Supplementary material S2

Authors: Jiří Landa, Milan Hokr
Paper title: Contaminant transport from the deep geological repository: lumped parameters derived from 3D hydrogeological model
Journal: Energies (ISSN 1996-1073)
September 2022

Algorithmic notation for the Integral method – lumped parameter evaluation procedure

This document is intended for detailed technical description for the procedure explained by conceptual ideas and word formulation in the paper. It is based on the data of a generic numerical method for a 3D hydrogeological model (groundwater flow and tracer transport problems), i.e. parameters and results assigned to the discretisation mesh of the model domain. We introduce a mathematical notation for these data. The processing method is composed of elementary algebraic operations or subset constructions, expressed in mathematical form, and of mesh search iterative algorithms expressed by pseudocode, with eventual double notation (mathematical and programmer). Besides the titles, the bold face text is used to remind the terms for quantities mentioned as results in Section 3.2. of the paper.

For the algorithm, it is convenient to consider a graph theory notation for the discretisation mesh, so that some features can be seen as analogues or modifications of well-known generic algorithms and easier to understand.

Quantities and data notation

Problem geometry

Ω model domain

Ω_S source subdomain (the repository)

Γ model boundary $\Gamma = \partial\Omega$

Γ_S source boundary $\Gamma_\mathrm{S} = \partial\Omega_\mathrm{S}$

Mesh objects

e_i elements

f_k sides (global index list)

f_{ij} a side common to the elements e_i and e_j (graph incidence notation)

$\Omega_e = \{e_i, \dots\}$ set of all mesh elements $\bigcup_{\Omega_e} e_i = \Omega$

$\Omega_e^S = \{e_i, \dots\} \subset \Omega_e$ set of source subdomain elements $\bigcup_{\Omega_e^S} e_i = \Omega_\mathrm{S}$

$\Phi_f = \{f_k, \dots\}$ set of all mesh element sides (faces)

$\Gamma_f = \{f_k, \dots\} \subset \Phi_f$	set of model boundary element sides $\bigcup_{\Gamma_f} f_k = \Gamma$
$\Gamma_f^S = \{f_k, \dots\} \subset \Phi_f$	set of source boundary element sides $\bigcup_{\Gamma_f^S} f_k = \Gamma_S$
$\Omega_e^B = \{e_i, \dots\} \subset \Omega_e$	set of "boundary elements" (at least one side of e_i is a part of the boundary Γ)
$\Omega_e^{Bcf} \subset \Omega_e^B$	"contaminated outflow boundary elements" (construction procedure below)
$F(e_i) \subset \Phi_f$	set of sides of a particular element
$N(e_i) \subset \Omega_e$	set of neighbours of a particular element

Data values

V_i	volume of element e_i
η_i	porosity of element e_i
$\vec{x}_i$	centre coordinates of element e_i, $\vec{x}_i = (x_i, y_i, z_i)$
c_i	tracer concentration in element e_i (asymptotic time – see details below)
S_k	area of side f_k (global index list)
S_{ij}	area of "internal" side f_{ij} (indexing through elements)
S_i^B	area of boundary side of element e_i
q_{ij}	water flux across side f_{ij} (positive from e_i to e_j)
q_i^{out}	total outflow from element $q_i^{out} = \sum_{\substack{e_j \in N(e_i) \\ q_{ij} > 0}} q_{ij}$ (note: equals to the total inflow into the element up to the sign)
q_i^B	outflow from element e_i to boundary (positive out from the domain)
m_{ij}	mass flux across side f_{ij} (positive from e_i to e_j)
m_i^B	mass flux from element e_i to boundary (positive out from the domain)

(note the specific notation of quantities related to boundary sides, which are not in the incidence relation to two elements but only to one)

Global parameters

δ_q	relative flux threshold (minimum share of a single side flux on the total element outflow)
δ_m	relative mass flux threshold (maximum deviation of the incomplete sum of fluxes)

