The Darcy-Weisbach Jacobian and Avoiding Zero Flow Failures in the Global Gradient Algorithm for the Water Network Equations

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ABSTRACT

This paper considers two issues related to iteratively solving the non-linear equations governing the flows and heads in a water distribution system network. The first concerns the use of the correct Jacobian for the Global Gradient Algorithm (GGA) when the Darcy-Weisbach head loss model is used. The second relates to dealing with zero flows in the iterative solution process. A regularization procedure for the GGA with the Hazen–Williams model is demonstrated on an example network which has zero flows but for which the (full) Jacobian is invertible.

INTRODUCTION

This paper[1] considers two aspects associated with solving the pipe network equations for a water distribution system. The first aspect relates to the way in which the variation of the Darcy-Weisbach (DW) friction factor with discharge is fully accounted for when the Jacobian matrix is computed in the Newton iteration. Using the correct DW Jacobian gives the iteration process the quadratic convergence which normally comes with Newton's method, unlike the implementation in EPANET (Rossman 2000).

The second issue relates to pipes that have zero flows. In the computation using the Global Gradient Algorithm (GGA) a key matrix becomes singular if any of the flows are zero when the Hazen–Williams (HW) head loss model is used. That prevents any further computation. In this paper a regularization of the GGA that allows for zero flows is discussed and demonstrated. Results from a case study network to demonstrate the effectiveness of the regularization are presented. By comparison, it will become evident that zero flows do not cause a failure when the DW head loss model is used.

THE PIPE HEAD LOSS EQUATIONS

Consider a water distribution network of n_p pipes, n_j junctions or nodes ($n_p < n_j$) and n_f fixed–head nodes. Suppose Q_j is the unknown flow for the pipe, p_j which has area of cross section A_j, length L_j, diameter D_j, and resistance factor r_j. All the pipes in the system are assumed to have the same head loss exponent, n, which is either $n = 1.852$ for the HW head loss model, or $n = 2$ for DW head loss model. Let H_i denote the unknown head at the i-th node, v_i.

We define the following quantities. Let $\boldsymbol{q} = (Q_1, Q_2, \ldots, Q_{n_p})^T$ denote the vector of unknown flows, $\boldsymbol{h} = (H_1, H_2, \ldots, H_{n_j})^T$ denote the vector of unknown heads,

[1] Some of the content of this paper draws on material published in Simpson & Elhay (2011) and Elhay & Simpson (2011).

$\boldsymbol{r} = (r_1, r_2, \ldots, r_{n_p})^T$ denote the vector of resistance factors for the pipes and $\boldsymbol{d} = (d_1, d_2, \ldots, d_{n_j})^T$ denote the vector of nodal demands.

Hazen-Williams head loss equation. The relation between the heads at two ends, node i and node k, of a pipe p_j and the flow in the pipe is defined by $H_i - H_k = r_j Q_j |Q_j|^{n-1}$where $n = 1.852$ and for SI units $r_j = 10.670 L_j/(C_j^{1.852} D_j^{4.871})$, and where C_j is the HW coefficient for pipe p_j. We define a diagonal matrix, $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{q}, \boldsymbol{r}) \in \mathbb{R}^{n_p \times n_p}$, for the *Hazen-Williams* formulation, by

$$[\boldsymbol{G}]_{jj} = r_j |Q_j|^{n-1},\ j = 1, 2, \ldots, n_p. \tag{1}$$

Darcy-Weisbach head loss equation. The DW head loss equation for pipe p_j is $h_{f_j} = f_j L_j V_j |V_j|/(2gD_j)$ where f_j is the DW friction factor, V_j denotes the average fluid velocity and g is the gravitational constant. Let ν denote the kinematic viscosity of water and let the Reynolds number be defined by $\mathcal{R} = |V|D/\nu$. The resistance factors for pipe p_j may be defined by

$$r_j = \begin{cases} \dfrac{128\nu}{\pi g} \dfrac{L_j}{D_j^4}, & \text{for laminar flow,} \\ \dfrac{8}{\pi^2 g} \dfrac{L_j f_j}{D_j^5}, & \text{for turbulent flow} \end{cases}. \tag{2}$$

The relation between the heads at two ends of a pipe and the flow is defined by

$$H_i - H_k = \begin{cases} r_j Q_j, & \text{for laminar flow,} \\ r_j Q_j |Q_j|^{n-1}, & \text{for turbulent flow} \end{cases} \tag{3}$$

where $n = 2$.

