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A fully interior penalty discontinuous Galerkin method for variable density groundwater flow problems

Ali Raeisi Isa-Abadi^a, Vincent Fontaine^b, Hamid-Reza Ghafouri^c, Anis Younes^d, Marwan Fahs^{d,*}

^aDepartment of Water Engineering, Shahrekord University, Shahrekord, Iran

^bDepartment of Building and Environmental Sciences, University of Réunion, Le Tampon, France

^cDepartment of Civil Engineering, Shahid Chamran University of Ahvaz, Ahvaz, Iran

^dUniversité de Strasbourg, CNRS, ENGEEES, LHYGES UMR 7517, F-67000 Strasbourg, France

Abstract

Discontinuous Galerkin (DG) methods due to their robustness properties, e.g. local conservation, low numerical dispersion, and well-capturing strong shocks and physical discontinuities, are well-suited for the simulation of Variable Density Flow (VDF) in porous media. This paper aims at introducing, in a unified format, the general class of Interior Penalty DG (IPDG) methods to solve the VDF equations. A combination of symmetric, non-symmetric and incomplete IPDG methods is used to discretize both head and concentration variables. Compatibility analysis is performed to prevent the loss of accuracy of the IPDG methods in simulations of coupled flow and transport equations. An accurate technique is used for time integration, based on a non-iterative procedure and adaptive time stepping with embedded error control. Several benchmarks are investigated to validate the proposed DG scheme and to examine its performance in simulating VDF problems. The new DG scheme reproduces better the experimental data than the conventional SEAWAT model. Its results are in excellent agreement with a recent semi-analytical solution of the Henry problem, dealing with seawater intrusion under convection-dominating conditions. The performance of the DG scheme is examined by simulating the challenging problem of natural convection in porous enclosure. The method is compared against a finite element solution obtained with COMSOL multi-physics. The numerical experiments indicate clearly that high-order DG method is much more appropriate than standard conforming Galerkin method in simulating VDF problems while at the same time, guaranteeing a better precision and high-fidelity solutions. The proposed numerical method can be extended to 3D problems.

Keywords: Variable density flow, Compatible algorithms, Advanced model, seawater intrusion, Natural convection in porous enclosures

1. Introduction

Numerical modeling of variable density flow (VDF) has an irreplaceable role in predicting the groundwater behaviour in several applications such as seawater intrusion, saltwater upconing, geothermal systems, underground nuclear waste disposal, and carbon sequestration. In such situations, a coupled nonlinear system of flow and transport equations is commonly used to describe the physical processes. Simulation

*Corresponding author
Email address: fahs@unistra.fr (Marwan Fahs)

6 of VDF problems requires accurate methods as numerical artifacts can affect the results, especially in un-
7 stable cases. This is also why benchmarking VDF numerical models is a common issue which has been
8 widely discussed in the literature [30, 65, 73, 74, 77, 84]. Clearly, in a numerical simulation, the level of
9 the solution accuracy profoundly depends on the applied numerical scheme.

10 In the literature, several studies investigated the different aspects of VDF numerical modelling. For
11 instance, Mazzia and Putti [56] validated the formulations resulting from the combination of two sets of
12 dependent variables, i.e. head/concentration and pressure/mass-fraction, and concluded that the latter one
13 is more accurate especially in long simulation periods. Comparison of conservative and non-conservative
14 formulations [62] and validity of Oberbeck-Boussinesq based formulation were also explored [36, 47, 49].
15 Younes et al. [92] studied the efficiency of high-order time integration schemes to solve the partial differential
16 equations of the VDF model. Different time-stepping techniques have been also investigated in Hirthe and
17 Graf [41], Younes and Ackerer [89]. Consistent velocity approximation is one of the numerical challenges
18 addressed by Albets-Chico and Kassinos [5], Diersch and Kolditz [20], Frolkovič [32], Herbert et al. [40], Voss
19 and Souza [85]. Another common challenge that the authors have encountered is the solution of the coupled
20 nonlinear systems obtained from numerical discretization. For example, Putti and Paniconi [66] presented
21 a partial Newton method in order to reduce the size of matrix systems equal to that of Picard. A new
22 coupling procedure was also proposed by Ackerer [2] to improve the rate of convergence in Picard method.
23 However, one of the most crucial questions for the numerical solution of the VDF model is the discretization
24 of the spatial derivatives. Numerous studies have been devoted to the various spatial discretization methods
25 such as the finite difference method [15, 37], the finite element method [19, 45, 72], the finite volume method
26 [33, 38], and the method of characteristics [63, 64]. However, using the conventional discretization methods
27 (especially standard Galerkin finite element and finite difference methods) for the transport equation leads
28 to numerical dispersion [57, 86], and using nonconservative methods for the flow equation in a coupled
29 system can result in erroneous solutions [21].

30 DG methods were firstly introduced in the middle of the seventies for the numerical approximation
31 of hyperbolic problems, and independently, in the context of elliptic and parabolic problems [see e.g.,
32 8, 9, 14]. For diffusion problems, Arnold [7] introduced a primal DG method inspired by the original work
33 of Nitsche (1971) using Interior Penalty (IP) technique to weakly enforce some regularity requirements of
34 the solution across the skeleton of the mesh. This derivation yields to the Symmetric Interior Penalty (SIP)
35 method and constitutes a milestone in the development of primal DG methods. In the late 1990s, numerous
36 variations of the SIP method have been proposed and studied in the literature. For instance, Oden et al. [61]
37 introduced the Oden–Babuška–Baumann (OBB) method for pure diffusion problems and then extended
38 it to convection-diffusion processes [11]. Compared to SIP, the differences lie in the use of consistency
39 and penalty terms at interfaces that are now skew-symmetric and null, respectively. Alternatively, penalty
40 terms have been added to the OBB formulation leading to the Non-symmetric Interior Penalty (NIP)
41 method analyzed by Rivière et al. [70]. Finally, we mention the Incomplete Interior Penalty (IIP) method

42 as introduced first by Dawson et al. [16]. Thus, symmetric, non-symmetric and incomplete interior Penalty
43 methods are the three most famous variations of the primal DG method, and they have been judiciously
44 combined to solve efficiently coupled single-phase flow and reactive transport problems [see e.g., 16, 80,
45 and the references therein]. The DG methods are numerically stable even for high Péclet numbers, able to
46 capture physical discontinuities well and to handle nonconforming and unstructured meshes [1, 31]. They
47 are locally adaptive in mesh and polynomial degrees and are well suited for efficient parallel implementations
48 [see e.g. 14, 57, 79, and references therein].

49 Since its introduction, and due to their advantages, DG methods have benefited from intensive research
50 and development, and they have been applied to a variety of physical issues and situations. In the context of
51 porous media, the DG method has been used to discretize the hyperbolic terms of the governing equations
52 in applications involving contaminant transfer in aquifers [88], two phase flow nonfractured domains [27,
53 34, 51, 94], two phase flow in fractured domains [42, 43, 58, 59, 93] and diffusion and natural convection in
54 fractured domains [44]. In this context, the combination of DG method and mixed finite element (MFE)
55 method has received particular attention. The former has been used to discretize the convective term of
56 the transport equation while the later has been used for flow. Sun et al. [78] used this combination with a
57 cut-off operator in DG method to make the method converge. Li and Riviere [55] developed a discretization
58 method based on the combination of MFE-DG without any slope limiter into heterogeneous media which
59 uses a high-order Runge-Kutta approximation for time.

60 The DG method has been also used to entirely solve the flow or transport (both hyperbolic and parabolic
61 terms) equations in porous media. Li and Riviere [54] used a weighted version of high-order IPDG methods
62 for simulation of miscible displacement problems. Besides, Rivière and Wheeler [69] described a full DG
63 method with slope limiter for miscible displacement. For a coupled system of flow and reactive transport,
64 a fully primal DG using a cut-off operator was developed by Sun and Wheeler [79]. Full primal DG
65 method was used to simulate two-phase flow in Arbogast et al. [6], Bastian [10], Epshteyn and Rivière
66 [23, 24, 25], Ern et al. [26], Jamei et al. [46], Kou and Sun [50], Mozolevski and Schuh [60]. The three primal
67 DG methods, namely IIP, SIP, and NIP methods were discussed in these works. Different DG methods
68 have been also used to investigate variably-saturated flow expressed by Richards equation [17, 22, 52, 53]
69 and reactive transport in porous media [79–83, 87].

70 This brief review shows an increasing interest in the development and utilization of the DG methods
71 in several applications related to flow and mass transfer in fractured/unfractured porous media. The
72 review paper by Miller et al. [57] estimated that, with the advancement of computing technology, DG
73 methods have great potential to be foundational technique for future simulators of multi-physical processes
74 in porous media and more generally for future solvers of physical partial differential equations. The dynamic
75 adaptivity properties and localized nature of DG methods, especially, are well-adapted for many VDF
76 situations where the dense physics/high spatial gradients occur only in a small space may vary continuously
77 over time. Thereby, a comparable memory and processing time can be saved. However, despite their

78 advantages, wide range of applications, increasing popularity and promising results, applications of DG
79 methods in VDF are limited and performance of these methods in such a configuration has been never
80 evaluated. For VDF, the DG methods have been only used for discretizing the convective terms of the
81 transport equation and has been coupled with other methods (mainly MFE) for discretizing the flow and
82 parabolic term of the transport equation [3, 4, 13, 92].

83 DG methods have never been used to solve the full VDF model while this could be very advantageous.
84 In a full DG model, one can efficiently solve pure diffusion, pure advection or any mixed situation with
85 one and only one mathematical formalism, no splitting operator techniques, no need to introduce different
86 variables for the diffusive and convective parts, and solution procedure can be efficiently accelerated using
87 parallel computing. This avoids splitting errors and allows for treating mixed boundary conditions in
88 accurate manner. Thus, the main aim of the present work is to show how DG methods can be used to solve
89 the full VDF model and to evaluate the performance and benefits of this class of methods in simulating
90 VDF problems. We develop a unified and coherent format of the general class of IPDG. We test symmetric,
91 non-symmetric and incomplete IPDG methods to discretize flow and transport variables (pressure head and
92 concentration). Flow and transport equations are solved sequentially. We implement an efficient scheme for
93 time integration based on adaptive time stepping with error control. The new developed numerical scheme
94 is validated against experimental data and semi-analytical solutions for problems involving VDF driven by
95 salinity gradients. A highly convective thermal-driven case is considered to evaluate the performance of the
96 developed DG scheme, by comparing it against standard finite element solution obtained with COMSOL
97 Multiphysics.

98 The paper is organized as follows: In section 2, we describe the governing equations. Section 3 is
99 devoted to the discretization of the governing equations using the IPDG method and to the numerical
100 scheme implemented to solve the discretized equations. Section 4 aims at validating and verifying the
101 new developed scheme by comparison against semi-analytical solutions (Henry and thermal porous-cavity
102 problems) and experimental data. To highlight the performance of the developed DG scheme, a convergence
103 analysis is presented in section 4. Finally, we end in section 5 with general conclusions.

104 2. Governing equations

105 The governing equations of variable density groundwater flow and solute transport are described follow-
106 ing [12, 45, 49]. The set of partial differential equations include (i) the generalized Darcy' law, (ii) continuity
107 equations of fluid and solute mass, and (iii) state equations for the bulk fluid density and/or viscosity. We
108 will propose an equivalent compact formulation of both original problems based on the introduction of
109 suitable variables. In the rest of the paper, we assume that previous coupled physical processes are given
110 in a bounded domain $\Omega \subset \mathbb{R}^2$ with a Lipschitz boundary $\partial\Omega$, and in time interval $[0, T]$, with $T > 0$.