Graph theory analogue

Graph vertices	Mesh elements
Graph edges	Mesh sides
Edge direction	Flux direction (sign)
Edge weights	Fluxes

3D model features

As described in the text, the 3D hydrogeological and tracer transport model is set by standard configuration of boundary condition. The flow model is steady-state with recharge, discharge, and no-flow conditions. The transport model has a constant-concentration condition in the source subdomain, and therefore the transient model asymptotically approaches to the steady state. With the used notation, the flow model discrete quantities are numbers (steady-state). The concentrations and mass fluxes would be functions of time, but the data from the final time of model run, corresponding to an approximation of the asymptotic steady state, are used under the introduced notation and within the algorithms below.

Conditional sum operations

The quantities below are obtained by cumulative operations of quantities over subsets defined by some conditions. The particular algorithmic procedure is analogue in all cases, i.e. a trivial cycle over the specified mesh objects listed above and application of the given condition.

Source areas:

S_S total source area $S_S = \sum_{f_k \in \Gamma_f^S} S_k$

S_S^{in} source inflow area $S_S^{in} = \sum_{f_{ij}} S_{ij}$ for $f_{ij} \in \Gamma_f^S$ such that $q_{ij} < 0$ for $e_i \in \Omega_e^S$ and $e_j \notin \Omega_e^S$

S_S^{out} source outflow area $S_S^{out} = \sum_{f_{ij}} S_{ij}$ for $f_{ij} \in \Gamma_f^S$ such that $q_{ij} > 0$ for $e_i \in \Omega_e^S$ and $e_j \notin \Omega_e^S$

Source water fluxes:

Q_S^{in} source water inflow rate $Q_S^{in} = \sum_{f_{ij}} q_{ij}$ for $f_{ij} \in \Gamma_f^S$ such that $q_{ij} < 0$ for $e_i \in \Omega_e^S$ and $e_j \notin \Omega_e^S$

Q_S^{out} source water outflow rate $Q_S^{out} = \sum_{f_{ij}} q_{ij}$ for $f_{ij} \in \Gamma_f^S$ such that $q_{ij} > 0$ for $e_i \in \Omega_e^S$ and $e_j \notin \Omega_e^S$

i.e. water inflow into the "geosphere" $Q_G^{in} = Q_S^{out}$

Source mass fluxes:

M_S^{in} source mass (tracer) inflow rate $M_S^{in} = \sum_{f_{ij}} q_{ij}\, c_j$ for $f_{ij} \in \Gamma_f^S$ such that $q_{ij} < 0$ for $e_i \in \Omega_e^S$ and $e_j \notin \Omega_e^S$

M_S^{out} source mass (tracer) outflow rate $M_S^{out} = c_S Q_S^{out}$ considering $c_i = c_S = const$ for all $e_i \in \Omega_e^S$

Backflow compensation

Considering mass balance in the asymptotic stead state, the mass outflow from the model must be equal to the mass outflow from the source reduced by the backflow (a part of the mass which actually sinks in the source subdomain, see the paper text). This is used for the compensation factor to evaluate the realistic **Geosphere inflow area** S_G^{in} (see the boundary flux M_B^{out} below):

$$S_G^{in} = S_S^{corr} = \frac{S_S^{out} \cdot M_B^{out}}{M_S^{out}}$$

Boundary areas

To define the outflow side of the constructed lumped parameter model, it is needed to determine a part of the boundary which is reached by the tracer (contaminant) and potentially in a contact with the biosphere, i.e. the set of "contaminated boundary outflow elements", $\Omega_e^{Bcf} \subset \Omega_e^B$. This would be theoretically based on conditions $q_i^B > 0$ and $c_i > 0\ \forall e_i \in \Omega_e^{Bcf}$, but a "numerical noise" of very small positive and negative numbers resulting typically from iterative algebraic solvers must be filtered out. A threshold condition applied directly on concentration would be a unit-dependent value. More practically, it can be done with a dimensionless value expressing a deviation from the total mass flux (M_B^{out}, see below), if an incomplete sum M_B^{lim} is considered, without the neglected "noise" fluxes. It was used in the paper example calculation with $1 - \delta_m = 0.999999$.

