated?	3	Again, start simple and increase complexity as for flow.
Unstructured grids	Is the model grid orthogonal only or can irregular meshes be used?	2	These would help deal with local scale issues, such as flow to boreholes / adits.
Capable of parallelisation	Has the code been parallelised already or how could it be made parallel?	2	
Language used	Computational language that the code is written in. Is it object-oriented?	2	Object oriented approach would be ideal, but not a barrier to use.
Open source	Is the source code available?	1	If we are to make these codes linkable within the Hydro-JULES framework then this is important.
Cost	Is the code freely available? What is price of obtaining the code?	1	
Linkability	Has the code been set up to able it to be linked to other codes at runtime?	1	This means that the code is set up to be controlled by other external

			software. See above for test code based on single layered 2D
Ease of use	How easy or difficult is it to run the code? Does it have a user interface / pre- and post-processing software?	1	This will need to be tested by using the code on test problems or based on personal experience; Can the model be incorporated into the JULES Rose interface?
Manual	Does on exist and what is it like?	2	
Code guardian	Who is responsible for the code and how accessible are they?	2	
Frequency of use	How well used it the model code? How many applications are reported in the peer-reviewed literature?	3	

3 Results of evaluation

3.1 COMMERCIAL GROUNDWATER MODELLING CODES

3.1.1 MARTHE

MARTHE is a finite-difference hydrodynamic software developed by BRGM (Bureau de Recherches Géologiques et Minières, the French geological survey) that allows calculating fluid flows and mass and heat transfers in a 3D porous medium. The software (written in Fortran 77/95 depending on the version) uses only structured grids and to the best of our knowledge, it has not been parallelised. Although the code is not free (its full version costs 7900 €), there is a free access version that can be downloaded that allows to do some computations with a limited size grid. This code has been coupled to other software such as the geochemical model Phreeqc and it is widely used (43 publications) by the BRGM survey.

Due to the fact that the code is not free, we do not plan to give further consideration to this particular software.

Table 2. Summary table of the MARTHE code.

Marthe		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	

Full 3d solution to the GW solute transport equation	Yes	MARTHE_Transport_Masse_7_5_RP-64765-FR.pdf (in french)
Full 3d solution to the GW heat transport equation	Yes	MARTHE_Transport_Masse_7_5_RP-64765-FR.pdf (in french)
Unstructured grids	No	Finite difference grids are used.
Capable of parallelisation	Unknown	Not reported
Language used	Fortran	Fortran 77/Fortran 95 (depending on the version)
Open source	No	
Cost	High	There is a free access version that can be downloaded that allows to do some computations with a limited size grid. Full version: 7900 € (excl. VAT). There is a limited version that costs 4000 € (excl. VAT).
Linkability	Not explicitly reported how but has been coupled to Phreeqc, for instance.	It has been coupled to PHREEQC (MARTHE_PHREEQC_RM_7_5_RP-65010-FR.pdf).
Ease of use	Good?	Pre-processor and post-processor through graphic interface. Input interface with 3D modellers:Multilayer ®, GDM ®, EarthVision ®, Éclipse ®, Surfer ®. Export to Mapinfo ®, Paraview, Tecplot ®, Winteracter-3Dview ®, Vrml QGis, ArcGis ® for 3D displays.
Manual	Yes	http://www.brgm.eu/sites/default/brgm/software/marthe/Tutorial_MARTHE_ENGLISH_V7_3.pdf
Code guardian	BRGM	Code from the French geological survey, Bureau de Recherches Géologiques et Minières
Frequency of use	43 publications according to the webpage (used by same team)	http://www.brgm.eu/scientific-output/scientific-software/reference-publications-on-marthe
Others		http://www.brgm.eu/scientific-output/scientific-software/marthe-modelling-software-groundwater-flows
Current version		7.1

Space discretisation		Finite difference
Comments:		

3.1.2 FEFLOW

FEFLOW is a widely used commercially available groundwater code, which includes an easy to use user interface. FEFLOW has been linked with MIKE SHE using OpenMI, and plugins can be written using C/C++ as a pre time-step call-back function.

