Journal of Hydraulic Engineering. Submitted October 27, 2009; accepted February 23, 2011;
posted ahead of print February 25, 2011. doi:10.1061/(ASCE)HY.1943-7900.0000411

Dealing With Zero Flows in Solving the Non-Linear Equations for Water Distribution Systems

Sylvan Elhay* Angus R. Simpson† M.ASCE

Abstract

Three issues concerning the iterative solution of the non-linear equations governing the flows and heads in a water distribution system network are considered. Zero flows cause a computation failure (division by zero) when the Global Gradient Algorithm of Todini and Pilati is used to solve for the steady–state of a system in which the head loss is modeled by the Hazen-Williams formula. We propose a regularization technique which overcomes this failure as a solution to this first issue. The second issue relates to zero flows in the Darcy-Weisbach formulation. We explain for the first time why zero flows do not lead to a division by zero where the head loss is modeled by the Darcy-Weisbach formula. We show how to handle the computation appropriately where there is laminar flow (the only instance in which zero flows may occur). However, as is shown, a significant loss of accuracy can result if the Jacobian matrix, necessary for the solution process, becomes poorly conditioned and so it is recommended that the regularization technique be used for the Darcy-Weisbach case as well. Only a modest extra computational cost is incurred when the technique is applied. The third issue relates to a new convergence stopping criterion for the iterative process based on the infinity-norm of the vector of nodal head differences between one iteration and the next. This test is recommended because it has a more natural physical interpretation than the relative discharge stopping criterion that is currently used in standard software packages such as EPANET. In addition, we recommend that the infinity norms of the residuals are checked once iteration has been stopped. The residuals test ensures that inaccurate solutions are not accepted.

*School of Computer Science, University of Adelaide, South Australia, 5005.
†School of Civil, Environmental and Mining Engineering, University of Adelaide, South Australia, 5005.

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INTRODUCTION

Water distribution systems analysis involves determination of flow rates and pressures in a network. The equations governing the flows and heads in a water distribution system are non-linear and often a Newton iterative solution algorithm is used in which a linearized set of equations is solved at each iteration. Since the advent of computers a number of papers have been written describing methods for solving the pipe network equations in a water distribution system (Martin & Peters 1963, Shamir & Howard 1968, Epp & Fowler 1970, Wood & Charles 1972, Wood & Rayes 1981, Ormsbee & Wood 1986, Nielsen 1989, Boulos & Wood 1990). Jeppson (1976) also detailed a number of solution methods in his book. The most commonly used formulation models the flow and head equations in terms of the unknown flows and unknown nodal heads. For this formulation Todini & Pilati (1988) developed a fast algorithm consisting of a two-step process where the heads and then flows are solved for, consecutively, at each iterative step during the solution procedure.

We consider three related issues which are associated with the solution of pipe network models. The first issue concerns the difficulty that arises in the solution method proposed by Todini & Pilati (1988), later called the Global Gradient Algorithm (GGA) (Todini 2006), when some of the pipes in a network, in which the head losses are modeled by the Hazen-Williams formula, have zero flows. When that happens a key matrix in the method becomes singular and prevents further computation. To overcome this difficulty we propose a new regularization method that is a variation of the standard GGA and allows for zero flows. Zero flows occur relatively commonly in networks especially at dead end branched sections that have zero demands. This is particularly true for "all pipes" models that include the offtakes to residences. If an extended period simulation is run to model water usage during the day then many of these offtakes will have zero demands and, hence, zero flows. Results from case study networks to demonstrate the effectiveness of the new algorithm are presented.

The second issue we address concerns the GGA applied to networks in which the head loss is modeled by the Darcy-Weisbach formula. We give a computational formula for the Jacobian which recognizes that the head loss for laminar flow is proportional to velocity, rather than the square of

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velocity as in turbulent flow. Thus, the method we propose avoids the failure that would otherwise occur with zero flows for this case.

The third issue discussed relates to the stopping test for convergence that is applied in the iterative process used to solve the non–linear equations. A test based on the infinity norm of the vector of nodal head differences between one iteration and the next is recommended because it has a more natural physical interpretation than the relative discharge stopping criterion that is currently used in standard software packages such as EPANET. In addition, we recommend that the infinity norms of the residuals are checked once iteration has been stopped. Any solution for which the residual is large can be rejected as inaccurate.

THE NETWORK EQUATIONS

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, for the Hazen-Williams head loss model using SI units, by $H_i - H_k = r_j Q_j |Q_j|^{n-1}$ where $n = 1.852$ and $r_j = 10.670 L_j / (C_j^n D_j^{4.871})$, where the pipe length is L_j, Hazen-Williams coefficient is C_j and diameter is D_j.

Denote the vector of flows by $\boldsymbol{q} = (Q_1, Q_2, \ldots, Q_{n_p})^T$, where n_p is the number of pipes. We define a square, diagonal matrix $\boldsymbol{G}$ which, for the Hazen-Williams formulation, has elements

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

Note that r_j in (1) does not depend on the flow Q_j.