For turbulent flow the DW friction factor, f_j, for pipe p_j may be modeled by the Swamee & Jain (1976) approximation

$$f_j = \frac{0.25}{\left[\log_{10}\left(\epsilon_j/3.7D_j + 5.74/\mathcal{R}_j^{0.9}\right)\right]^2}, \tag{4}$$

where ϵ_j is the roughness height. Note that $\mathcal{R}$, the Reynolds number can also be written as

$$\mathcal{R} = 4|Q|/(\pi \nu D). \tag{5}$$

Importantly, we note here from (5) and (4) that r_j in (2) depends, for turbulent flow, on the discharge Q_j. We define a diagonal matrix, $\boldsymbol{G} = \boldsymbol{G}(\boldsymbol{q}, \boldsymbol{r}) \in \mathbb{R}^{n_p \times n_p}$, for the *Darcy-Weisbach* formulation, by

$$[\boldsymbol{G}]_{jj} = \begin{cases} r_j, & \text{for laminar flow} \\ r_j |Q_j|^{n-1}, & \text{for turbulent flow} \end{cases}, j = 1, 2, \ldots, n_p, \tag{6}$$

THE GLOBAL GRADIENT ALGORITHM RELATIONS

Todini & Pilati (1988) proposed a smart algorithm, now referred to as the GGA, to solve the pipe network equations that resulted in a particularly fast algorithm. We now briefly rederive the GGA equations.

We define $\boldsymbol{O}$ as an n_j square, zero matrix, $\boldsymbol{o}$ as an $n_p \times n_j$ zero matrix, and $\boldsymbol{I}_k$ as a k–square identity matrix. Define also (i) $\boldsymbol{F}$ a diagonal $n_p \times n_p$ matrix in which each diagonal element is the derivative with respect to Q of the corresponding element of $\boldsymbol{G}$, (ii) the full column–rank, unknown–head node–arc incidence matrix $\boldsymbol{A}_1$ of dimension $n_p \times n_j$, and (iii) the fixed–head, node–arc incidence matrix, $\boldsymbol{A}_2$, of dimension $n_p \times n_f$. Let $\boldsymbol{u}$ denote the vector of dimension n_f of fixed-head elevations left-multiplied by the matrix $\boldsymbol{A}_2$. The matrices $\boldsymbol{A}_1$ and $\boldsymbol{A}_2$ are sparse and have non-zero entries ± 1.

The steady state flows and heads in the system are the solutions of the energy and continuity equations:

$$\boldsymbol{f}(\boldsymbol{q},\boldsymbol{h}) = \begin{pmatrix} \boldsymbol{G}(\boldsymbol{q}) & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} - \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{d} \end{pmatrix} = \boldsymbol{o}. \tag{7}$$

The block equations are

$$\boldsymbol{G}(\boldsymbol{q})\boldsymbol{q} - \boldsymbol{A}_1\boldsymbol{h} - \boldsymbol{u} = \boldsymbol{o}, \tag{8}$$

$$-\boldsymbol{A}_1^T\boldsymbol{q} - \boldsymbol{d} = \boldsymbol{o}. \tag{9}$$

Denote by $\boldsymbol{J}$ the Jacobian of $\boldsymbol{f}(\boldsymbol{q},\boldsymbol{h})$

$$\boldsymbol{J}(\boldsymbol{q},\boldsymbol{h}) = \begin{pmatrix} \boldsymbol{F}(\boldsymbol{q}) & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix}. \tag{10}$$

The Newton iteration for (7) proceeds by taking given starting values $\boldsymbol{q}^{(0)}$, $\boldsymbol{h}^{(0)}$ and repeatedly computing, for $m = 0, 1, 2, \ldots$, the iterates $\boldsymbol{q}^{(m+1)}$ and $\boldsymbol{h}^{(m+1)}$ from

$$\begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m+1)} - \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m+1)} - \boldsymbol{h}^{(m)} \end{pmatrix} = -\left(\begin{pmatrix} \boldsymbol{G} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m)} \end{pmatrix} - \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{d} \end{pmatrix} \right) \tag{11}$$

until, if the iteration converges, the difference between successive iterates is sufficiently small. We can rewrite (11) as

$$\begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m+1)} \\ \boldsymbol{h}^{(m+1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F} - \boldsymbol{G} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{d} \end{pmatrix}. \tag{12}$$