Table 3. Summary table of the FEFLOW groundwater modelling code.

FEFLOW		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	
Full 3d solution to the GW solute transport equation	Yes	
Full 3d solution to the GW heat transport equation	Yes	
Unstructured grids	Yes	quadrilateral or unstructured triangular meshes
Capable of parallelisation	limited	using the SAMG solver allows parallelization on multicore or multiprocessor systems. PARADISO solver: parallel sparse direct solver.
Language used	C/C++	
Open source	no	
Cost	expensive	? ~ 17 k for a network licence, but not the code
Linkability	limited	with MIKE SHE over OpenMI. Plug-ins written in C/C++ can be used, which is a pre timestep callback function
Ease of use	good	good user interface. Model and set-up, mesh and output are stored in one file I think, which makes working with larger models tricky.

Manual	yes	
Code guardian	MIKE DHI	
Frequency of use		3880 in google scholar
Others		https://www.mikepoweredbydhi.com/products/feflow
Current version		
Space discretisation		Finite element
Comments:		

3.1.3 TOUGH2

TOUGH is a software code to numerically simulate the coupled transport of water, vapour, gas and heat in porous and fractured media. This code (whose current version is 3) is developed at the Lawrence Berkeley National Laboratory (LBNL) and written in Fortran. It can deal with unstructured finite volume meshes if the WinGridder mesh generator is used. A parallel version (MP) can be used with version 2 (TOUGH2-MP). The code is not open-source. It has been the topic of more than 500 peer-reviewed journal articles, conference proceedings and project reports, where its capabilities of being linked to other codes at runtime have been shown.

Table 4. Summary table of Tough2 modelling code.

Tough2		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	
Full 3d solution to the GW solute transport equation	Yes	
Full 3d solution to the GW heat transport equation	Yes	
Unstructured grids	Yes	WinGridder
Capable of parallelisation	Yes	TOUGH2-MP
Language used	Fortran	
Open source	No	
Cost	Expensive	
Linkability	Yes	
Ease of use	No	No graphical interfaces are part of the TOUGH distribution, and only minimal support for model setup and mesh generation is built into the simulators

Manual	Yes	
Code guardian	Lawrence Berkeley National Laboratory	
Frequency of use	good	
Others		https://tough.lbl.gov/software/tough3/
Current version		3
Space discretisation		
Comments:		

3.1.4 ESTEL

ESTEL is a groundwater flow model solving Richard's equation and contaminant transport and has been developed by the University of Bristol and the Research and Development unit at Electricité de France. ESTEL is part of the TELEMAC system. The ESTEL-3D contains a prototype model solving advection-dispersion equation using the random walk method. It is not clear however, whether the code is open source. Attempts to contact the named code guardian at Bristol University were not successful and further enquiries determined that the code was no longer being developed.

Table 5. Summary table of ESTEL groundwater modelling code.

ESTEL		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	Richard's equation in mixed form
Full 3d solution to the GW solute transport equation	Yes	Advection-dispersion equation using the random walk method
Full 3d solution to the GW heat transport equation	No??	
Unstructured grids	Yes	2D: unstructered meshes of triangles. 3D unstructured meshes of tetrahedra. Mesh generation using ANSYC ICE CFD
Capable of parallelisation	Yes	Using MPI
Language used	Fortran	uses the TELEMAC system (http://www.opentelemac.org/)
Open source	No	Using subversion https://source.ggy.bris.ac.uk/wiki/Install_the_TELEMAC_system

Cost	No	ESTEL is available commercially from the distributors of the TELEMAC system. Research licenses are also available.
Linkability	?	
Ease of use	?	
Manual	Yes	https://source.ggy.bris.ac.uk/uploads/5/5f/ESTEL-3D_v5p6_User_Manual.pdf dated 2006
Code guardian	Bristol, Malcolm Anderson, JP Renaud	
Frequency of use	some	Bates et al., 2000; Claxton et al., 2003; Renaud et al. 2003, Cloke et al., 2003, 2006a, 2006b
Others		https://source.ggy.bris.ac.uk/wiki/Official_ESTEL_Documentation
Current version	v5p9	
Space discretisation		Finite element
Comments:		

3.2 CODES FOR THERMO-HYDRO-CHEMICAL MODELLING

3.2.1 OpenGeoSys

OPENGEOSYS (OGS) is a scientific open source project for the development of numerical methods for the simulation of thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media. Current version is OpenGeoSys-6.