111 *2.1. Variable density flow equation*

112

113 The generalized Darcy' law can be written in term of the reference head variable $\varphi = p/(\rho_0 g) + z$ where
 114 p corresponds to the dynamic pressure $[ML^{-1}T^{-2}]$, ρ_0 the reference fluid density $[ML^{-3}]$, z the vertical
 115 elevation above some datum level $[L]$, and g the gravity acceleration $[LT^{-2}]$. Namely,

$$116 \quad \mathbf{q} = -\mathbf{K} \left(\nabla\varphi + \frac{\rho - \rho_0}{\rho_0} \nabla z \right) \quad \text{in } \Omega \times (0, T], \quad (1)$$

117 where \mathbf{q} denotes the Darcy's velocity $[LT^{-1}]$ and ρ is the fluid density $[ML^{-3}]$. Here, $\mathbf{K} = \frac{\rho_0 g \mathbf{k}}{\mu}$ is defined
 118 as hydraulic conductivity where \mathbf{k} is the permeability tensor of the porous material $[L^2]$, and μ the bulk
 119 fluid viscosity $[ML^{-1}T^{-1}]$. Following Huyakorn et al. [45], the time-dependent mass balance equation of
 120 the fluid in a porous medium is given by:

$$121 \quad \rho s \partial_t \varphi + \phi \partial_c \rho \partial_t c + \nabla \cdot (\rho \mathbf{q}) = 0, \quad \text{in } \Omega \times (0, T], \quad (2)$$

122 where s is the specific storativity of the porous medium related to head change $[L^{-1}]$, c the solute mass
 123 fraction $[-]$, ϕ the kinematic porosity $[-]$, and ∂_x the partial derivative operator with respect to the x -
 124 variable. The boundary $\partial\Omega$ is divided into a Dirichlet part, $\partial\Omega_D$, and a Neumann part, $\partial\Omega_N$, such that
 125 $\partial\Omega_D \cup \partial\Omega_N = \partial\Omega$ and $\partial\Omega_D \cap \partial\Omega_N = \emptyset$. Thus, the boundary and initial conditions for the flow process are
 126 given by:

$$127 \quad \varphi = \varphi_D, \quad \text{on } \partial\Omega_D \times (0, T], \quad (3a)$$

$$128 \quad \rho \mathbf{q} \cdot \mathbf{n} = q_N, \quad \text{on } \partial\Omega_N \times (0, T], \quad (3b)$$

$$129 \quad \varphi(\cdot, 0) = \varphi^0, \quad \text{in } \Omega \times \{0\}, \quad (3c)$$

131 where \mathbf{n} is the outward unit normal vector on $\partial\Omega$, φ_D and q_N are prescribed functions on $\partial\Omega_D$ and $\partial\Omega_N$,
 132 respectively.

133 *2.2. Solute transport equation*

134 The solute transport process is governed by a time-dependent advection-dispersion equation,

$$135 \quad \partial_t(\phi \rho c) + \nabla \cdot (\rho \mathbf{q} c - \rho \mathbf{D} \nabla c) = 0, \quad \text{in } \Omega \times (0, T]. \quad (4)$$

136 Here \mathbf{D} corresponds to the hydrodynamic dispersion tensor $[L^2 T^{-1}]$ given by,

$$137 \quad \mathbf{D} = (\alpha_T |\mathbf{q}| + \phi D_m) \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{q} \otimes \mathbf{q}}{|\mathbf{q}|}, \quad (5)$$

138 where \otimes denotes the dyadic product, $|\cdot|$ the Euclidean norm, D_m the molecular diffusion coefficient $[L^2 T^{-1}]$,
 139 \mathbf{I} the identity tensor, and α_L and α_T the longitudinal and transverse dispersivity, respectively $[L]$. The
 140 domain boundary is now splitted into the inflow part, $\partial\Omega_{\text{in}} := \{\mathbf{x} \in \partial\Omega : \mathbf{q} \cdot \mathbf{n} < 0\}$, and the outflow part,

141 $\partial\Omega_{\text{out}} := \partial\Omega \setminus \partial\Omega_{\text{in}}$, such that $\partial\Omega_{\text{in}} \cup \partial\Omega_{\text{out}} = \partial\Omega$ and $\partial\Omega_{\text{in}} \cap \partial\Omega_{\text{out}} = \emptyset$. Thus, the boundary and initial
 142 conditions for the solute transport process are given by:

$$143 \quad (\rho c \mathbf{q} - \rho \mathbf{D} \nabla c) \cdot \mathbf{n} = \rho_{\text{in}} c_{\text{in}} \mathbf{q} \cdot \mathbf{n}, \quad \text{on } \partial\Omega_{\text{in}} \times (0, T], \quad (6a)$$

$$144 \quad -\mathbf{D} \nabla c \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega_{\text{out}} \times (0, T], \quad (6b)$$

$$145 \quad c(\cdot, 0) = c^0, \quad \text{in } \Omega \times \{0\}, \quad (6c)$$

146
 147 where ρ_{in} and c_{in} are the specified inflow density and mass fraction at the inflow boundary $\partial\Omega_{\text{in}}$, respectively.

148 2.3. State equation for the bulk fluid density

149 The state equations represent fundamental thermodynamic relationships reflecting some properties and
 150 physical characteristics of a fluid using state variables. In practice, the mathematical dependencies of the
 151 bulk fluid density and viscosity quantities are usually derived by using a total derivative representation
 152 with respect to the set of state variables. Here, we assume that the bulk fluid density and viscosity depend
 153 only on the mass fraction variable, i.e., $\rho = \rho(c)$ and $\mu = \mu(c)$, on the whole domain. We consider the
 154 simplest linearized model for the density :

$$155 \quad \rho = \rho_0 (1 + \beta_0 c), \quad \text{in } \Omega \times (0, T], \quad (7)$$

156 where $\beta_0 = \rho_0^{-1} \partial_c \rho$ corresponds to the expansivity coefficient resulting from a change of the solute mass
 157 fraction $[-]$. Different mathematical models of state equations have been proposed in the literature, in-
 158 cluding the thermal effect and based on a polynomial expansion of the state variables. The viscosity is
 159 considered as constant in the numerical simulations developed in this work, but the developed DG model
 160 can handle variable viscosity.

161 2.4. Mathematical model

162 In this section, we propose to rewrite the set of partial differential equations governing variable-density
 163 flow with the corresponding initial and boundary conditions in a compact form. To this aim, we introduce
 164 suitable variables for the description of each of both processes. Thus, we use the following notations:

$$165 \quad (\text{Flow}) \quad s^* = \rho s, \quad \beta_0^* = \rho_0 \phi \beta_0, \quad \mathbf{q}^* = \rho \mathbf{q} \quad \text{and} \quad \mathbf{K}^* = \rho \mathbf{K}, \quad (8a)$$

$$166 \quad (\text{Transport}) \quad \phi^* = \rho \phi, \quad \mathbf{D}^* = \rho \mathbf{D} \quad \text{and} \quad c_{\text{in}}^* = \frac{\rho_{\text{in}} c_{\text{in}}}{\rho}. \quad (8b)$$

167
 168 Respecting the previous notations, the flow problem is now described by the simplified set of equations:

$$169 \quad s^* \partial_t \varphi + \beta_0^* \partial_t c + \nabla \cdot \mathbf{q}^* = 0, \quad \text{in } \Omega \times (0, T], \quad (9a)$$

$$170 \quad \mathbf{q}^* = -\mathbf{K}^* (\nabla \varphi + \beta_0 c \nabla z), \quad \text{in } \Omega \times (0, T], \quad (9b)$$

171
 172 where the initial and Dirichlet boundary conditions (3a)-(3c) remain unchanged, and the Neumann condi-
 173 tion (3b) becomes:

$$174 \quad \mathbf{q}^* \cdot \mathbf{n} = q_N, \quad \text{on } \partial\Omega_N \times (0, T]. \quad (10a)$$

175

176 The time-dependent advection-dispersion equation now can be written as follows:

$$177 \quad \gamma \partial_t(c) + \nabla \cdot (\mathbf{q}^* c - \mathbf{D}^* \nabla c) = 0, \quad \text{in } \Omega \times (0, T], \quad (11)$$

178 where $\gamma(c) = \phi^* + \beta_0^* c$, with the following boundary conditions

$$179 \quad (c\mathbf{q}^* - \mathbf{D}^* \nabla c) \cdot \mathbf{n} = c_{\text{in}}^* \mathbf{q}^* \cdot \mathbf{n}, \quad \text{on } \partial\Omega_{\text{in}} \times (0, T], \quad (12a)$$

$$180 \quad -\mathbf{D}^* \nabla c \cdot \mathbf{n} = 0, \quad \text{on } \partial\Omega_{\text{out}} \times (0, T]. \quad (12b)$$

182 Let us underline that the initial condition (6c) remains unchanged as well as the definitions of inflow $\partial\Omega_{\text{in}}$
183 and outflow $\partial\Omega_{\text{out}}$ boundary parts since $\rho > 0$.

184 3. Interior penalty discontinuous Galerkin methods

185 The class of Interior Penalty discontinuous Galerkin (IPDG) methods is now derived to solve the coupled
186 non-linear system of partial differential equations. Precisely, we consider the Incomplete Interior Penalty
187 (IIP), the Symmetric Interior Penalty (SIP) and the Non-symmetric Interior Penalty (NIP) variants for
188 each physical process leading to nine possible combinations schemes. The main difference between these
189 three IP variants lies in the symmetrization term used in the discrete bilinear form [68]. Before establishing
190 the weak formulations, let us introduce some conventional notations that will be used throughout the
191 remainder of the paper.

192 3.1. Some notations

193 We denote by $0 = t_0 < t_1 < t_2 < \dots < t_N = T$ a non-uniform partition of the simulation time
194 interval $(0, T]$. Let $\mathcal{E}_h = \{E_i\}_{N_h}$ be a partition of the domain $\bar{\Omega}$ into a set of quasi-uniform conforming
195 triangular elements, E denotes an element with the boundary ∂E and area $|E|$, and $h = \max_{E \in \mathcal{E}_h} h_E$ where
196 $h_E = \text{diam}(E)$. Let N_{loc}^H and N_{loc}^c be the number of degrees of freedom (DOFs) per element for head and
197 mass fraction, respectively. Let \mathcal{F}_h be the set of all edges comprising interior and boundary edges such
198 that $\mathcal{F}_h = \mathcal{F}_h^I \cup \mathcal{F}_h^B$. Let Γ be an interior edge $\Gamma \in \mathcal{F}_h^I$ with size $|\Gamma|$, then there exist two adjacent elements
199 E_{Γ}^{\pm} such that $\Gamma = \partial E_{\Gamma}^- \cap \partial E_{\Gamma}^+$. Further, we denote $\mathbf{n}_{\Gamma}^{\pm}$ the unit normal vector on Γ pointing exterior to
200 E_{Γ}^{\pm} , respectively (see e.g., Fig. 1), and \mathbf{n}_{Γ} is coincident with \mathbf{n}_{Γ}^+ . Let Γ be a boundary edge $\Gamma \in \mathcal{F}_h^B$, then
201 there exist an element $E \in \mathcal{E}_h$ such that $\Gamma = \partial E \cap \partial\Omega$. We define the set of Dirichlet, Neumann, inflow and
202 outflow edges such that $\mathcal{F}_h^B = \mathcal{F}_h^D \cup \mathcal{F}_h^N = \mathcal{F}_h^{\text{in}} \cup \mathcal{F}_h^{\text{out}}$. For clarity purposes, we denote by $\mathcal{F}_h^0 := \mathcal{F}_h^I \cup \mathcal{F}_h^D$
203 for the flow problem, and by $\mathcal{F}_h^+ := \mathcal{F}_h^I \cup \mathcal{F}_h^{\text{out}}$ for the solute transport problem. The DG method is based
204 on the use of discontinuous approximations of discrete variables. To this aim, let us introduce the broken
205 polynomial space \mathcal{V}_h^p which is a finite dimensional space of discontinuous piecewise polynomial functions
206 belonging to the broken Sobolev space $\mathcal{H}^s(\mathcal{E}_h)$ with $s \geq 1$,

$$207 \quad \mathcal{V}_h^p := \{v \in L^2(\Omega) : v|_E \in \mathbb{P}_p(E) \quad \forall E \in \mathcal{E}_h\},$$

208 where $\mathbb{P}_p(E)$ corresponds to the space of all polynomials of total degree $\leq p$ on E . Let ψ_Γ^\pm be the traces
 209 of function ψ on the edge Γ between E_Γ^\pm . Therefore, p_φ and p_c are taken to be the total degrees of
 discontinuous polynomials for approximating reference head and mass fraction, respectively. The jump and

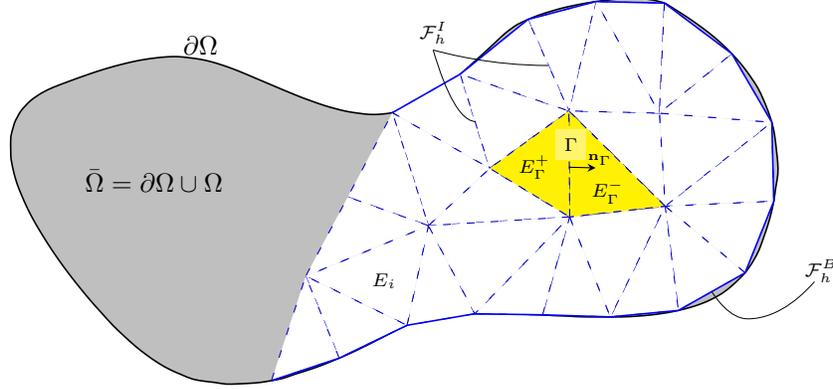


Fig. 1. Schematic discretization of $\bar{\Omega}$ and representation of elements, interior and boundary edges

210

211 average of ψ on Γ can be now defined on the skeleton \mathcal{F}_h as follows,

$$212 \quad \llbracket \psi \rrbracket := \begin{cases} \psi_\Gamma^- \mathbf{n}_\Gamma^- + \psi_\Gamma^+ \mathbf{n}_\Gamma^+, & \text{if } \Gamma \in \mathcal{F}_h^I, \\ \psi \mathbf{n}, & \text{if } \Gamma \in \mathcal{F}_h^B, \end{cases} \quad (13a)$$

213

$$214 \quad \{\!\!\{ \psi \}\!\!\} := \begin{cases} (\psi_\Gamma^- + \psi_\Gamma^+) / 2, & \text{if } \Gamma \in \mathcal{F}_h^I, \\ \psi, & \text{if } \Gamma \in \mathcal{F}_h^B. \end{cases} \quad (13b)$$

215 Let us precise that previous definitions of trace operators can be easily extended to any vector-valued
 216 functions ψ in the same way. For all $\mathbf{x} := (x_1, \dots, x_p) \in \mathbb{R}^p$ with $p \geq 1$, we define the uniform norm of \mathbf{x}
 217 by $\|\mathbf{x}\|_\infty := \max_{1 \leq i \leq p} |x_i|$.