The block equations of (12) are

$$\boldsymbol{F}\boldsymbol{q}^{(m+1)} - \boldsymbol{A}_1\boldsymbol{h}^{(m+1)} = (\boldsymbol{F} - \boldsymbol{G})\boldsymbol{q}^{(m)} + \boldsymbol{u}, \tag{13}$$

$$-\boldsymbol{A}_1^T\boldsymbol{q}^{(m+1)} = \boldsymbol{d}. \tag{14}$$

Multiplying (13) on the left by $-\boldsymbol{A}_1\boldsymbol{F}^{-1}$ and rearranging gives

$$\boldsymbol{A}_1^T\boldsymbol{F}^{-1}\boldsymbol{A}_1\boldsymbol{h}^{(m+1)} = -\boldsymbol{A}_1\boldsymbol{F}^{-1}\left((\boldsymbol{F} - \boldsymbol{G})\boldsymbol{q}^{(m)} + \boldsymbol{u}\right) + \boldsymbol{A}_1^T\boldsymbol{q}^{(m+1)}.$$

Replacing the last term on the right–hand–side by $-\boldsymbol{d}$ using (14) gives

$$\boldsymbol{V}\boldsymbol{h}^{(m+1)} = -\boldsymbol{A}_1\boldsymbol{F}^{-1}\left((\boldsymbol{F} - \boldsymbol{G})\boldsymbol{q}^{(m)} + \boldsymbol{u}\right) - \boldsymbol{d} \tag{15}$$

if we denote $\boldsymbol{V} = \boldsymbol{A}_1^T\boldsymbol{F}^{-1}\boldsymbol{A}_1$. Once $\boldsymbol{h}^{(m+1)}$ is determined, the next flow iterate $\boldsymbol{q}^{(m+1)}$ can be found from (13) as

$$\boldsymbol{q}^{(m+1)} = \boldsymbol{q}^{(m)} + \boldsymbol{F}^{-1}\left(\boldsymbol{A}_1\boldsymbol{h}^{(m+1)} - \boldsymbol{G}\boldsymbol{q}^{(m)} + \boldsymbol{u}\right). \tag{16}$$

THE DARCY-WEISBACH JACOBIAN

In the original paper Todini and Pilati considered only the HW head loss model. EPANET (Rossman 2000) uses the HW Jacobian ($\boldsymbol{F} = n\boldsymbol{G}$) when the DW head loss model is used. The GGA nevertheless converges to the correct solution, albeit with linear rather than the usual quadratic convergence, because using this Jacobian is equivalent to replacing the Newton method by an approximation called the Chord Method (see Simpson & Elhay (2011) for details).

In the HW case the Jacobian matrix of (10) has diagonal elements in the (1,1) block which are the derivatives of terms of the form $r_j Q_j |Q_j|$ in which the resistance factors r_j are independent of flow. As a result the matrix $\boldsymbol{F}$ in (10) has the simple form $\boldsymbol{F} = n\boldsymbol{G}$. However, recall that when the DW head loss model is used, the resistance factors r_j of (2) depend on the flow. This dependency leads to a more complicated form of the matrix $\boldsymbol{F}$ which we now develop.

The formulae in (2) and (3) show two flow types: laminar and turbulent. A third type of flow, which we shall refer to as transitional, is usually considered necessary to allow a smooth passage from laminar to turbulent flow in computer codes. The resulting three ranges of Reynolds numbers we consider are shown in the first column of Table 1. For these three ranges of $\mathcal{R}$ we have the following formulae for friction factors, resistance factors and terms on the diagonal of the matrix $\boldsymbol{G}$:

Case 1: Laminar flow $\mathcal{R} \leq 2000$ For this range of $\mathcal{R}$ the Hagen-Poiseuille formula is applicable and so the term on the diagonal of the matrix $\boldsymbol{G}$ in (6) is just $[\boldsymbol{G}]_{jj} = r_j$. Importantly, this term does not depend on the pipe flow.

Case 2: Transitional flow $2000 < \mathcal{R} < 4000$ We use Dunlop's interpolating cubic splines (Dunlop 1991) (expressed in a slightly different form). The following representation gives exactly the same Dunlop cubic spline approximation as that used in EPANET and which is discussed on pages 189-190 in the EPANET User's Manual (Rossman 2000): $f = \sum_{k=0}^{3} (\alpha_k + \beta_k/\theta)\,\eta^k$ where α_k, β_k are defined in Table 2, and where we have introduced the new variables $\eta = \mathcal{R}/2000$,

$$\theta = \frac{\epsilon}{3.7D} + \frac{5.74}{\mathcal{R}^{9/10}} = \frac{b\epsilon}{D} + c\left|\frac{D}{Q}\right|^{9/10}, \quad \hat{\theta} = \frac{b\epsilon}{D} + \frac{5.74}{4000^{9/10}}, \tag{17}$$

where $b = 1/3.7$ and $c = 5.74\,(\pi\nu/4)^{9/10}$. With this representation the term on the diagonal of the matrix $\boldsymbol{G}$ in (6) is that given in the third column of Table 1.