It can be used to solve the GW flow equation (see command GROUNDWATER_FLOW), the GW solute transport equation (see command MASS_TRANSPORT) and the GW heat transport equation (see command HEAT_TRANSPORT). OGS (coded in C++) is able to deal with complex geometrical domains by means of the pre- and post-processor GINA, developed by the German Federal Institute for Geosciences and Natural Resources (BGR). This meshing software is only free for teaching and research. So, further research is needed to analyse whether this is a viable option for our purposes. To increase its computational efficiency, the OGS code has been parallelized (Wang et al., 2009). The code has been linked to other software (see Kalbacher et al., 2012; Kolditz et al., 2012; He et al., 2015), and it needs pre- and post-processor tools since there is no interface.

Table 6. Summary table of OpenGeoSys code.

OpenGeoSys		
Criteria	**Answer**	**Comments**

Full 3d solution to the GW flow equation	Yes	See command GROUNDWATER_FLOW
Full 3d solution to the GW solute transport equation	Yes	See command MASS_TRANSPORT
Full 3d solution to the GW heat transport equation	Yes	See command HEAT_TRANSPORT
Unstructured grids	Yes	It is done through GINA (see page 13 of the tutorial)
Capable of parallelisation	Yes	See Wang et al. (2009) and pages 6,9,10 of the manual
Language used	Yes (C++)	
Open source	Yes	Source code can be dowbnloaded from a Git repositroy (https://www.opengeosys.org/docs/userguide/basics/introduction/)
Cost	0	But needs other software that is only free for research and teaching (GINA, for the model geometry)
Linkability	Yes	See He et al. (2015), Kalbacher et al (2012) and Kolditz et al (2012). It has been coupled to external geochemical solvers such as OGS-PHREEQC, OGS-GEMs, OGS-BRNS and OGS-ChemApp, see page 7 of the tutorial for more information about this.
Ease of use	No	Preprocessing needs to be done via other software (such as GINA for the model geometry). Postprocessing needs to be done via ParaView.
Manual	Yes	https://ogsstorage.blob.core.windows.net/web/Books/Computational-Hydrology-III/Computational-Hydrology-III.pdf
Code guardian	OpenSource	https://www.opengeosys.org/docs/userguide/basics/introduction/
Frequency of use	Well used	126 documents according to Scopus mentioning OpenGeoSys in title/asbstract or keywords.
Others		https://www.opengeosys.org/
Current version		6
Space discretisation		FEM
Comments:		

3.2.2 Dumux

DUMUX is a parallel open-source multiphase flow simulator implemented in C++. It is able to solve the 3D GW flow, the 3D GW solute transport and the 3D GW heat transport equation. DUMUX can deal with structured grids itself and with unstructured grids if an external library (GM) is used. As with OGS, the software has been linked to other software (Ahusborde et al., 2017) and it needs pre- and post-processor tools since there is no interface.

Table 7. Summary table of the DUMUX flow simulator.

Dumux		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	
Full 3d solution to the GW solute transport equation	Yes	
Full 3d solution to the GW heat transport equation	Yes	
Unstructured grids	Yes	Structured grids can be created with Dumux itself. Unstructured grids can be created with external libraries.
Capable of parallelisation	Yes	It is a parallel open-source simulator
Language used	C++	
Open source	Yes	Source can be downloaded from https://dumux.org/download
Cost	0	
Linkability	It has been coupled to some chemistry modules for instance	See for instance Ahusbordeetal2017.pdf
Ease of use	No	Preprocessing needs to be done via other software if unstructured meshes are desired. Postprocessing needs to be done via ParaView.
Manual	Yes	dumux-handbook-master.pdf
Code guardian	OpenSource	
Frequency of use	Well used	https://dumux.org/publications
Others		https://dumux.org/
Current version		3

Space discretisation		FVM
Comments:		

3.2.3 PFLOTRAN

PFLOTRAN is an open source subsurface flow and reactive transport code. The code, written in object oriented FORTRAN 2003, is parallelized. PFLOTRAN's capabilities are extensive and include thermo-hydro-chemical problems with multiple continuums for heat, porous media and discrete fracture networks, multiphase ice-water-vapour flow, mineral precipitation and dissolution, subsurface flow and reactive transport coupling. PFLOTRAN is under development to be coupled to the Community Land Model CLM.