218 3.2. Spatial discretization of the flow process

219 The IPDG weak formulations for flow and transport are derived by multiplying the corresponding
 220 governing equation by appropriate test functions, integrating by parts over an element $E \in \mathcal{E}_h$ (via the
 221 Green theorem), summing-up over all elements of the partition, and finally by imposing initial and boundary
 222 conditions. By performing the afore-mentioned operations on the flow problem (9), the weak form (in
 223 continuous time) is achieved and consists to seek, for any compatible $c_h(\cdot, t) \in \mathcal{V}_h^{p_c}$, the discrete variable
 224 $\varphi_h(\cdot, t) \in \mathcal{V}_h^{p_\varphi}$ such that,

$$225 \quad (s^* \partial_t \varphi_h, v_h)_{\mathcal{E}_h} + (\beta_0^* \partial_t c_h, v_h)_{\mathcal{E}_h} + a_h^{(\epsilon_f)}(\varphi_h, v_h; c_h) = l_f^{(\epsilon_f)}(v_h; c_h) \quad \forall v_h \in \mathcal{V}_h^{p_\varphi}, \quad (14)$$

226 where $\epsilon_f \in \{0, \pm 1\}$ is a symmetrization parameter, and the discrete operators $a_h^{(\epsilon_f)}$ and $l_f^{(\epsilon_f)}$ are given by:

$$227 \quad a_h^{(\epsilon_f)}(\varphi_h, v_h; c_h) = (\mathbf{K}^*(c_h) \nabla \varphi_h, \nabla v_h)_{\mathcal{E}_h} - \langle \{\!\!\{ \mathbf{K}^*(c_h) \nabla \varphi_h \}\!\!\}, \llbracket v_h \rrbracket \rangle_{\mathcal{F}_h^0} - \epsilon_f \langle \{\!\!\{ \mathbf{K}^*(c_h) \nabla v_h \}\!\!\}, \llbracket \varphi_h \rrbracket \rangle_{\mathcal{F}_h^0} + \langle \sigma_\Gamma^f \llbracket \varphi_h \rrbracket, \llbracket v_h \rrbracket \rangle_{\mathcal{F}_h^0}, \quad (15)$$

$$\begin{aligned}
l_f^{(\epsilon_f)}(v_h; c_h) &= -(\mathbf{K}^*(c_h)\beta_0 c_h \nabla z, \nabla v_h)_{\mathcal{E}_h} + \langle \{\{\mathbf{K}^*(c_h)\beta_0 c_h \nabla z\}\}, \llbracket v_h \rrbracket \rangle_{\mathcal{F}_h^D} - \epsilon_f \langle \mathbf{K}^*(c_h) \nabla v_h \cdot \mathbf{n}_\Gamma, \varphi_D \rangle_{\mathcal{F}_h^D} \\
&+ \langle \sigma_\Gamma^f \varphi_D, v_h \rangle_{\mathcal{F}_h^D} - \langle q_N, v_h \rangle_{\mathcal{F}_h^N}.
\end{aligned} \tag{16}$$

The second, third and fourth terms on the right-hand side of (15) are respectively called *consistency*, *symmetry* and *penalty* terms. The role of the parameter ϵ_f consists of regulating the symmetry term impact inside the bilinear form. Here, σ_Γ^f corresponds to the penalty parameter on Γ , and it is defined on the mesh skeleton as follows:

$$\sigma_\Gamma^f = \begin{cases} \frac{2\tau_\Gamma^- \tau_\Gamma^+}{\tau_\Gamma^- + \tau_\Gamma^+} & \text{if } \Gamma \in \mathcal{F}_h^I \\ \tau_{E,\Gamma} & \text{if } \Gamma \in \mathcal{F}_h^D \end{cases} \tag{17}$$

where $\tau_\Gamma^\pm = \tau_{E^\pm, \Gamma}$ denotes the transmissibility coefficient on $\Gamma = \partial E^- \cap \partial E^+$. For all $E \in \mathcal{E}_h$, and for any $\Gamma \in \partial E$, this parameter is given by,

$$\tau_{E,\Gamma} = \sigma_0^f \frac{|\Gamma|}{|E|} (p_\varphi + 1)(p_\varphi + 2) \kappa_{E,\Gamma}, \tag{18}$$

where $\kappa_{E,\Gamma} = \mathbf{n}_\Gamma \mathbf{K}_E^* \mathbf{n}_\Gamma$ represents the normal diffusivity on Γ and $\sigma_0^f \geq 0$ is a user-dependent parameter. The unified DG formalism of the variable density flow problem (14) includes the Incomplete Interior Penalty (IIP), the Symmetric Interior Penalty (SIP), the Non-symmetric Interior Penalty (NIP), and the Oden–Babuška–Baumann (OBB) methods. All these variants are deduced by choosing precisely both parameters ϵ_f and σ_0^f : IIP ($\epsilon_f = 0$ and $\sigma_0^f > 0$), SIP ($\epsilon_f = 1$ and $\sigma_0^f > 0$), NIP ($\epsilon_f = -1$ and $\sigma_0^f > 0$), and OBB ($\epsilon_f = -1$ and $\sigma_0^f = 0$). Regardless of the choice of IP methods, it is a fundamental aspect at this stage to reconstruct the Darcy’s velocity field \mathbf{q}^* . To this aim, we shall use the favourable local conservation properties associated with IPDG methods. Let us denote by $\tilde{\mathbf{q}}_h^*$ the discrete approximation of the velocity field \mathbf{q}^* on the partition \mathcal{E}_h . Two description levels are used to approximate \mathbf{q}^* (i) at the element-level E of the mesh \mathcal{E}_h , and (ii) at the edge-level Γ of the mesh skeleton \mathcal{F}_h .

$$\tilde{\mathbf{q}}_h^* = \begin{cases} \mathbf{q}_h^*, & \text{for all } E \in \mathcal{E}_h, \\ \hat{\mathbf{q}}_h^* & \text{for all } \Gamma \in \mathcal{F}_h, \end{cases} \tag{19}$$

where $\mathbf{q}_h^* = -\mathbf{K}^*(c_h) (\nabla \varphi_h + \beta_0 c_h \nabla z)$ and the numerical flux $\hat{\mathbf{q}}_h^*$ is defined as follow:

$$\hat{\mathbf{q}}_h^* = \begin{cases} \{\{\mathbf{q}_h^*\}\} + \sigma_\Gamma^f \llbracket \varphi_h \rrbracket, & \text{if } \Gamma \in \mathcal{F}_h^I \\ \mathbf{q}_h^* + \sigma_\Gamma^f (\varphi_h - \varphi_D) \mathbf{n}_\Gamma, & \text{if } \Gamma \in \mathcal{F}_h^D \\ q_N \mathbf{n}_\Gamma, & \text{if } \Gamma \in \mathcal{F}_h^N \end{cases} \tag{20}$$

3.3. Spatial discretization of the transport process

This section is devoted to the presentation of the IPDG discretization of the transport equation respecting the imposed boundary conditions. We use a similar approach to the previous section to handle the

254 dispersive part that we combine with a traditional upwind-strategy to control the advective part. Thus, the
 255 spatial discretization of the transport problem (in continuous time) consists to seek, for any reconstructed
 256 $\tilde{\mathbf{q}}_h^*(\cdot, t)$, the discrete variable $c_h(\cdot, t) \in \mathcal{V}_h^{p_c}$ such that,

$$257 \quad (\gamma \partial_t c_h, w_h)_{\mathcal{E}_h} + b_h^{(\epsilon_t)}(c_h, w_h; \tilde{\mathbf{q}}_h^*) = l_t^{(\epsilon_t)}(w_h; \tilde{\mathbf{q}}_h^*), \quad \forall w_h \in \mathcal{V}_h^{p_c}, \quad (21)$$

258 where $\epsilon_t \in \{0, \pm 1\}$, the discrete bilinear form $b_h^{(\epsilon_t)}$ is given by,

$$259 \quad b_h^{(\epsilon_t)}(c_h, w_h; \tilde{\mathbf{q}}_h^*) = (\mathbf{D}^*(\hat{\mathbf{q}}_h^*) \nabla c_h - c_h \hat{\mathbf{q}}_h^*, \nabla w_h)_{\mathcal{E}_h} + \langle \hat{\mathbf{q}}_h^* \llbracket c_h \rrbracket, \llbracket w_h \rrbracket \rangle_{\mathcal{F}_h^+} - \langle \llbracket \mathbf{D}^*(\hat{\mathbf{q}}_h^*) \nabla c_h \rrbracket, \llbracket w_h \rrbracket \rangle_{\mathcal{F}_h^I} \\ - \epsilon_t \langle \llbracket \mathbf{D}^*(\hat{\mathbf{q}}_h^*) \nabla w_h \rrbracket, \llbracket c_h \rrbracket \rangle_{\mathcal{F}_h^I} + \langle \sigma_\Gamma^t \llbracket c_h \rrbracket, \llbracket w_h \rrbracket \rangle_{\mathcal{F}_h^I}, \quad (22a)$$

260 and the linear form $l_t^{(\epsilon_t)}$ by,

$$261 \quad l_t^{(\epsilon_t)}(w_h; \tilde{\mathbf{q}}_h^*) = - \langle (\hat{\mathbf{q}}_h^* \cdot \mathbf{n}_\Gamma) c_{\text{in}}, w_h \rangle_{\mathcal{F}_h^{\text{in}}}. \quad (22b)$$

262 Here, $\sigma_\Gamma^t \geq 0$ corresponds to the penalty parameter for the advective-dispersive problem and we assume
 263 that it can be decomposed into a dispersive and advective parts,

$$264 \quad \sigma_\Gamma^t = \frac{2\tau_\Gamma^- \tau_\Gamma^+}{\tau_\Gamma^- + \tau_\Gamma^+} + \frac{1}{2} |\hat{\mathbf{q}}_h^* \cdot \mathbf{n}_\Gamma|, \quad \forall \Gamma \in \mathcal{F}_h^I, \quad (23)$$

265 where the parameters $\tau_\Gamma^\pm = \tau_{E^\pm, \Gamma}$ are now derived using the hydrodynamic dispersion tensor \mathbf{D}^* and the
 266 polynomial order p_c of the discrete variable c_h . For all $E \in \mathcal{E}_h$, and for any $\Gamma \in \partial E$, it is given by,

$$267 \quad \tau_{E, \Gamma} = \sigma_0^t \frac{|\Gamma|}{|E|} (p_c + 1)(p_c + 2) \kappa_{E, \Gamma}, \quad (24)$$

268 where $\kappa_{E, \Gamma} = \mathbf{n}_\Gamma \mathbf{D}_E^* \mathbf{n}_\Gamma$ represents the normal dispersion on Γ and $\sigma_0^t \geq 0$ is a user-dependent parameter.
 269 Despite the natural skew-symmetry of the advection-dispersion operator, we have included the additional
 270 symmetry term of the dispersive operator which is controlled here by the parameter ϵ_t . The resulting DG
 271 method is also called IIP, SIP, and NIP discretizations of the solute transport problem if ϵ_t is equal to 0,
 272 1, and -1, respectively [18, 48, 68].