Table 1: The terms on the diagonal of $\boldsymbol{G}$ and their sources (from Simpson & Elhay (2011)).

Case	Range of $\mathcal{R}$	Diagonal element of $\boldsymbol{G}$	Formula source
1	$\mathcal{R} \leq 2000$	$\frac{128\nu}{\pi g}\frac{L}{D^4}$	Hagen-Poiseuille
2	$2000 < \mathcal{R} < 4000$	$\lvert Q\rvert \left(\frac{8}{\pi^2 g}\right) \frac{L}{D^5} \sum_{k=0}^{3} (\alpha_k + \beta_k/\theta)\,\eta^k$	Dunlop α_k, β_k as in Table 2
3	$\mathcal{R} \geq 4000$	$\lvert Q\rvert \left(\frac{2\ln^2 10}{\pi^2 g}\right) \frac{L}{D^5}\frac{1}{\ln^2\theta}$	Swamee-Jain (see (4))

Table 2: Coefficients of the cubic interpolating spline defining the friction factor for $2000 < \mathcal{R} < 4000$. The constants are $\tau = 0.00514215$ and $\xi = -0.86859$ (from Simpson & Elhay (2011)).

k	α_k	β_k
0	$5/(\xi^2 \ln^2 \hat{\theta})$	$\tau/(\xi^3 \ln^3 \hat{\theta})$
1	$0.128 - 12/(\xi^2 \ln^2 \hat{\theta})$	$-5\tau/(2\xi^3 \ln^3 \hat{\theta})$
2	$-0.128 + 9/(\xi^2 \ln^2 \hat{\theta})$	$-2\tau/(\xi^3 \ln^3 \hat{\theta})$
3	$0.032 - 2/(\xi^2 \ln^2 \hat{\theta})$	$-\tau/(2\xi^3 \ln^3 \hat{\theta})$

Table 3: The diagonal terms[†] of the matrix $\boldsymbol{F}$ (from Simpson & Elhay (2011)).

Case	Range of $\mathcal{R}$	The diagonal terms in $\boldsymbol{F}$
1*	$\mathcal{R} \leq 2000$	$\left(\frac{128\nu}{\pi g}\right) \frac{L}{D^4}$
2	$2000 < \mathcal{R} < 4000$	$\left(\frac{8}{\pi^2 g}\right) \frac{L}{D^5} \lvert Q \rvert \sum_{k=0}^{3} \left\{ \frac{9c}{10} \frac{\beta_k}{\theta^2} \left\lvert \frac{D}{Q} \right\rvert^{9/10} + (2+k)\left(\alpha_k + \beta_k/\theta\right) \right\} \eta^k$
3	$\mathcal{R} \geq 4000$	$\left(\frac{2\ln^2 10}{\pi^2 g}\right) \frac{L}{D^5} \frac{\lvert Q \rvert}{\ln^2 \theta} \left(1 + \left(\frac{9c}{5\theta \ln \theta}\right) \left\lvert \frac{D}{Q} \right\rvert^{9/10}\right)$

* Note that for Case 1 the diagonal term in $\boldsymbol{F}$ is constant and is independent of Q.
† For details of the derivations of the terms in $\boldsymbol{F}$ see Simpson & Elhay (2011).

Case 3: Turbulent flow $\mathcal{R} \geq 4000$ The DW friction factor of (4) can be rewritten as $f = \ln^2 10/(4 \ln^2 \theta)$ with θ defined in (17).

The calculations in this paper have been performed using two programs: one written by the authors in Matlab (Mathworks 2008), and the other the package EPANET V2.00.12 written by L. Rossman. Both codes use IEEE standard double precision arithmetic.

The stopping tests in our implementation of the Newton method use the one–norm and the infinity–norm of a k–dimensional vector $\boldsymbol{x}$, defined, respectively, by $\|\boldsymbol{x}\|_1 = \sum_{j=1}^{k} |x_j|$ and $\|\boldsymbol{x}\|_\infty = \max_j |\boldsymbol{x}_j|$. The EPANET algorithm is designed to keep iterating until the *relative flow* is smaller than a preset stopping parameter δ_{stop}

$$\phi^E(\boldsymbol{q}^{(m)}) \stackrel{\text{def}}{=} \frac{\left\|\boldsymbol{q}^{(m)} - \boldsymbol{q}^{(m-1)}\right\|_1}{\|\boldsymbol{q}^{(m)}\|_1} = \frac{\sum_{k=1}^{n_p} \left|Q_k^{(m)} - Q_k^{(m-1)}\right|}{\sum_{k=1}^{n_p} |Q^{(m)}|} \leq \delta_{stop}. \tag{18}$$