Table 8. Summary code of PFLOTRAN code.

3.3 OPEN SOURCE GROUNWATER MODELLING CODES

3.3.1 MODLFOW

MODFLOW is the U.S. Geological Survey's modular hydrologic model and was first published in 1984. There have been six different versions, of which MODFLOW-2005 and the newly released MODFLOW 6 in 2018 are currently maintained by the USGS Office of Groundwater.

MODFLOW-2005 consists of modular programming components, Packages and Processes. MODFLOW-2005 solves the full 3D groundwater flow equation, and has a groundwater transport package (GWT) and a package for unstructured grids (MODFLOW-USG), however, heat flow cannot be simulated. There have been some efforts in parallelisation of MODFLOW (Dong and Li, 2009; Ji et al., 2014). An advantage of MODFLOW-2005 is its demonstrated ability to be linked to other codes at runtime, as for the PCR-GLOBWB-MODFLOW (De Graaf et al., 2015), Hydrus-MODFLOW (Beegum et al., 2018a; Beegum et al., 2018b), SWAT-MODFLOW (e.g. Aliyari et al., 2019).

Table 9. Summary table of MODFLOW-2005 groundwater modelling code.

MODFLOW-2005		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	
Full 3d solution to the GW solute transport equation	Yes	SEAWAT combines version of MODFLOW and MT3DMS for simulating variable-desnity groundwater flow and transport. GWT package incorporates the capability to simulate solute transport with MODFLOW.
Full 3d solution to the GW heat transport equation	No	

Unstructured grids	Yes	MODFLOW-USG: an unstructured grid version of MODFLOW for simulating groundwater flow and tightly coupled processes using a control volume finite-difference formulation
Capable of parallelisation	Yes	E.g. OpenMP programming used to parallelize the PCG solver (Dong et al 2009). Or using the J Adaptive Structured Mesh application Infrastructure (Cheng et al 2013)
Language used	Fortran	
Open source	Yes	
Cost	Free	
Linkability	Yes	e.g. PCR-GLOBWB-MODFLOW, Hydrus-MODFLOW, SWAT-MODFLW
Ease of use	Yes	Preprocessors/Postprocessors: Flow-Py, GW_CHART, ModelMuse, ModelViewer, Zomebudget, GMS
Manual	Yes	
Code guardian	USGS	
Frequency of use	Well	22000 results on google scholar
Others		https://water.usgs.gov/ogw/modflow/index.html
Current version		MODFLOW 6v / MODFLOW 2005
Space discretisation		Cartesian
Comments:		

MODFLOW 6 has been completely rewritten using an object-oriented design, and currently only supports the Groundwater Flow Process. MODFLOW 6 main advantage lies in the design that any number of models can be included in the simulation, which can be independent of one another with no interaction, they can exchange information with each other, or they can be tightly coupled at the matrix level. The object oriented framework of MODFLOW 6 allows, unlike MODFLOW-2005, that multiple GWF Model object can be used in a single simulation and can be hydraulically connected using GWF-GWF Exchange objects. This allows grid refinement consisting of parent and child models or to couple adjacent GWF Models. Multiple models and their exchanges can be incorporated into a single solution object and tightly coupled at the matrix level.

Table 10. Summary table of MODFLOW 6 groundwater modelling code.