273 3.4. Time-discretization of coupled flow-transport problem

274 The IPDG approach for solving the coupled flow-transport process yields to a set of differential and
 275 algebraic equations. To this aim, let us consider the discrete variables $\varphi_h(\cdot, t) \in \mathcal{V}_h^{p_\varphi}$ and $c_h(\cdot, t) \in \mathcal{V}_h^{p_c}$ that
 276 we decompose as follows:

$$277 \quad \varphi_h = \sum_{i=1}^{N_f} \varphi_i(t) v_i \quad \text{and} \quad c_h = \sum_{i=1}^{N_c} c_i(t) w_i \quad (25)$$

278 where $N_f = \dim(\mathcal{V}_h^{p_\varphi})$ and $N_c = \dim(\mathcal{V}_h^{p_c})$. Here, $(v_i)_{i=1, \dots, N_f}$ and $(w_i)_{i=1, \dots, N_c}$ denote the set of trial
 279 functions of approximation spaces $\mathcal{V}_h^{p_\varphi}$ and $\mathcal{V}_h^{p_c}$, respectively. The matrix form of the global discrete
 280 problem can be recast as follows:

$$281 \quad \begin{bmatrix} \mathbb{S} & \mathbb{C} \\ 0 & \mathbb{T} \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{\varphi}}_h \\ \dot{\mathbf{c}}_h \end{bmatrix} + \begin{bmatrix} \mathbb{A}^{(\epsilon_f)} & 0 \\ 0 & \mathbb{B}^{(\epsilon_t)} \end{bmatrix} \begin{bmatrix} \boldsymbol{\varphi}_h \\ \mathbf{c}_h \end{bmatrix} = \begin{bmatrix} \mathbf{L}_f \\ \mathbf{L}_t \end{bmatrix} \quad (26)$$

282 where the *dot* symbol denotes the partial time-derivative operator, and $\varphi_h^t = [\varphi_1, \dots, \varphi_{N_f}]$ and $c_h^t =$
 283 $[c_1, \dots, c_{N_c}]$, the vector of degrees of freedom of the discrete variable φ_h and c_h , respectively. The block-
 284 matrices associated with (26) are given by,

$$285 \quad \mathbb{S}_{|ij} = (s^*(c_h)v_j, v_i)_{\mathcal{E}_h}, \quad (27a)$$

$$286 \quad \mathbb{C}_{|ik} = (\beta_0^*(c_h)w_k, v_i)_{\mathcal{E}_h}, \quad (27b)$$

$$287 \quad \mathbb{T}_{|kl} = (\gamma(c_h)w_l, w_k)_{\mathcal{E}_h}, \quad (27c)$$

$$288 \quad \mathbb{A}_{|ij}^{(\epsilon_f)} = a_h^{(\epsilon_f)}(v_j, v_i; c_h), \quad (27d)$$

$$289 \quad \mathbb{B}_{|kl}^{(\epsilon_t)} = b_h^{(\epsilon_t)}(w_l, w_k; \tilde{\mathbf{q}}_h^*), \quad (27e)$$

$$290 \quad \mathbf{L}_{f|i} = l_f^{(\epsilon_f)}(v_i; c_h), \quad (27f)$$

$$291 \quad \mathbf{L}_{t|k} = l_t^{(\epsilon_t)}(w_k; \tilde{\mathbf{q}}_h^*). \quad (27g)$$

293 where indexes $i, j = 1, \dots, N_f$, $k, l = 1, \dots, N_c$, and block-matrices $\mathbb{A}, \mathbb{S} \in \mathbb{R}^{N_f} \times \mathbb{R}^{N_f}$, $\mathbb{B}, \mathbb{T} \in \mathbb{R}^{N_c} \times \mathbb{R}^{N_c}$,
 294 and $\mathbb{C} \in \mathbb{R}^{N_f} \times \mathbb{R}^{N_c}$. Due to the discontinuous nature of $\mathcal{V}_h^{p_\varphi}$ and $\mathcal{V}_h^{p_c}$, all computations (matrix assembly)
 295 can be done locally at the element level. We underline that the IPDG method leads to a very compact
 296 discretization stencil consist of a given mesh element and its direct neighbors. A popular way for solving
 297 the coupled differential-algebraic system (26) consists in splitting the numerical treatment of both physical
 298 sub-processes (flow and transport) and to treat them sequentially via an adapted flux reconstruction.
 299 Usually, for each time step, an iterative procedure is applied between the flow and transport operators
 300 until convergence. This approach could be more efficient in CPU time than the fully coupled approach
 301 that proceeds by solving both flow and transport operators simultaneously. However, the slow convergence
 302 of the iterative procedure between both operators affects significantly the performance of the solution.
 303 To avoid this problem, we use the non-iterative approach suggested by Younes and Ackerer [89]. In this
 304 paper, the time discretization is performed by a first-order Backward Differentiation Formula (BDF₁) and
 305 a direct solver using an unsymmetric-pattern multifrontal method and a direct sparse LU factorization
 306 (UMFPACK) is implemented for solving linear systems. Accuracy of the time discretization is insured
 307 using a proper time step management where the time step length is controlled by the temporal truncation
 308 error. Note that high order BDF can also be used and allow large time steps which may further improve the
 309 efficiency of the simulations [92]. The main steps of the non-iterative procedure used to solve the coupled
 310 flow and transport operators are described here. We denote by c_h^n and φ_h^n the discrete approximation of
 311 $c(\cdot, t_n)$ and $\varphi(\cdot, t_n)$ at the instant t_n with $0 \leq n \leq N$, respectively. Similarly, we denote by φ_h^n and c_h^n the
 312 corresponding vector of degrees of freedom. We describe below the staggered procedure for switching from
 313 t_n to t_{n+1} and calculating the $(n+1)$ -th time step Δt^{n+1} .

314 • **Step 1.** Solve the transport problem: Given c_h^n and $\hat{\mathbf{q}}_h^{*n}$, seek c_h^{n+1} solving the equation,

$$315 \quad \left[\frac{\mathbb{T}(c_h^n)}{\Delta t^n} + \mathbb{B}^{(\epsilon_t)}(\hat{\mathbf{q}}_h^{*n}) \right] c_h^{n+1} = \mathbf{L}_t(c_h^n) + \frac{\mathbb{T}(c_h^n)}{\Delta t^n} c_h^n, \quad (28)$$

where $\Delta t^n = t_{n+1} - t_n$.

- **Step 2. Solve the flow problem:** Given initial values \mathbf{c}_h^{n+1} , seek φ_h^{n+1} solving the equation,

$$\left[\frac{\mathbb{S}(\mathbf{c}_h^{n+1})}{\Delta t^n} + \mathbb{A}^{(\epsilon_f)}(\mathbf{c}_h^{n+1}) \right] \varphi_h^{n+1} = \mathbf{L}_f(\mathbf{c}_h^{n+1}) + \frac{\mathbb{S}(\mathbf{c}_h^{n+1})}{\Delta t^n} \varphi_h^n - \frac{\mathbb{C}(\mathbf{c}_h^{n+1})}{\Delta t^n} (\mathbf{c}_h^{n+1} - \mathbf{c}_h^n). \quad (29)$$

- **Step 3. Flux reconstruction:** Given \mathbf{c}_h^{n+1} and φ_h^{n+1} , we reconstruct the global velocity field $\tilde{\mathbf{q}}_h^{*n+1} = [\mathbf{q}_h^{*n+1}, \hat{\mathbf{q}}_h^{*n+1}]$ on the whole domain as follows :

– Mesh element: For all $A \in \mathcal{E}_h$, we compute interior approximations as follows,

$$\mathbf{q}_h^{*n+1} = -\mathbf{K}^*(c_h^{n+1}) (\nabla \varphi_h^{n+1} + \beta_0 c_h^{n+1} \nabla z). \quad (30)$$

– Mesh skeleton: For all $\Gamma \in \mathcal{F}_h^0$, we compute boundary approximations as follows,

$$\hat{\mathbf{q}}_h^{*n+1} = \begin{cases} \{\{\mathbf{q}_h^{*n+1}\}\} + \sigma_\Gamma^f \llbracket \varphi_h^{n+1} \rrbracket, & \text{if } \Gamma \in \mathcal{F}_h^I, \\ \mathbf{q}_h^{*n+1} + \sigma_\Gamma^f (\varphi_h^{n+1} - \varphi_D^{n+1}) \mathbf{n}_\Gamma, & \text{if } \Gamma \in \mathcal{F}_h^D. \end{cases} \quad (31)$$

- **Step 4. Update the time step:** The truncation error e^{n+1} measures the difference between first- and second-order temporal approximations of the concentration [89]:

$$e^{n+1} := \frac{1}{2} \left[\mathbf{c}_h^{n+1} - \left(\mathbf{c}_h^n + \frac{\Delta t^n}{\Delta t^{n-1}} (\mathbf{c}_h^n - \mathbf{c}_h^{n-1}) \right) \right]. \quad (32)$$

The uniform norm $\|e^{n+1}\|_\infty$ is used to accept or reject the time step with respect to the user tolerance γ^{tol} (set at 10^{-3} in this work).

– If $\|e^{n+1}\|_\infty \leq \gamma^{\text{tol}}$, the time step is accepted and the next one is estimated using,

$$\Delta t^{n+1} = \Delta t^n \min \left(\kappa \sqrt{\frac{\gamma^{\text{tol}}}{\|e^{n+1}\|_\infty}}, r_{\max} \right), \quad (33)$$

where $\kappa (= 0.95)$ is a safety factor and $r_{\max} (= 2)$ is the maximum allowed time step.

– Else, the time step is repeated with a smaller step size using the latest error estimate:

$$\Delta t_{j+1}^n = \Delta t_j^n \max \left(\kappa \sqrt{\frac{\gamma^{\text{tol}}}{\|e_j^{n+1}\|_\infty}}, r_{\min} \right), \quad (34)$$

where j indexes the consecutive time step estimates and $r_{\min} (= 0.1)$ is the minimum allowed time step.

- **Step 5. Update the initial guess:** $n \leftarrow n + 1$, $\mathbf{c}_h^n \leftarrow \mathbf{c}_h^{n+1}$, $\varphi_h^n \leftarrow \varphi_h^{n+1}$, $\Delta t^n \leftarrow \Delta t^{n+1}$ and back to **Step 1**.

339 *3.5. Compatibility analysis & Frolkovič-Knabner procedure*

340 Traditional algorithms employ operator-splitting to treat the coupled flow and transport processes
 341 sequentially and separately. However, when solving coupled processes, the discretization method employed
 342 to solve the flow is crucial since the approximate velocity field can strongly influence the positive features of
 343 the transport method. In 2003, Dawson et al. [16] analyzed compatible DG-algorithms for the coupled flow
 344 and transport problem. Specifically, they established some minimal requirements on the flow DG schemes
 345 to maintain optimal accuracy and conservation properties of the DG algorithms used for transport. Firstly,
 346 the authors proved that DG methods employed for the transport process must imperatively respect the
 347 *zero-order accuracy* requirement. This latter condition measures the ability of the DG method to reproduce
 348 a constant field by replacing the true velocity field \mathbf{q}^* by its discrete approximation $\tilde{\mathbf{q}}_h^*$ in the transport
 349 process. Particularly, Sun and Wheeler [79] analyzed this criterion in the context of primal IPDG methods,
 350 and they established that all schemes namely, IIP-, NIP- and SIP-DG variants, verify it. However, it also
 351 imposes that the discrete velocity field verifies a *compatibility* requirement, implying that the DG method
 352 employed for the resolution of flow can not be chosen arbitrarily i.e.,

$$353 \quad (\mathbf{q}_h^*, \nabla w_h)_{\mathcal{E}_h} + \langle \hat{\mathbf{q}}_h^*, \llbracket w_h \rrbracket \rangle_{\mathcal{F}_h} = \langle \mathbf{q}^* \cdot \mathbf{n}_\Gamma, w_h \rangle_{\mathcal{F}_h^{\text{in}}} \quad \forall w_h \in \mathcal{V}_h^{p_c}. \quad (35)$$

354 Let us note that the *compatibility* condition (35) corresponds here to a stronger form of the local conservative
 355 principle since it holds for any polynomial functions in the space $\mathcal{V}_h^{p_c}$, and not only for piecewise constants.
 356 Thus, in virtue of (35), the IIP-DG scheme method for flow is the only one compatible with primal IPDG
 357 methods for transport in the sense defined in [16]. In compliance with Sun and Wheeler [79], the total
 358 number of permissible combinations to solve VDF equations is now reduced from nine to three compatible
 359 ones: IIP-IIP, IIP-SIP, and IIP-NIP. Any other combination of (non-compatible) methods can cause severe
 360 struggles such as a loss of accuracy or conservative properties, and may not even converge. For solving
 361 the VDF equations, we can choose related polynomial degrees of approximation for flow and transport i.e.,
 362 $p_\varphi \sim p_c$, however, optimal or nearly optimal solution convergence can be attained when $p_\varphi = p_c$, in coupled
 363 flow and transport processes [79].