The test (18) considers only the flows but from a practical standpoint it might be considered appropriate as an alternative, to cease iterating when all the heads in a network differ by a sufficiently small margin from one iteration to the next. To implement this test one keeps iterating until

$$\phi^\infty(\boldsymbol{h}^{(m)}) \stackrel{\text{def}}{=} \left\|\boldsymbol{h}^{(m)} - \boldsymbol{h}^{(m-1)}\right\|_\infty = \max_i \left|H_i^{(m)} - H_i^{(m-1)}\right| \leq \epsilon_{stop}, \tag{19}$$

where ϵ_{stop} is a predetermined stopping parameter. Thus, in a practical setting one might be satisfied when the greatest difference between heads from one iteration to the next is no greater than, say, 1 mm. This is achieved, in SI units, by setting

$\epsilon_{stop} = 10^{-3}$ m but in this paper we will use much smaller tolerances in order to better illustrate the points we wish to make.

Example 1 To illustrate the difference between using $\boldsymbol{F} = n\boldsymbol{G}$ and the correct terms for $\boldsymbol{F}$ given in Table 3 in the performance of the GGA, we compared the number of iterations taken by the two versions on some example networks. The example networks were generated by the program GRIDNETS (Berghout & Kuczera 1997). The stopping tolerances for both EPANET and the Matlab implementations were set to 10^{-10} m. The column in Table 4 headed n_i^c shows the number of iterations required by the method with $\boldsymbol{F} = n\boldsymbol{G}$ and that headed by n_i^v shows the number of iterations required by the method with the correct Jacobian.

The convergence data for Network 3 of Table 4 are shown in Table 5 for illustrative purposes. □

Table 4: Comparison of the number of iterations required to achieve convergence with the DW head loss model. The stopping test used $\epsilon_{stop} = 10^{-10}$ m.

ID	n_p	n_j	n_i^c	n_i^v
1	553	290	15	12
2	1054	538	21	12
3	2625	1333	25	12
4	5187	2617	31	14
5	10354	5187	29	15

REGULARIZATION IN THE CASE OF ZERO FLOWS

Consider the $(1,1)$ block, $\boldsymbol{F}$ of the Jacobian (10) for the HW model. From relations (15), (16) it is clear that the GGA method cannot continue if, at some stage in the iterations, any of the diagonal elements of the matrix $\boldsymbol{F}$ become zero because then neither the matrix $\boldsymbol{F}^{-1}$ nor $\boldsymbol{V} = \boldsymbol{A}_1^T\boldsymbol{F}^{-1}\boldsymbol{A}_1$ exist. A diagonal element of $\boldsymbol{F}$ becomes zero when the flow in the corresponding pipe becomes zero. In computational terms this occurs whenever the Reynolds number for a flow falls below a threshold predetermined by the modeler.

It is worth discussing the connection between the invertibility of the $\boldsymbol{F}$ and the invertibility of the whole Jacobian $\boldsymbol{J}$ for the HW head loss equations.

Provided that $\boldsymbol{F}$ is invertible, the matrix $\boldsymbol{J}$ of (10) admits the factoring

$$\begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} = \begin{pmatrix} \boldsymbol{I}_{n_p} & \boldsymbol{o} \\ -\boldsymbol{A}_1^T\boldsymbol{F}^{-1} & \boldsymbol{I}_{n_j} \end{pmatrix} \begin{pmatrix} \boldsymbol{F} & \boldsymbol{o} \\ \boldsymbol{o}^T & -\boldsymbol{V} \end{pmatrix} \begin{pmatrix} \boldsymbol{I}_{n_p} & -\boldsymbol{F}^{-1}\boldsymbol{A}_1 \\ \boldsymbol{o}^T & \boldsymbol{I}_{n_j} \end{pmatrix}$$

so $\det(\boldsymbol{J}) = \det(\boldsymbol{F})\det(-\boldsymbol{V})$. Thus, if $\boldsymbol{F}$ is invertible then $\boldsymbol{J}$ is invertible if and only if $\boldsymbol{V}$ is invertible.

From (1) we see that all the elements on the diagonal of $\boldsymbol{F}$ are non-negative.

Suppose for a moment that none of the flows is zero. Then all the elements on the diagonal of $\boldsymbol{F}$ are positive and so $\boldsymbol{F}$ is invertible. Now, the matrix $\boldsymbol{A}_1$ has full column

Table 5: The convergence data for Case 3 from Table 4.This network has $n_p = 2625$ pipes and $n_j = 1333$ nodes. The stopping test limit was set to $\epsilon_{stop} = 10^{-10}$ m.