MODFLOW 6		
Criteria	**Answer**	**Comments**

Full 3d solution to the GW flow equation	Yes	
Full 3d solution to the GW solute transport equation	not yet	
Full 3d solution to the GW heat transport equation	no	
Unstructured grids	Yes	irregular mesh. E.g. triangular grid using the DISV package
Capable of parallelisation		Not mentioned in manual
Language used	Fortran	object oriented
Open source	Yes	
Cost	free	
Linkability		A key feature of the new MODFLOW 6 framework is the ability to solve multiple, tightly coupled, numerical models in a single system of equations. These may be multiple models of the same type or of different types. MODFLOW 6 is an entirely new version of MODFLOW. Transfer of information between models is isolated to exchange objects, which allow models to be developed and used independently of one another. Within this new framework, a regional-scale groundwater model may be coupled with multiple local-scale groundwater models. Or, a surface-water flow model could be coupled to multiple groundwater flow models. The framework naturally allows for future extensions to include the simulation of solute transport.
Ease of use	not sure	
Manual		https://doi.org/10.3133/tm6A57. https://doi.org/10.3133/tm6A55 https://doi.org/10.3133/tm6A56
Code guardian	USGS	
Frequency of use		new
Others		https://pubs.er.usgs.gov/publication/tm6A55
Current version		MODFLW 6
Space discretisation		Control-volume finite difference

Comments:		

3.3.2 SUTRA

SUTRA is a USGS groundwater model for saturated-unsaturated, variable density groundwater flow with solute or energy transport. SUTRA itself is an open source code and freely available, however the creation of input files is commonly done using the SutraGUI, for which uses the commercially available software ArgusONE. We have tested the use of SutraGUI for the use of 2D models, however for large scale models with complex geology it is questionable whether this is the most suitable form of preparing the input files. Therefore, if SUTRA is taken for further consideration, this would have to be tested or potentially another form of preparing the input files has to be found.

Table 11. Summary table of the SUTRA groundwater modelling code.

SUTRA		
Criteria	**Answer**	**Comments**
Full 3d solution to the GW flow equation	Yes	saturated/unsaturated constant-density or density-dependent groundwater flow user-programmable unsaturated flow functions
Full 3d solution to the GW solute transport equation	Yes	transport of either thermal energy or a single species single solute or thermal energy zeroth- and first-order solute production/decay; zeroth-order energy production/decay linear, Freundlich, or Langmuir adsorption
Full 3d solution to the GW heat transport equation	Yes	see above
Unstructured grids	Yes	hybrid Galerkin-finite-element and integrated-finite-difference method quadrilateral (2D) or generalized hexahedral (3D) finite elements fully implicit finite-difference time discretization hybrid Galerkin-finite-element and integrated-finite-difference method quadrilateral (2D) or generalized hexahedral (3D) finite elements fully implicit finite-difference time discretization

Capable of parallelisation	?	no evidence
Language used	Fortran-90	The FORTRAN-90 coding stresses clarity and modularity rather than efficiency, providing easy access for later modifications.
Open source	Yes	To use and modify
Cost	Free	
Linkability	Limited	Limited. Linking SUTRA and MANHAM
Ease of use	Good	Argus One preprocessor to create model input files (commercial, we have one licence). SutraPrep, Model Viewer.
Manual	Yes	
Code guardian		USGS Cliff Voss, Alden Provost
Frequency of use	Yes	2790 hits for "SUTRA groundwater model" in google scholar
Others	Yes	https://water.usgs.gov/nrp/gwsoftware/sour/overview/overview.htm
Current version	2.2	
Space discretisation		hybrid Galerkin-finite-element and integrated-finite-difference method quadrilateral (2D) or generalized hexahedral (3D) finite elements
Comments:		Boundary conditions in SUTRA are limited: Fluid sources or sinks Solute mass or energy sources or sinks Specified pressures Specified solute concentrations or temperatures

3.3.3 HST3D / PHAST

HST3D is an open-source computer code for simulation of groundwater flow and associated heat and solute transport in three dimensions. Developed by USGS (the US geological survey) and written in Fortran is able to deal with structured grids but to best of our knowledge, no unstructured grids can be employed and no parallel versions have been developed. According to USGS webpage, 10 peer-reviewed publications can be found where the use of HST3D is reported.