364 Besides, in buoyancy-driven problems, existence of additional gravity term in Darcy's velocity make a
 365 constraint on use of equal degrees of approximation for flow and transport due to the confliction between
 366 the head gradient and gravity terms of Darcy in parts of the domain where the velocity is zero or nearly zero
 367 [see e.g. 20, 32, 85]. To overcome this problem, a consistent velocity approximation based on Frolkovič-
 368 Knabner (FK) approximation [32] was developed for the IPDGs presented here for different polynomial
 369 degrees. The FK allows us to approximate flow and transport with the same degree of polynomials and
 370 also reduces the computational effort, considerably.

4. Results and discussion

A new numerical scheme is developed to solve the VDF equations with the DG method. This scheme is implemented in a numerical code. The first goal of this section is to validate the new developed scheme and to verify the correctness of the developed code. To do so, we use common benchmarks dealing with different configurations and applications of VDF and we compare the results of the new code against experimental results and semi-analytical solutions. The first benchmark is the Goswami-Clement laboratory experimental problem [35] that deals with saltwater intrusion in a rectangular experimental tank. This problem is used to test the new developed code in the case of specified-head boundary conditions (Dirichlet type). The comparison against experimental data would give an overall assessment of the robustness of the mathematical model in reproducing physical processes but cannot confirm the accuracy of the developed numerical solution and the correctness of the developed numerical code. The later can be well assessed by comparing numerical results against exact-analytical solutions. As there is no analytical solution for the VDF model, we compare the results of the new developed code against the semi-analytical solution of the Henry problem [39], which is a common benchmark for seawater intrusion. Several semi-analytical solutions of the Henry problem have been suggested in the literature [39, 71, 75, 90, 95], here we use the recent solution developed by Fahs et al. [28] as, in contrast to the previous solutions, it involves velocity-dependent dispersion. The Henry problem allows not only comparison against semi-analytical solution but also checking the model in a case dealing with specified-flux boundary conditions (Neumann type). Both Goswami-Clement and Henry problems deal with mixed convection as the flow is generated by a head gradient or forced conditions. In order to investigate the new developed code in a case involving purely natural convection, we consider the problem of natural convection in porous square cavity with vertically heated walls. In this case, VDF is thermally driven. The flow is generated by the temperature gradient. This problem is commonly used to represent natural convection in porous media in either cases of vertical (horizontally heated walls) or horizontal temperature gradient (vertically heated walls). We do not consider horizontally heated wall as the problem could be unstable. Unstable problems are not suitable for benchmarking as they could have multiple solutions [65]. Our new developed code is compared against the stable semi-analytical solution developed by [29]. For validation, we consider cases dealing with relatively small Rayleigh number. Beside verification, the problem of porous square cavity would also highlight the flexibility of the new developed model in treating either solute or thermal problems and even coupled thermohaline problems.

The Results section aims also at highlighting the performance and accuracy of the developed DG scheme in solving VDF equations. To do so, we consider a case of the porous cavity problem with high Rayleigh number and we compare the new developed model against a commercial model based on standard finite element method (COMSOL Multiphysics). Fahs et al. [29] have shown that such a case is computationally challenging as accurate solution of this case is beyond the capacity of current models. Standard numerical techniques used in current models could lead to spurious oscillations or numerical diffusion.

407 4.1. Validation: The Goswami-Clement experimental problem

408 Herein, to validate our model we simulate the laboratory experiments originally performed by Goswami
 409 and Clement [35]. These experiments have been developed with the purpose of evaluating the density-
 410 dependent models. The experimental setup composed of a rectangular flow tank comprising three distinct
 411 chambers. The central chamber contains an unconfined, homogeneous, porous medium and two constant-
 412 head chambers on the left and right sides containing saltwater and freshwater, respectively. Goswami
 413 and Clement [35] completed their experiments by recording the data in both transient and steady state
 414 conditions. As a result, in addition to the steady state validation, the transient test of numerical models
 415 is also possible. The saltwater intrusion experiments were conducted under three transient phases ended
 416 with steady state conditions. The first phase was established by setting the right freshwater head equal to
 417 26.7 cm and fixing the left equivalent freshwater head proportional to the saltwater head of 25.5 cm. Under
 418 these conditions, the first steady state condition (SS₁) was obtained for the salt wedge (initial phase). Then
 419 the freshwater head was instantaneously reduced to 26.2 cm and maintained until the second steady state
 420 condition (SS₂) is reached (advancing phase). Finally, the freshwater head was increased to 26.55 cm which
 421 forces the salt wedge to recede and the conditions was kept until the third steady state condition (SS₃) was
 422 established (receding phase).

423 In the present study, we tested our DG model by comparing the simulation results against experiments
 424 data in both transient and steady state conditions. For numerical simulations, the unconfined porous
 425 medium was assumed to be confined with the boundary conditions depicted in Fig. 2, [35]. The domain
 426 was discretized using 44K structured right-angled triangles with equal grid spacing and linear polynomial
 427 approximations were used for both variables i.e., head and mass fraction. The initial mass fraction and
 428 freshwater head were set to zero and 26.7 cm, respectively. Table 1 illustrates the physical parameters used
 for simulation of the experiments.

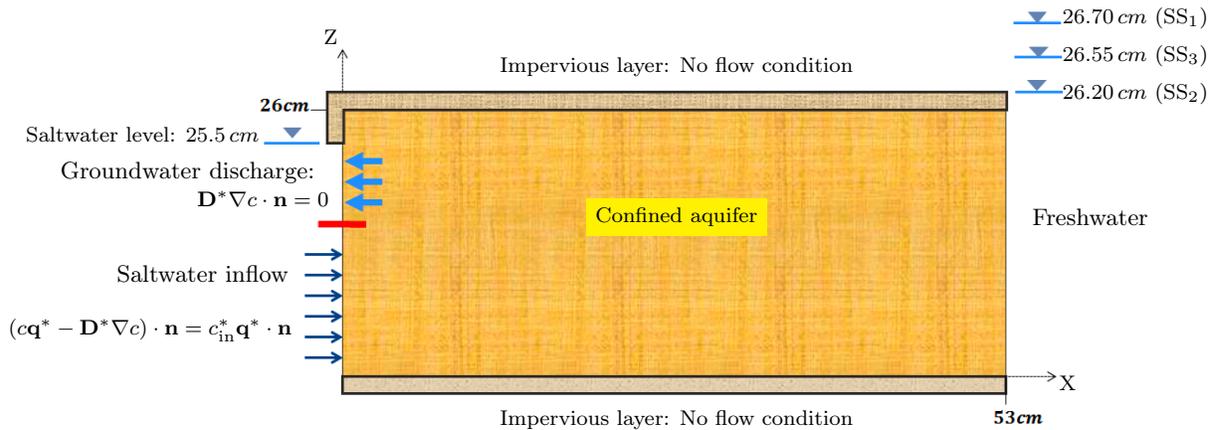


Fig. 2. Geometry and boundary conditions for the Goswami-Clement experimental setup

429

430 Fig. 3 illustrates the 10, 50 and 90 % isochlors predicted in steady state condition for three phases, SS₁

Table 1. Physical parameters for the Goswami-Clement experimental problem

Parameter	Value	Unit
\mathbf{K}	0.0122	ms^{-1}
D_m	1.0×10^{-9}	m^2s^{-1}
α_L	0.001	m
α_T	0.0001	m
s	1.0×10^{-5}	m^{-1}
ϕ	0.385	—
ρ_0	1000	$kg\ m^{-3}$
ρ_s	1026	$kg\ m^{-3}$
μ_0	0.001	$kg\ m^{-1}\ s^{-1}$
β_μ	0	—
β_0	0.026	—

431 to SS_3 . In addition to the experimental data from measurements of salt wedge location, the numerical
 432 results of SEAWAT [35] were superimposed for comparison. As can be seen, our results are in excellent
 433 agreement with the experimental data. The maximum difference between the results and experimental
 434 data respects to SS_2 . This is while for the SEAWAT model, the difference exists for all the three steady
 435 state conditions. In general, our model can provide a closer prediction of salt wedge, particularly in the
 toe, for SS_1 to SS_3 . Note that the results from IIP-IIP, IIP-SIP and IIP-NIP were closely similar [67].

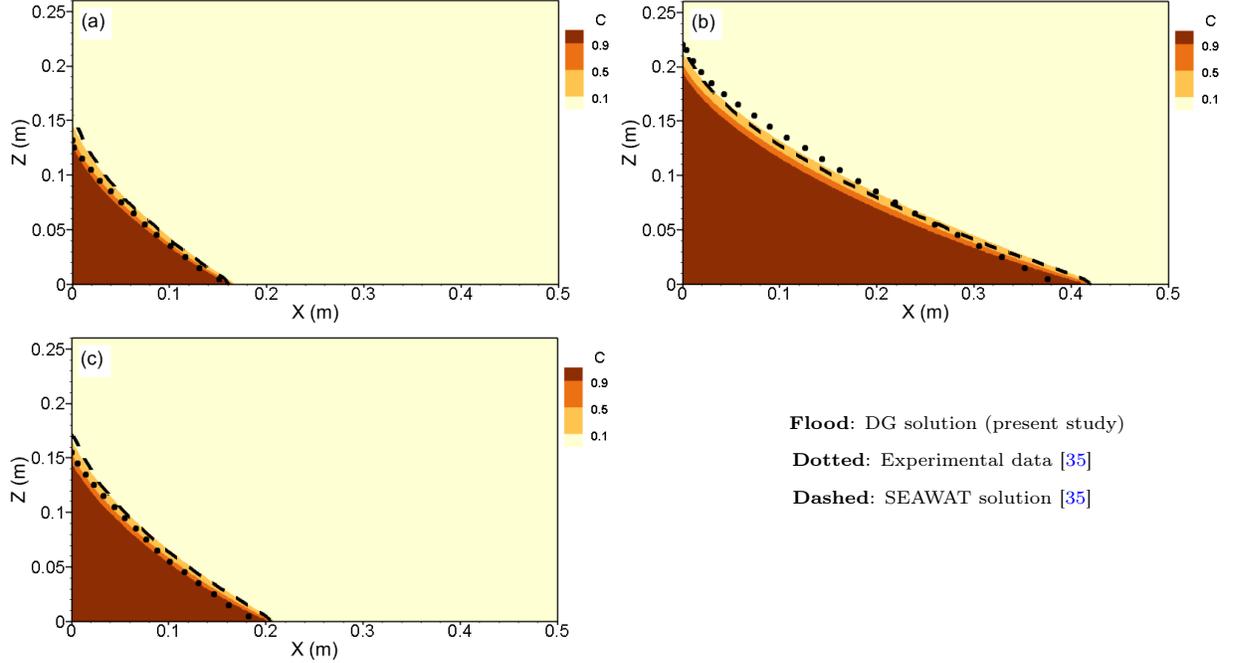


Fig. 3. 10%, 50% and 90% isochlors of DG solution in comparison with Goswami experimental data [35] and 50% SEAWAT isochlor [35] in the (a) first steady state (SS_1), (b) second steady state (SS_2), and (c) third steady state (SS_3) conditions

436

437 Here, for the first transient test, the advancing phase of salt wedge was also considered. Fig. 4 compares
 438 the results of numerical simulations with experimental measurements at times 5, 15, 55 *min* after starting
 439 the second phase. Similar to the steady state test, the results match well with the experimental data at the

440 different times. The results show that the more salt wedge advances over time, the less agreement appears
 441 due to approaching to SS_2 position. The results of SEAWAT model were also presented in the figure for
 442 comparison. Similarly, for SEAWAT, the differences was increased in the later times. As a second part of
 443 transient test, we performed a comparison of numerical results with experimental data in receding phase.
 444 Again, the most difference is observed when the salt wedge is closer to SS_2 position (Fig. 5). This condition
 is also true for SEAWAT [67].