	DW without correction (flow independent f)		DW with correction (flow dependent f)	
m	$\phi^\infty(\boldsymbol{q}^{(m)})$	$\phi^\infty(\boldsymbol{h}^{(m)})$	$\phi^\infty(\boldsymbol{q}^{(m)})$	$\phi^\infty(\boldsymbol{h}^{(m)})$
1	$1.6e+000$	$2.9e+002$	$1.7e+000$	$2.9e+002$
2	$7.1e-001$	$1.3e+002$	$7.5e-001$	$1.3e+002$
3	$3.0e-001$	$3.4e+001$	$3.2e-001$	$3.7e+001$
4	$1.1e-001$	$2.7e+001$	$1.2e-001$	$2.4e+001$
5	$4.8e-002$	$1.6e+001$	$6.4e-002$	$1.4e+001$
6	$2.0e-002$	$2.8e+000$	$3.0e-002$	$2.8e+000$
7	$8.8e-003$	$4.5e-001$	$1.3e-002$	$6.0e-001$
8	$1.7e-003$	$8.8e-002$	$4.2e-003$	$1.8e-001$
9	$2.4e-004$	$1.3e-002$	$5.2e-004$	$2.6e-002$
10	$3.5e-005$	$1.6e-003$	$1.2e-004$	$1.7e-003$
11	$3.2e-006$	$1.1e-004$	$1.3e-007$	$4.0e-006$
12	$6.0e-007$	$1.3e-005$	$6.6e-013$	$2.7e-011$
13	$2.3e-007$	$3.1e-006$	–	–
14	$1.0e-007$	$7.4e-007$	–	–
15	$4.3e-008$	$2.6e-007$	–	–
16	$1.9e-008$	$1.1e-007$	–	–
17	$8.2e-009$	$4.9e-008$	–	–
18	$3.6e-009$	$2.1e-008$	–	–
19	$1.6e-009$	$9.2e-009$	–	–
20	$6.8e-010$	$4.0e-009$	–	–
21	$3.0e-010$	$1.8e-009$	–	–
22	$1.3e-010$	$7.6e-010$	–	–
23	$5.7e-011$	$3.4e-010$	–	–
24	$2.5e-011$	$1.4e-010$	–	–
25	$1.1e-011$	$7.0e-011$	–	–

rank and, since $\boldsymbol{F}$ is positive definite, then $-\boldsymbol{V}$ is symmetric, negative definite and so it too is invertible. Thus, if $\boldsymbol{F}$ is invertible then $\boldsymbol{J}$ is invertible.

Suppose now that we allow zero flows. If one or more of the flows is zero then neither $\boldsymbol{F}^{-1}$ nor $\boldsymbol{V}$ exist and relations (15) and (16) cannot be used. In fact, the singularity of the matrix $\boldsymbol{F}$ does not, of itself, imply the singularity of the Jacobian matrix (10). Certainly, if more than n_j of the flows are zero then the Jacobian $\boldsymbol{J}$ is necessarily singular. However, if fewer than n_j of flows are zero then the Jacobian matrix may be invertible even though $\boldsymbol{F}$ is singular. See Appendix I of Elhay & Simpson (2011) for details.

Thus, a mechanism for dealing with the case where a sufficiently small number of flows are zero while $\boldsymbol{J}$ remains invertible is desirable. In Elhay & Simpson (2011) a *regularization* method is proposed. The method is applied at each iteration by identifying those elements on the diagonal of the $\boldsymbol{F}$ matrix corresponding to pipes in the network that have flows sufficiently small enough to present a difficulty and defining a corrective element which counteracts the problem.

Suppose the n_p–square matrix $\boldsymbol{T}$ is such that

$$\boldsymbol{T} = \text{diag}\left\{t_1, t_2, \ldots, t_{n_p}\right\} \text{ where } \begin{cases} t_i = 0 & \text{if } Q_i \neq 0, \\ t_i > 0 & \text{if } Q_i = 0. \end{cases} \tag{20}$$

The iteration

$$\begin{pmatrix} \boldsymbol{F}+\boldsymbol{T} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m+1)} \\ \boldsymbol{h}^{(m+1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{d} \end{pmatrix} \tag{21}$$

has the same solution as (7).