Sort $e_i \in \Omega_e^B$ by m_i^B descending

$\Omega_e^{Bcf} \coloneqq \{\}$ *//initialization*

For i such that $e_i \in \Omega_e^B$

$M_B^{lim} \coloneqq M_B^{lim} + m_i^B$

$\Omega_e^{Bcf} \coloneqq \Omega_e^{Bcf} \cup \{e_i\}$

If $M_B^{lim} > M_B^{out}(1 - \delta_m)$ break

S_B^{out} **contaminated** (boundary) **outflow area** $S_B^{out} = \sum_{e_i \in \Omega_e^{Bcf}} S_i^B$

Boundary fluxes

Q_B^{out} boundary **outflow rate of contaminated water** $Q_B^{out} = \sum_{e_i \in \Omega_e^{Bcf}} q_i^B$

M_B^{out} boundary mass flux $M_B^{out} = \sum_{\substack{e_i \in \Omega_e^B \\ m_i^B > 0}} m_i^B$

Transport path search algorithm

This algorithm is analogue of graph traversal in the graph theory. The form here corresponds to the "depth-first search" (easier to express in a recursive form), besides the second choice of the "breadth-first search". The algorithm is formulated for a generic graph (not necessary a tree, no edge weights, no directions). Applying the additional conditions based on the model physics (groundwater flow results), we actually construct and search a directed tree sub-graph representing the flux path from the (undirected) graph expression of the whole discretisation mesh at the same time.

As the results, **volume and porosity of the path** are calculated, V and η respectively, and the minimum and maximum elemental porosities found, i.e. η_{min}, η_{max}.

Define procedure Path_search (element e_i)

Mark element as visited, $P \coloneqq P \cup \{e_i\}$

$V \coloneqq V + V_i$, $V^p \coloneqq V^p + V_i \eta_i$

If $\eta_i > \eta_{max}$ then $\eta_{max} \coloneqq \eta_i$

If $\eta_i < \eta_{min}$ then $\eta_{min} \coloneqq \eta_i$

For all (neighbour e_j) of element // ($e_j \in N(e_i)$)

If ($q_{ij} > q_i^{out} \cdot \delta_q$) and ($e_j \notin \Omega_e^B$) and $e_j \notin P$
// positive flux higher then threshold, not reaching the boundary, and not visited

Path_search (neighbour) *// recursive call of the same procedure*

$P \coloneqq \{\}$ Path element set initialization (mark all elements as unvisited)

$V \coloneqq 0$ Total volume initialization

$\eta_{min} \coloneqq 0, \eta_{max} \coloneqq 1$ Min/max search initialization

For all element in Ω_e^S *//starting in source subdomain*

Path_search (element)

$\eta = \frac{V^p}{V}$ // porosity

Output $P, V, \eta, \eta_{min}, \eta_{max}$

Length of the transport path

This algorithm is similar concept to a standard particle tracking in the reverse direction (from the boundary to the source). All relevant "particle paths" are aggregated by averaging with e.g. boundary mass fluxes m_i^B used as weights.

For all elements e_i in Ω_e^{Bcf}

$L_i(e_i) \coloneqq 0$

$e_j := e_i$ *// initial path element for given boundary element*

While $e_j \not\subset \Omega_S$ *// until the path reaches the source domain*

Find e_k maximizing m_{kj} on $N(e_j)$
// highest mass flux from k (next upstream) to j (current)

$L_i := L_i + |\vec{x}_k - \vec{x}_j|$

$e_j := e_k$ *// take this element for the next step*

L = (weighted) average of $L_i(e_i)$ over $e_i \in \Omega_e^B$