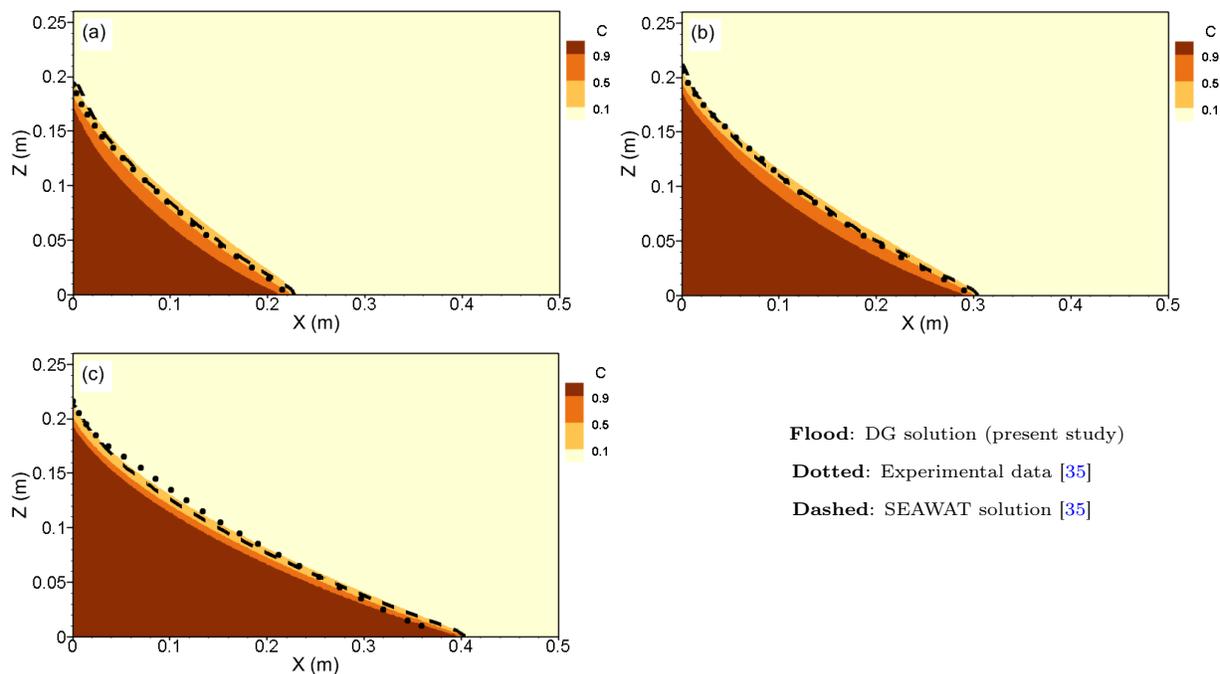


Fig. 4. 10%, 50% and 90% isochlors of DG solution in comparison with Goswami experimental data [35] and 50% SEAWAT isochlor [35] at (a) 5 min, (b) 15 min, and (c) 55 min of advancing phase (moving from SS_1 toward SS_2)

445
 446 Finally, a flux test was also presented to compare the freshwater fluxes predicted by the model against
 447 the steady state flux measurements. Table 2 reports the measured fluxes and the results from our DG
 448 code and SEAWAT. For the DG, the most difference is happened in SS_3 , though, this is not significant and
 449 is less than 2 percent. Generally, the fluxes estimated by our model compared to SEAWAT have closer
 agreement with the experimental measurements.

Table 2. Numerical fluxes ($cm^3 \cdot s^{-1}$) in comparison with the experimental data and SEAWAT for the three steady state conditions of Goswami-Clement problem

	SS_1	SS_2	SS_3
Experimental measurement [35]	1.42	0.59	1.19
DG (present study)	1.41	0.6	1.17
SEAWAT [35]	1.46	0.59	1.13

450

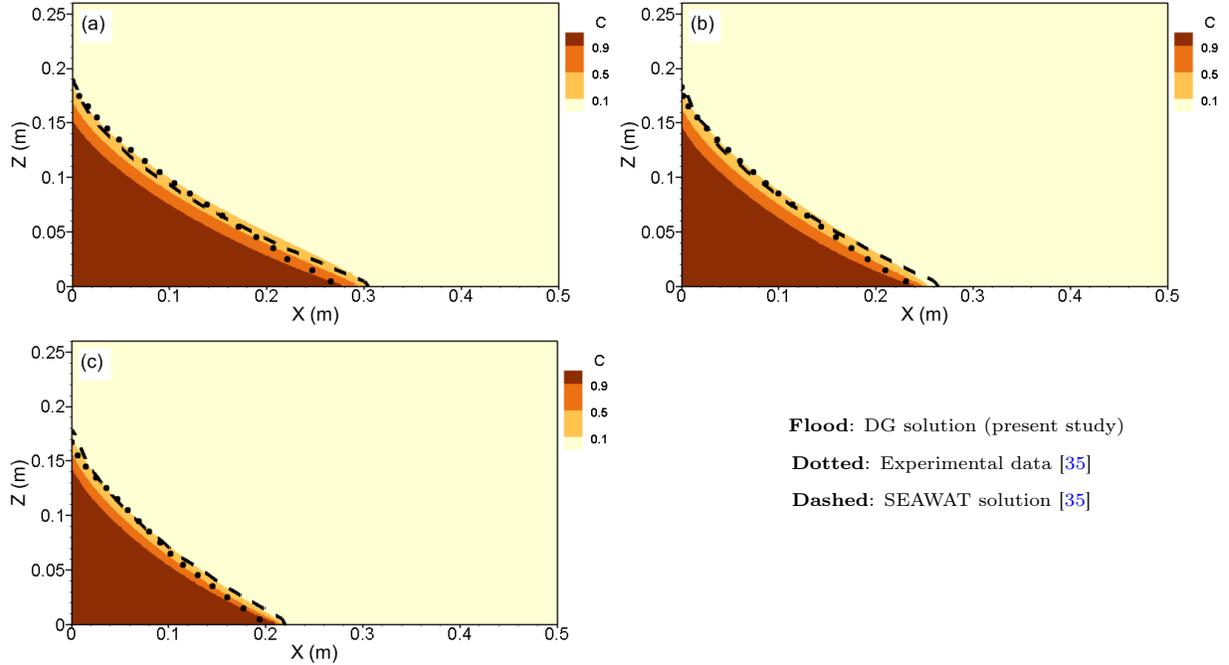


Fig. 5. 10%, 50% and 90% isochlors of DG solution in comparison with Goswami experimental data [35] and 50% SEAWAT isochlor [35] at (a) 10 min, (b) 15 min, and (c) 25 min of advancing phase (moving from SS₂ toward SS₃)

4.2. Verification against semi-analytical solution: The Henry problem

Henry [39] was the first to model seawater intrusion phenomenon in a variable density system. His simplified rectangular model is constructed based on a confined, homogeneous, isotropic 2D aquifer in a vertical section (Fig. 6). As shown, the left landward boundary is recharged by a constant rate of freshwater (Q) and the right boundary is ended to the sea such that the top aquifer boundary is just leveled at the sea surface. Saltwater intrudes from the seaside until an equilibrium is established with the landward inflowing freshwater. Henry developed a semi-analytical solution based on the double Fourier series for the problem under the steady state condition. Due to the availability of the analytical solution, for many years, various attempts have been made [see the review in 76, 95] aimed at utilizing the Henry problem as benchmark for variable density flow models. The first semi-analytical solution, developed by Henry [39], has been limited to high diffusion for which the buoyancy processes are dominated by diffusion. Voss et al. [84] showed that this solution is a necessary but not a sufficient test for a simulator to present variable-density physics. Several further studies suggested new semi-analytical solutions that are more sensitive to the variable-density flow physics by reducing the imposed inland flow or the diffusion coefficient [76, 91, 95].

Here we use the semi-analytical solution developed by Fahs et al. [28] that includes velocity-dependent dispersion. This solution is more realistic than previous solutions in representing seawater intrusion processes. It is more suitable for code verification as it includes velocity dependent dispersion. Here for verification purposes, we consider the three cases presented in Fahs et al. [28]. The first one is similar to the standard solution suggested by Henry [39]. It deals with pure molecular diffusion. The second one in-

470 cludes velocity-dependent dispersion, but with exaggerated dispersion coefficients leading to a wide mixing
 471 zone. These two cases are relatively simple from computational point of view as they do not involve sharp
 472 solutions. They are useful in verifying the correctness of the developed code. The third case deals with
 473 small dispersion coefficients, leading to a very narrow mixing zone. As shown in Fahs et al. [28], this case is
 474 computationally challenging because of its high sensitivity to the numerical scheme. Fahs et al. [28] showed
 475 that, for this case, standard finite element method leads to inaccurate results due to numerical diffusion.
 476 The physical parameters used in the three test cases are given in Table 3. Note that the three cases can be
 477 derived from the standard Henry problem by changing one or more of the following parameters: domain
 478 length (l), molecular diffusion (D_m) and dispersion coefficients (α_L , α_T).

479 For the purpose of numerical solution, following Fahs et al. [28], the domain was discretized using
 480 structured meshes comprising 7500, 12288 and 76800 triangles for test cases 1 to 3, respectively. For all
 481 the test cases except the third one which utilizes quadratic polynomial for head, the linear polynomial
 482 approximations were applied for both variables. The imposed boundary conditions are depicted in Fig. 6.
 483 All combinations of DG schemes are used for the simulation of Henry problem, however, we observed no
 484 significant difference between the results. Main isochlors (10%, 50% and 90%) as well as the velocity field
 485 for the three test cases are represented on Fig. 7. It can be observed that there is an excellent agreement
 486 between generated DG isochlors and those of semi-analytical solution throughout the total aquifer thickness.
 487 The third case highlights the capacity of the developed DG solution in reproducing a narrow mixing zone
 488 that could be very sensitive to numerical dispersion [28]. A more quantitative comparison is performed
 489 using scalar indicators representing the seawater intrusion metrics. The results are summarized in Table 4.
 490 For test case 1, the difference between the DG and semi-analytical solutions is less than 1.5%. The
 491 highest difference is observed for the width of the mixing zone. The post treatment procedure used for
 492 the evaluation of this zone depends on the computational mesh. For the second and third test cases, the
 493 discrepancy between the solutions is less than 6%, except for the mixing zone and the total flux. The
 494 small discrepancies between the solutions regarding L_s and L_{toe} confirms that DG avoids the problem of
 495 numerical dispersion. In fact, numerical dispersion could overestimate the diffusion processes and leads to
 496 an overestimation of L_{toe} and L_s .

497 4.3. Verification against semi-analytical solution: The problem of natural convection in a porous enclosure

498 An important application of the VDF is in natural convection in porous enclosure. In this case, the
 499 density variation is related to a thermal gradient. This problem can be modeled by a system of equations
 500 equivalent to the solute VDF problems. For thermal problems, the porosity is analogue to the equivalent
 501 specific heat of the porous domain and the molecular diffusion is analogue to the equivalent thermal
 502 diffusivity of the porous domain. In thermal application, the expansion coefficient in (7), should be negative
 503 as the density decreases with the increase of temperature. Thus the developed DG scheme can be applied
 504 to solve thermal density-driven problems. The previous test cases deal with mixed convection as the flow

Table 3. Physical parameters used for the simulations of the three test cases of the Henry problem

Parameter	Value			Unit
	Case 1	Case 2	Case 3	
\mathbf{K}	$0.01 \times \mathbf{I}$	$0.01 \times \mathbf{I}$	$0.01 \times \mathbf{I}$	ms^{-1}
D_m	18.86×10^{-6}	9.43×10^{-8}	9.43×10^{-8}	$m^2 s^{-1}$
α_L	0.0	0.1	0.001	m
α_T	0.0	0.01	0.0001	m
s	0	0	0	m^{-1}
ϕ	0.35	0.35	0.35	–
ρ_0	1000	1000	1000	$kg m^{-3}$
ρ_s	1025	1025	1025	$kg m^{-3}$
Q	6.6×10^{-5}	6.6×10^{-5}	6.6×10^{-5}	ms^{-1}
μ	0.001	0.001	0.001	$kg m^{-1} s^{-1}$
β_0	0.025	0.025	0.025	–

Table 4. Computed seawater intrusion metrics for Henry test cases [28]

Metrics*	Test case 1		Test case 2		Test case 3	
	DG	Semi-analytical	DG	Semi-analytical	DG	Semi-analytical
L_{Toe}	0.624	0.624	1.246	1.256	1.604	1.594
L_s	0.752	0.751	0.393	0.368	0.087	0.088
W_{mz}	0.756	0.757	0.323	0.295	0.088	0.09
Z_1	0.425	0.419	0.51	0.527	0.691	0.684
Q_s	1.066	1.068	1.069	1.061	0.35	0.3

* Adapted from [28]:

L_{toe} is the dimensionless distance to the seaside boundary that seawater intrudes along the aquifer bottom (measured based on 50% isochlor),

L_s is the dimensionless distance between 10 and 90% isochlors along the aquifer bottom,

W_{mz} is the vertically dimensionless average width of the mixing zone,

Z_1 is the dimensionless vertical coordinate of the point at which flow direction at seaside boundary alters adversely,

Q_s is the saltwater inflow flux from seaside boundary divided by freshwater recharge (Q).