Denoting $\boldsymbol{W} = \boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1$, the iteration equations corresponding to (15) and (16) are now

$$\boldsymbol{h}^{(m+1)} = -\boldsymbol{W}^{-1}\left(\boldsymbol{d} + \boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\left[(\boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T})\,\boldsymbol{q}^{(m)} + \boldsymbol{u}\right]\right) \tag{22}$$

and

$$\boldsymbol{q}^{(m+1)} = (\boldsymbol{F}+\boldsymbol{T})^{-1}\left(\boldsymbol{A}_1\boldsymbol{h}^{(m+1)} + \left[(\boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T})\boldsymbol{q}^{(m)} + \boldsymbol{u}\right]\right). \tag{23}$$

Provided $\boldsymbol{J}$ remains invertible, relations (22) and (23) can be used even if some of the flows are zero because, with the elements of the diagonal matrix $\boldsymbol{T}$ chosen as in (20), the submatrix $\boldsymbol{F}+\boldsymbol{T}$ is always invertible.

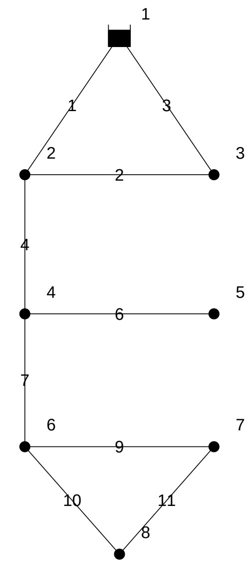
How to chose the elements of $\boldsymbol{T}$ to optimize the performance of the algorithm remains an open question but in Elhay & Simpson (2011) a bound minimization strategy is proposed which gives good results on all the networks that were tested.

We note that this modification of the Newton scheme, however, is no longer a true Newton iteration and convergence, if it occurs, cannot be expected to have quadratic order. However, our experience suggests that a suitable choice of the $\boldsymbol{T}$ matrix can lead to order of convergence which is higher than linear.

Define the *2–norm condition number* (see Golub & Loan (1989)) of $\boldsymbol{A}$, $cond(\boldsymbol{A}) = \|\boldsymbol{A}\|_2\left\|\boldsymbol{A}^{-1}\right\|_2$. Roughly speaking, one decimal digit of reliability in the solution of the well–scaled system of equations $\boldsymbol{Ax} = \boldsymbol{b}$ is lost for every power of ten in the condition number.

The strategy, sometimes used, of replacing a zero diagonal element of $\boldsymbol{F}$ by a small non-zero number to avoid singularity changes $cond(\boldsymbol{F})$ from a value of ∞ (when the

Figure 1: The network discussed in Example 2. Pipe 6 has zero flow.



matrix is singular) to a very large finite number. This means that the solution computed in (22) which uses $\boldsymbol{V}$ is unreliable. More importantly, this strategy is equivalent to solving the equation

$$\begin{pmatrix} n(\boldsymbol{G}+\boldsymbol{T}) & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} = \begin{pmatrix} (n-1)(\boldsymbol{G}+\boldsymbol{T}) & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} + \begin{pmatrix} \boldsymbol{u} \\ \boldsymbol{d} \end{pmatrix}, \tag{24}$$

with the non–zero t_i of (20) set to some small number and this equation has a solution that is different from that which we seek, the solution of (7).

We now illustrate the use of this modified method.

Example 2 In this example we consider the symmetric network shown in Figure 1.

The network has one reservoir at 40 m elevation and all other nodes are at zero elevation. All pipes have diameters, D_j, of 250 mm and lengths of L_j of 1000 m. Node 8 has a demand of 80 L/s and all other nodes have zero demands.

The head loss is modeled by the HW equation and each pipe has a HW coefficient of $C = 120$. The computation was set to use the stopping test defined by (19) and the stopping tolerance was set at $\epsilon_{stop} = 10^{-10}$ m.

The network has a dead–end pipe (pipe 6) which has zero–demand at node 5. The pipe to this node necessarily has zero flow. Pipe–node configurations which have dead–end pipes with zero demands are known to occur in real networks and so they can present problems to program codes not designed to handle zero flows.

In Table 6 we show the convergence data for the case where no regularization is used. The iterates move towards the solution but their approach causes an increase in the condition numbers of the $\boldsymbol{F}$ and $\boldsymbol{W}$ matrices, shown in Columns 5 and 6, and so the iterates then move away from the correct solution. When $\boldsymbol{W}$, has a condition number of about 10^{14} then, roughly speaking, only one, or possibly two, digits in the solution produced by (22) are reliable.

The data shown in Table 7 demonstrate that convergence is restored and the solution is found in 6 iterations when regularization, with $\boldsymbol{T}$ chosen as described in Elhay & Simpson (2011), is applied. □

By contrast, it follows that zero flows cannot cause zero elements in the matrix $\boldsymbol{F}$ for the Darcy-Weisbach head loss model if the formula for laminar flow is implemented as in Table 3.