4 Summary and recommendation for next steps

The codes are ranked according the priorities listed in Section 2, whereas the properties for the first priority get 3 points, the second priority 2 points and the third priority 1 point (Table 12). The codes with the highest ranking are MODFLOW, OpenGeoSys, followed by Dumux, PFLOTRAN and SUTRA.

Since the code of the commercial codes MARTHE, FEEFLOW, TOUGH2 and ESTEL are not freely available, these codes are unsuitable to be shared within the Hydro-Jules community. Therefore, these codes are discarded from the selection process at this point.

The choice of implementing a generic code that has the potential to simulate thermo-hydro-chemical problems, or an open source groundwater modelling code, depends on the science question asked by the user community. If the code is required to have the capability to simulate coupled flow, heat and transport processes, then OpenGeoSys, Dumux, or PFLOTRAN could be a good choice to be built into Hydro-Jules. However, since their ease of use is unknown, we suggest benchmarking these codes on a well-known setting before making a final decision. The pre- and/or post-processing generally requires other tools, e.g ParaView, Tecplot (commercial), GnuPlot, or MatPlotLib.

If the scope of the project however, is predominantly within simulating the hydrological cycle, e.g. to represent groundwater flooding and drought conditions, the use of a well-established groundwater modelling code is the ideal option, since their use for groundwater related processes is well known. Within the open-source groundwater modelling codes, MODFLOW-2005 or MODFLOW 6 are the choices with the highest ranking. MODFLOW-2005 is a widely used code which has been tested extensively, it has been coupled to the Land-Surface-Model PCR-GLOBWB-MODFLOW, and BGS has the experience in applying this code. Post-processing with MT3D allows for transport modelling capabilities. The newly developed MODFLOW-6, written in an object oriented framework could also be a good choice, however, this code is new and has not been tested within BGS yet. Therefore, before deciding on MODFLOW-6, it will need to be tested. SUTRA ranks lower than MODFLOW for this, since no example of parallelisation, and limited linking with other codes has been found. In addition, use-cases focus on coupled systems of either heat and groundwater or groundwater transport often represented in cross-sections. The frequency of use of HST3D is limited, and therefore less recommended.

Over the course of compiling this review, the focus of the codes has shifted from being able to simulate Nitrate and Heat to simulating drought and floods during the example period of the 2013/2014. Considering a focus on saturated groundwater flow, we would suggest to use either an off the shelf groundwater flow model, such as MODFLOW-2005 or MODFLOW 6, or write a BGS in house code that can solve the groundwater flow equation using moving grids.

If the aim is to code the groundwater model directly into Hydro-JULES, the code should be written in FORTRAN, which is the case for MODFLOW, SUTRA, HST3D and ESTEL.

Table 12. Ranking of the saturated model codes for Hydro-JULES. The weight of the ranking is from the priorities listed in Section 2.

Model	3d GW flow	3d GW solute transport	3d GW heat	Un-structured grids	Parallel-isation	Language	Open source	Cost	Linkability	Ease of use	Manual	Code guardian	Frequency of use	Sum
MODFLOW	3	2	0	2	1	F	3	3	3	2	1	Open source, USGS	1	21
OpenGeoSys	3	2	1	2	2	C	3	3	3	0	1	Free	1	21
Dumux	3	2	1	2	2	C	3	3	2	0	1	Free	1	20
PFLOTRAN	3	2	1	2	2	F	3	3	2	0	1	Open source	1	20
SUTRA	3	2	1	2	0	F	3	3	2	2	1	Open source, USGS	1	20
MODFLOW 6	3	0	0	2	1	F	3	3	3	1	1	Open source, USGS	0	17
HST3D	3	2	1	0	2	F	3	3	2	0	1	Open source, USGS	0	17
FEFLOW	3	2	1	2	1	C	0	0	2	3	1	MIKE DHI	1	16
Tough2	3	2	1	2	2	F	0	0	3	0	1	LBNL	1	15
ESTEL	3	2	0	2	2	F	0	0	0	0	1	Bristol	0	10
Marthe	3	2	1	0	0	F	0	0	2	0	1	BRGM	1	10

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