505 is either imposed or generated by an imposed pressure gradient. The main goal of this section is to test
506 the new developed scheme in cases involving natural convection, where flow is induced by density gradient.
507 Thus, we consider the well-known benchmark of natural convection in a porous cavity (Fig. 8). The
508 domain of the problem is a unit square filled with homogeneous porous medium. All sides are impervious
509 respective to fluid. Right and left sides of the domain have different temperatures with 1 and 0 dimensionless
510 temperatures, respectively. Other boundary conditions and data are depicted in Fig. 8. The main factor
511 of fluid density changes is the temperature differences due to heating the fluid from the boundaries. The
512 convective flow and heat transfer processes are governed by the dimensionless Rayleigh number ($Ra =$
513 $\mathbf{K}l\beta_0\Delta c/\phi D_m$, where l is the domain length) expressing the ratio of the buoyancy forces to the viscous-
514 diffusion effects.

515 Fahs et al. [29] developed a semi analytical solution for this problem which is used here to verify the
516 proposed DG scheme. We consider cases dealing with low and average Rayleigh numbers ($Ra = 100$ and
517 $Ra = 1000$). The physical parameters used in the simulations are given in Table 5.

518 In the previous test for Henry problem, DG was evaluated for linear approximation. Here, higher order

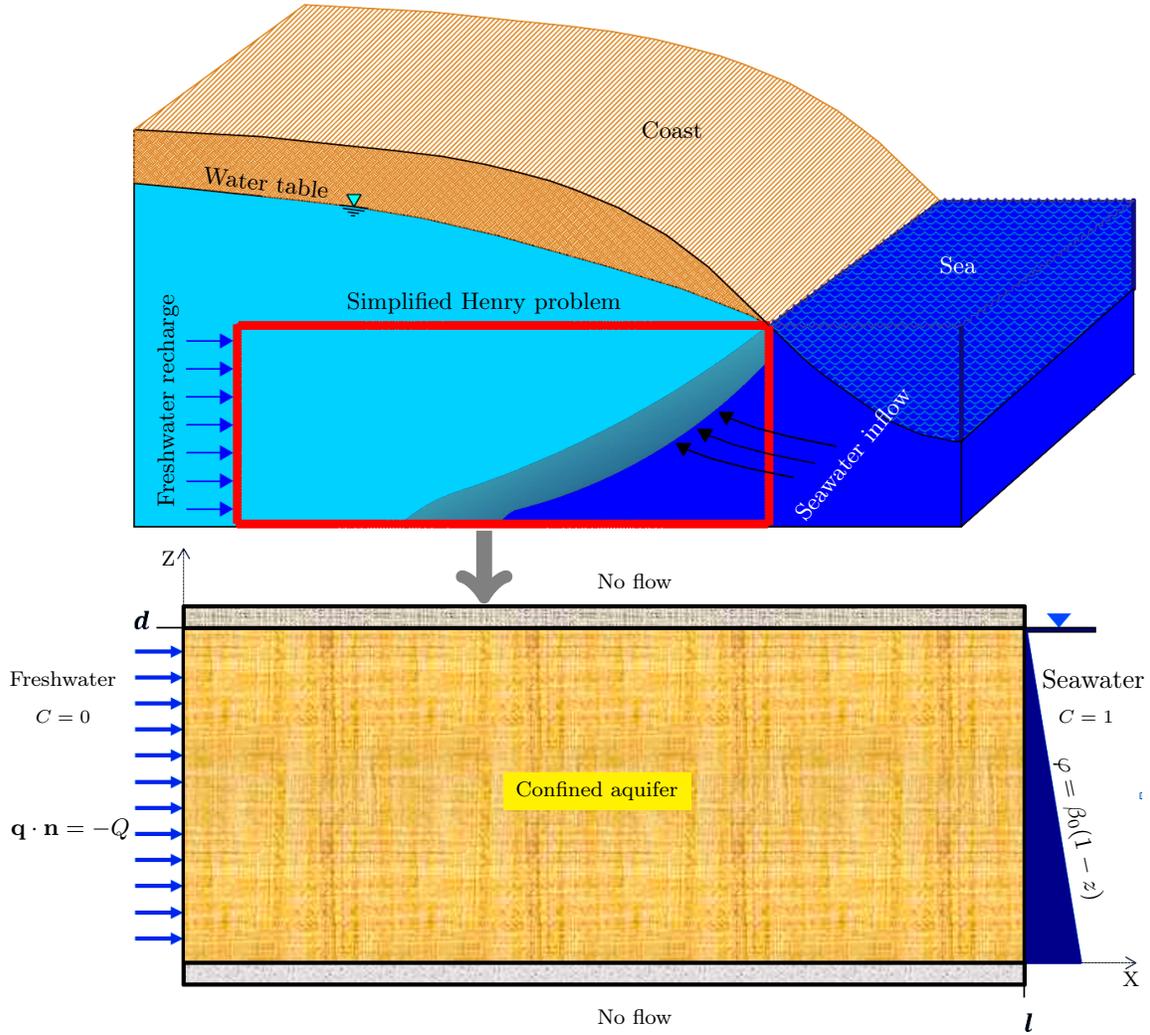


Fig. 6. Simplification of seawater intrusion by Henry [39] and the implemented boundary conditions

519 approximations of DG are examined. Accordingly, the domain is discretized by 2500 and 6400 uniform
 520 triangular elements for $Ra = 100$ and $Ra = 1000$, respectively, and the developed DG code is used for
 521 a wide range of polynomial degrees (from 1 to 4). The isotherms 0.2, 0.4, 0.6, 0.8 and the velocity field
 522 are depicted in Fig. 9 in comparison with those of semi-analytical solution of Fahs et al. [29]. This figure
 523 shows the occurrence of convective cells. The temperature gradient generates a clockwise rotating flow.
 524 The increase of the Rayleigh number accelerates the rotating flow. Convection dominates the heat transfer
 525 processes and the isotherms become more dependent on the flow structure. As can be seen, DG solution
 526 perfectly match the semi-analytical solutions.

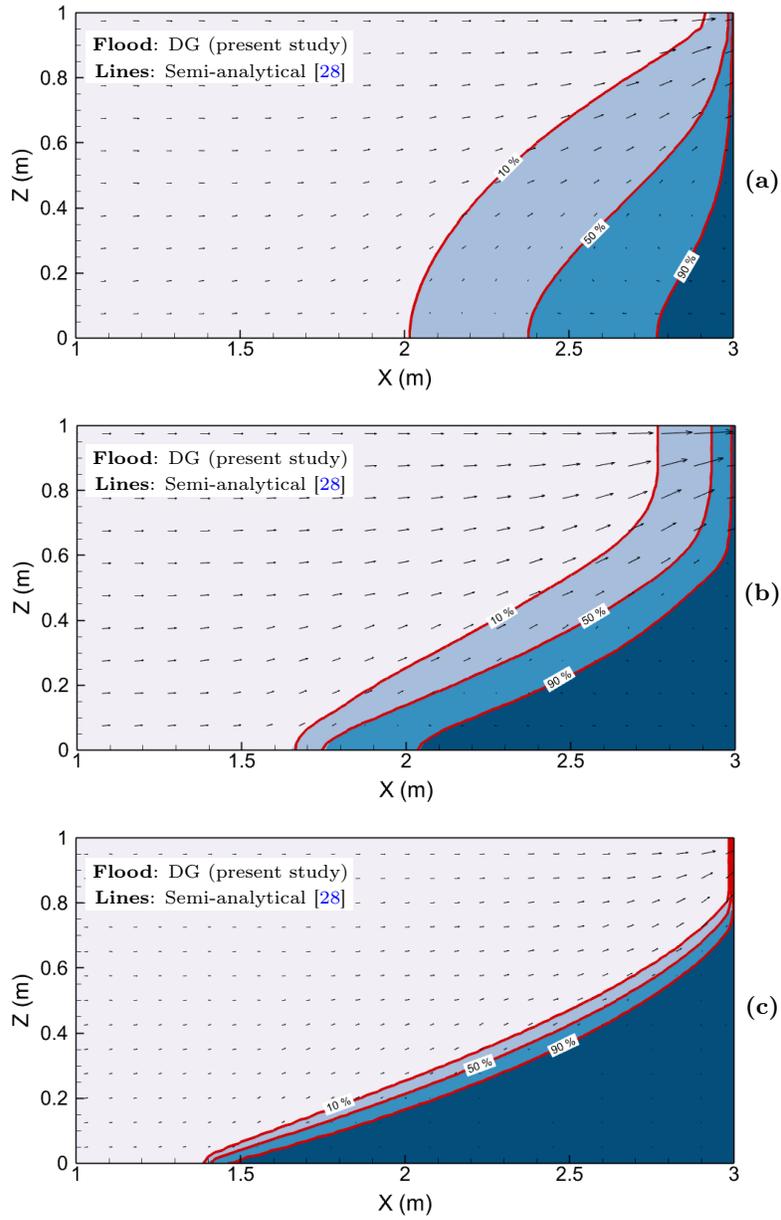


Fig. 7. Main isochlors and velocity field for the test case 1 (a), test case 2 (b), and test case 3 (c) of the Henry problem: comparison between the DG and semi-analytical solutions

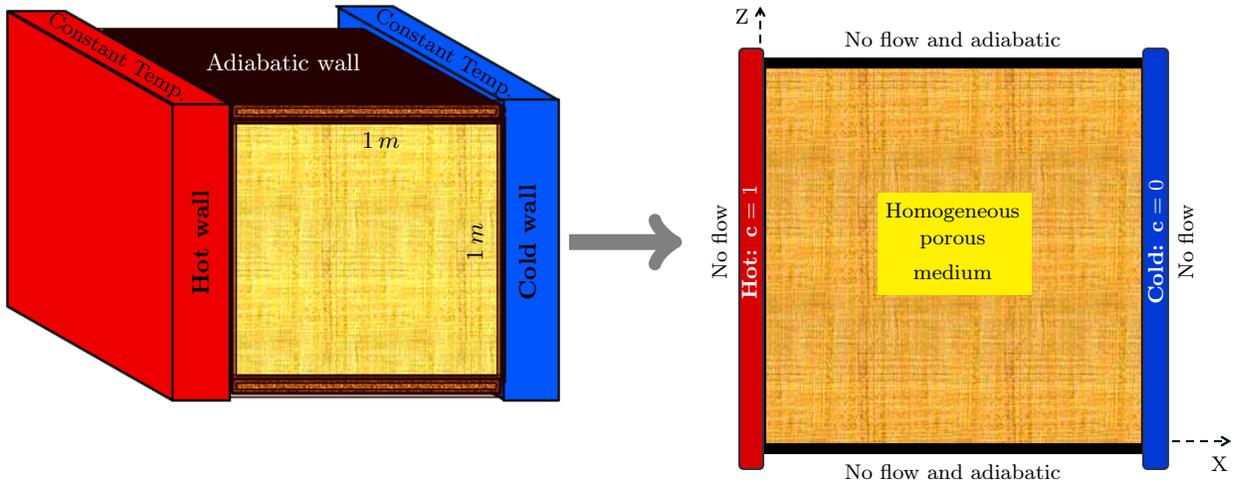


Fig. 8. Geometry and boundary conditions of the problem of natural convection in porous cavity

Table 5. Physical parameters for simulation of the problem of natural convection in porous cavity

Parameter	Value	Unit
\mathbf{K}	$0.01 \times \mathbf{I}$	$m s^{-1}$
D_m	1×10^{-6} ($Ra = 100$), 1×10^{-7} ($Ra = 1000$), 1×10^{-8} ($Ra = 10000$)	$m^2 s^{-1}$
α_L	0	m
α_T	0	m
s	0	m^{-1}
ρ_0	1000	$kg m^{-3}$
μ	0.001	$kg m^{-1} s^{-1}$
β_0	-0.01	-