Table 6: The convergence data for network shown in Figure 1 with no regularization.

HW head loss model

m	$\phi^\infty(\boldsymbol{q}^{(m)})$	$\phi^\infty(\boldsymbol{h}^{(m)})$	$\phi^E(\boldsymbol{q}^{(m)})$	$cond(\boldsymbol{F})$	$cond(\boldsymbol{W})$
1	$6.5e-002$	$3.9e+001$	$8.0e-001$	$1.0e+000$	$5.4e+001$
2	$8.6e-003$	$1.7e+001$	$9.5e-002$	$6.5e+012$	$1.2e+014$
3	$3.2e-004$	$2.1e-001$	$3.1e-003$	$3.5e+002$	$6.5e+003$
4	$2.0e-005$	$1.5e-003$	$7.0e-005$	$1.5e+012$	$2.9e+013$
5	$2.0e-005$	$1.2e-003$	$7.1e-005$	$1.2e+003$	$2.2e+004$
6	$9.1e-006$	$3.5e-003$	$5.7e-005$	$1.0e+012$	$1.9e+013$
7	$2.5e-005$	$3.1e-003$	$1.1e-004$	$1.9e+012$	$3.6e+013$
8	$2.5e-005$	$4.2e-004$	$7.1e-005$	$9.7e+002$	$1.8e+004$
9	$3.7e-006$	$4.9e-004$	$1.7e-005$	$2.9e+011$	$5.3e+012$
10	$3.7e-006$	$4.9e-004$	$1.7e-005$	$5.0e+003$	$9.3e+004$
11	$2.1e-007$	$8.1e-005$	$1.3e-006$	$3.5e+010$	$6.5e+011$
12	$4.5e-007$	$1.7e-004$	$2.8e-006$	$6.7e+010$	$1.3e+012$
13	$1.6e-006$	$6.0e-004$	$9.7e-006$	$1.3e+011$	$2.4e+012$
14	$1.5e-006$	$5.8e-004$	$9.4e-006$	$2.5e+011$	$4.7e+012$
15	$6.3e-006$	$1.8e-003$	$4.6e-005$	$4.9e+011$	$9.2e+012$
16	$6.3e-006$	$1.9e-003$	$4.8e-005$	$3.1e+003$	$5.9e+004$
17	$7.9e-006$	$3.0e-003$	$4.9e-005$	$8.4e+011$	$1.6e+013$
18	$5.6e-006$	$2.1e-003$	$3.5e-005$	$1.6e+012$	$3.0e+013$
19	$4.7e-005$	$1.8e-002$	$2.9e-004$	$3.1e+012$	$5.9e+013$
20	$5.2e-005$	$2.0e-002$	$3.3e-004$	$6.1e+012$	$1.1e+014$

CONCLUSIONS

This paper considers two issues related to iteratively solving the non-linear equations governing the flow and head in a water distribution system network. The first concerns the use of the correct Jacobian for the GGA when the DW head loss model is used. A range of networks with up to 10,354 pipes of different sizes were considered and show that the quadratic convergence typical of the Newton method is restored.

The second issue relates to dealing with zero flows in the iterative solution process. A regularization procedure for the GGA with Hazen-Williams head loss model was demonstrated on an example network which has zero flows but for which the (full) Jacobian is invertible. It was shown that, by contrast, zero flows with the Darcy-Weisbach head loss model do not lead to singularity of the $\boldsymbol{F}$ matrix.

Table 7: The convergence data for network shown in Figure 1 with the regularization method (22) and (23) applied. Rapid convergence is restored by the regularization.

HW head loss model

m	$\phi^{\infty}(\boldsymbol{q}^{(m)})$	$\phi^{\infty}(\boldsymbol{h}^{(m)})$	$\phi^{E}(\boldsymbol{q}^{(m)})$	$cond(\boldsymbol{F}+\boldsymbol{T})$	$cond(\boldsymbol{W})$
1	$6.5e-002$	$3.9e+001$	$8.0e-001$	$1.0e+000$	$5.4e+001$
2	$8.5e-003$	$1.7e+001$	$9.5e-002$	$1.0e+003$	$1.9e+004$
3	$3.2e-004$	$2.0e-001$	$2.9e-003$	$1.0e+003$	$1.9e+004$
4	$4.1e-007$	$2.4e-004$	$3.3e-006$	$1.0e+003$	$1.9e+004$
5	$6.8e-013$	$3.9e-010$	$5.4e-012$	$1.0e+003$	$1.9e+004$
6	$1.5e-014$	$5.8e-012$	$1.3e-013$	$1.0e+003$	$1.9e+004$

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