527 *4.4. Performance and accuracy of the developed DG solution: Natural convection with a high Rayleigh*
528 *number*

529 This section aims at examining the performance of the new developed DG scheme against conventional
530 methods. Thus, we consider a computationally challenging case and we simulate this case with the DG
531 scheme and with a standard finite element solution obtained using COMSOL. We simulate the case on
532 natural convection in porous enclosure under high Rayleigh regime ($Ra = 10000$). Fahs et al. [29] showed
533 that in this case, conventional numerical methods suffer from numerical dispersion and/or nonphysical
534 oscillations. They showed that accurate simulation of this test case is beyond the capacity of conventional
535 models. In their work, the author proposed a reference solution based on the Fourier series method. We
536 simulate this case using the DG scheme and COMSOL. For the DG scheme we use a computational mesh
537 of 10K elements and we test different polynomial orders from 1 to 4. In COMOS, we use two levels of
538 mesh refinement consisting of about 100K and 600K elements. COMSOL simulations are performed with
539 first polynomial order. We use the average Nusselt number to evaluate the performance of both models.
540 The average Nusselt number represents the dimensionless heat flux to the domain. It is calculated by:

541
$$\overline{Nu} = \int_{\partial\Omega} \overline{Nu}_{|x=0} = \int_{\partial\Omega} \nabla c \cdot \mathbf{n} \quad [29].$$

542 Table 6 summarizes the Nusselt number for the DG scheme in comparison with those of semi-analytical

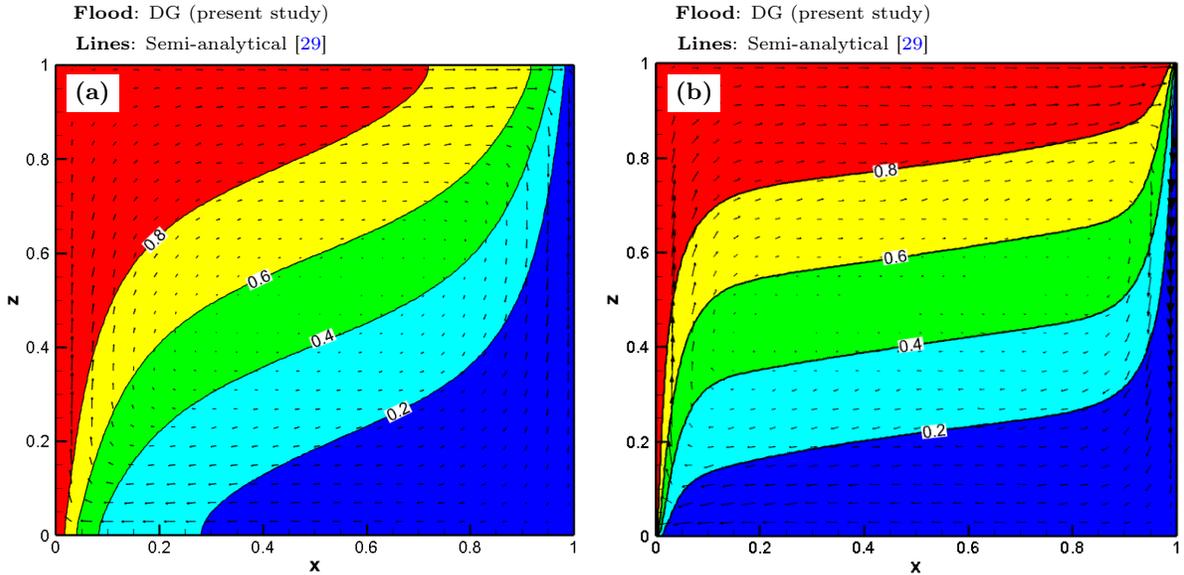


Fig. 9. Comparison of DG solution with that of semi-analytical for (a) $Ra = 100$ and $Ra = 1000$

Table 6. Nusselt number achieved for different number of DOFs per each variable

	DG				COMSOL-Multiphysics		Semi-analytical
	Order 1	Order 2	Order 3	Order 4	Order 1	Order 1	
Number of elements	10,000	10,000	10,000	10,000	100,110	655,752	—
Number of DOFs	60,000	120,000	200,000	300,000	201,022	1,313,506	—
\overline{Nu}	33.14	50.45	45.24	46.15	38.07	44.9	46.14

543 solution and COMSOL-Multiphysics. We should mention that, by default in COMSOL, second polynomial
544 order is used for flow and first order is used for transport. As shown, the \overline{Nu} achieved for DG approaches
545 to that of analytical as the order of polynomial approximation (the number of DOFs) is increased until at
546 order 4 including totally 300,000 DOFs, \overline{Nu} is extremely close to analytical value. Fig. 10 pinpoints how
547 the relative error on Nusselt number decreases as the number of DOFs is increased. COMSOL-Multiphysics
548 is a standard finite element software and its results were also included to demonstrate how DG is superior
549 to standard finite element method. We observe for high order DG solution, \overline{Nu} is more close to the
550 analytical value, though, less than a quarter of the number of COMSOL-Multiphysics' DOFs was used.
551 The DG scheme intrinsically has less numerical dispersion and this is why a more accurate solution is
552 achieved for, even with a much less number of DOFs. Fig. 11 depicts the isotherms for both models against
553 the semi-analytical solution. As illustrated, DG isotherms (for order 4) have closer agreement with the
554 semi-analytical solution than COMSOL.

555 The results of this test case show clearly a significant improvement in the accuracy of the solution due
556 to the DG method. This is in agreement with several previous studies on flow and transport in porous
557 media, confirming the high accuracy of the DG methods. However, in general the DG method is seen to be

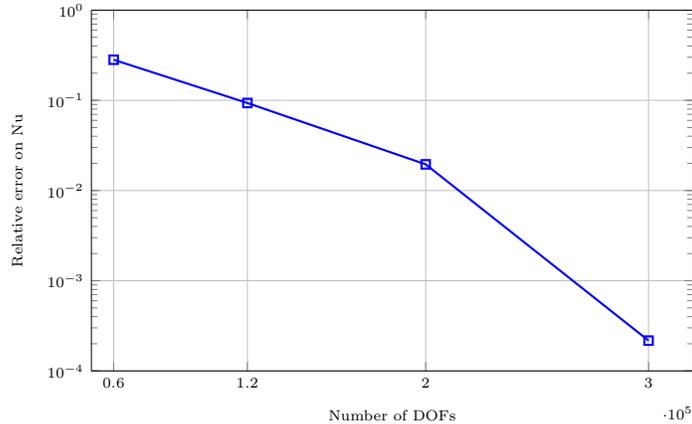


Fig. 10. Relative error on \overline{Nu} versus number of DOFs

558 more consuming in CPU time and memory than standard methods, due to the high number of DOFs per
 559 element of the computational mesh. The results here show that for VDF problems, this is not totally true.
 560 In fact, a reliable comparison should respect the balance between computational efficiency and solutions
 561 accuracy. In this logic, Table 6 confirms the superiority of the DG methods for the simulation of VDF
 562 problems.

563 5. Conclusion

564 Several recent studies have highlighted the advantages of the DG methods in solving partial differential
 565 equations governing flow or transport processes in porous media. This method has been never used to solve
 566 the full system of VDF equations. Yet, simulations of VDF requires high accurate numerical methods as
 567 the accuracy of the numerical solutions is highly sensitive to the numerical scheme. The first objective of
 568 this work is to show how the equations of VDF can be solved with the DG method. This requires extension
 569 of the DG method to solve nonlinear equations coupling flow and convective/dispersive transport equations
 570 under variable density. We develop, in a unified format, the general class of Interior Penalty DG (IPDG)
 571 methods to solve VDF equations. We test symmetric, non-symmetric and incomplete IPDG methods to
 572 discretize both head and concentration variables. Numerical experiments are performed to validate the
 573 developed DG scheme and to examine its performance in solving VDF problems.

574 The developed numerical scheme is implemented in a numerical code which is used to simulate common
 575 benchmarks dealing with VDF. The simulations are performed to validate and verify the developed DG
 576 scheme. The benchmarks are selected to cover different types of boundary conditions and convective flow
 577 processes (either, mixed, natural, solute or thermal). Validation is performed by comparing the results of
 578 the developed DG scheme with experimental data, based on the Goswami-Clement experimental problem.
 579 Good agreement has been found. The new developed DG scheme reproduces the experimental data better
 580 than the finite element SEAWAT code. Verifications are performed by comparing the code against the semi-

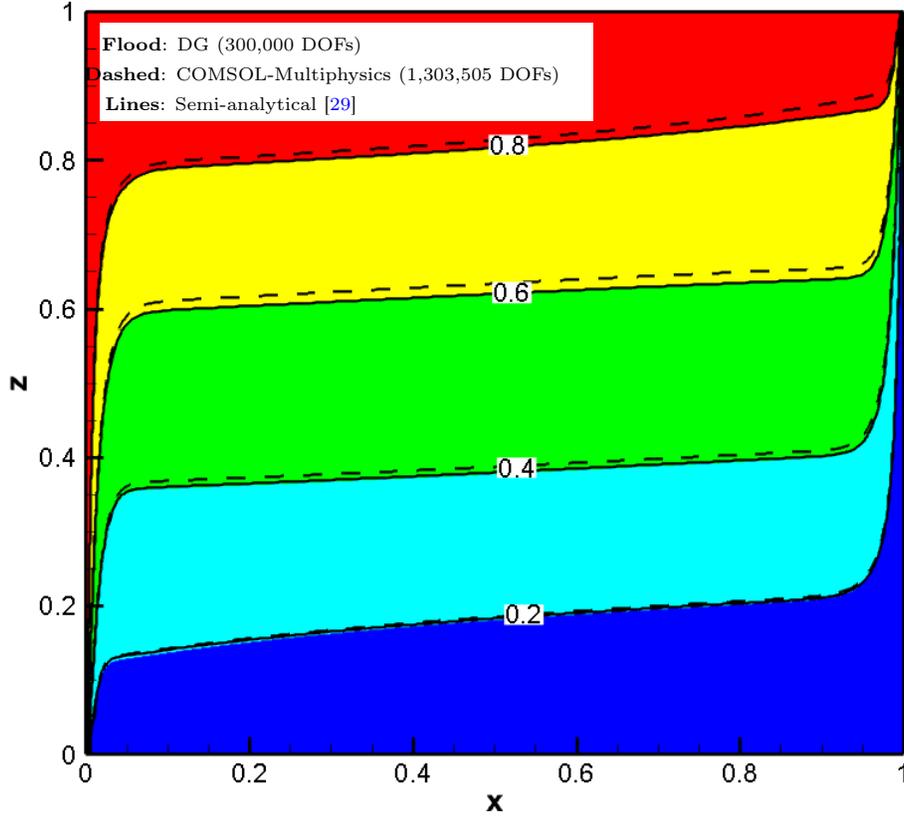


Fig. 11. Isotherms concluded from DG compared to that of analytical and COMSOL-Multiphysics

581 analytical solutions of the dispersive Henry problem dealing with seawater intrusion in coastal aquifers and
 582 the problem of thermal natural convection in a porous enclosure. Excellent agreement has been obtained
 583 with semi-analytical solutions for cases involving wide mixing zone or small Rayleigh numbers. This
 584 confirms the correctness of the developed code and DG scheme. Furthermore, close agreement has been
 585 obtained for Henry problem in the case of narrow mixing, which illustrates the promising results of the
 586 DG method in solving VDF with sharp fronts. These numerical experiments show that, whole algorithm
 587 combinations, i.e. IIP-IIP, IIP-SIP, and IIP-NIP have no significant differences in the solutions.

588 To highlight the performance of the DG method in solving the equations of VDF, we simulate the
 589 problem of natural convection at a high Rayleigh number (10,000). Accurate solution of this problem is
 590 out of the capacity of current models based on conventional methods. We compared the DG results to
 591 a semi-analytical solution and to a finite element solution obtained using COMOSL multi-physics. The
 592 results prove the promising performance of the DG method at high polynomial order as it provides higher
 593 accuracy than standard finite element method with reduced number of degree of freedom. The DG method
 594 outperforms the conventional method that we tested.

595 This study is the first step towards application of DG methods in the area of VDFs. Future work should
 596 target applying other nice properties of DG such as adaptivity in mesh and polynomial approximation

597 (hp-version) to even more reduce the computational cost. The proposed method is generic and can be
598 extended to 3D, which is an ongoing research project of this work.

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602 available on the GitHub repository: <https://github.com/fahs-LHYGES>

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