The flow and head equations

The energy and continuity equations describing the flows and nodal heads in a water distribution system are

$$\boldsymbol{Gq} - \boldsymbol{A}_1 \boldsymbol{h} - \boldsymbol{A}_2 \boldsymbol{e}_\ell \quad = \quad \boldsymbol{0}, \tag{2}$$

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$$-\boldsymbol{A}_1^T \boldsymbol{q} - \boldsymbol{d}_m \quad = \quad \boldsymbol{0}, \tag{3}$$

where $\boldsymbol{A}_1$ is the $n_p \times n_j$ *unknown head node incidence matrix*, n_j is the number of unknown head nodes, $\boldsymbol{h} = (H_1, H_2, \ldots, H_{n_j})^T$ is the vector of unknown heads, $\boldsymbol{A}_2$ is the $n_p \times n_f$ *fixed head node incidence matrix*, n_f is the number of fixed head nodes, $\boldsymbol{e}_\ell$ is the n_f–dimension vector of fixed head node elevations and $\boldsymbol{d}_m$ is the n_j–dimension vector of nodal demands.

Equations (2) and (3) can be written more conveniently in matrix form as

$$\boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} \boldsymbol{G} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} - \begin{pmatrix} \boldsymbol{A}_2 \boldsymbol{e}_\ell \\ \boldsymbol{d}_m \end{pmatrix} = \boldsymbol{0}, \tag{4}$$

where $\boldsymbol{x} = (\boldsymbol{q}^T, \boldsymbol{h}^T)^T$ is the $n_p + n_j$ dimensional, real vector of unknown flows and heads in the system, and $\boldsymbol{O}$ is an $n_j \times n_j$ zero matrix. Todini & Pilati (1988) presented the GGA to solve (4) for the Hazen-Williams head loss formulation. The matrix $\boldsymbol{A}_1$ is constant but $\boldsymbol{G}$ usually depends on the unknown pipe flows in $\boldsymbol{q}$ and this makes the system in (4) non–linear.

Solving the non–linear pipe network equations

Systems of non–linear equations $\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$ in (4) are frequently solved by Newton's iterative method $\boldsymbol{J}(\boldsymbol{x}^{(m)})(\boldsymbol{x}^{(m+1)} - \boldsymbol{x}^{(m)}) = -\boldsymbol{f}(\boldsymbol{x}^{(m)})$, $m = 0, 1, 2, \ldots,$ with $\boldsymbol{x}^{(0)}$ prescribed and $\boldsymbol{J}(\boldsymbol{x})$ the Jacobian of $\boldsymbol{f}(\boldsymbol{x})$, which in the case of (4) can be written

$$\boldsymbol{J} = \begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix}. \tag{5}$$

For the Hazen-Williams head loss model this matrix has the form

$$\boldsymbol{F} = n\boldsymbol{G} = 1.852\boldsymbol{G}, \tag{6}$$

with the diagonal elements of $\boldsymbol{G}$ given by (1).

AN ALTERNATIVE CONVERGENCE CRITERION

We now propose (i) the use of a new test based on the infinity norm of the nodal head differences from one iteration to the next to stop the iteration process and (ii) that the equation residuals be examined when iteration has ceased to avoid accepting an inaccurate solution. Define the infinity–norm of the vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)^T$ by $\|\boldsymbol{x}\|_\infty = \max_{1\le j\le k} |x_j|$. In the proposed test one would stop iterating when the infinity norm of the vector of nodal heads differences satisfies

$$\phi^\infty(\boldsymbol{h}^{(m)}) \stackrel{\text{def}}{=} \left\|\boldsymbol{h}^{(m)} - \boldsymbol{h}^{(m-1)}\right\|_\infty = \max_i \left|H_i^{(m)} - H_i^{(m-1)}\right| \le \epsilon_{stop}, \quad (7)$$

where ϵ_{stop} is a preset stopping parameter.

Once the iterative solution process has been stopped by (7), the residuals of the computed solution for equation (4) should be checked. Residuals that are too large indicate an inaccurate solution. The *energy residual*

$$\rho_e(\boldsymbol{q}, \boldsymbol{h}) = \boldsymbol{G}\boldsymbol{q} - \boldsymbol{A}_1\boldsymbol{h} - \boldsymbol{A}_2\boldsymbol{e}_\ell,$$

and the *continuity residual*

$$\rho_c(\boldsymbol{q}, \boldsymbol{h}) = \boldsymbol{A}_1^T\boldsymbol{q} + \boldsymbol{d}_m$$

will both be zero at the exact solution. A computed solution which satisfies (7) should be considered unacceptable if

$$\|\rho_e(\boldsymbol{q}, \boldsymbol{h})\|_\infty > u_1\epsilon_{stop} \text{ or } \quad \|\rho_c(\boldsymbol{q}, \boldsymbol{h})\|_\infty > u_2\epsilon_{mach}, \quad (8)$$

where ϵ_{mach} is defined in (20) and where $u_1 = 1$ and $u_2 = 100$ have been found by the authors to be suitable choices for networks with up to 10,000 pipes. Rejecting any solution for which one or both of (8) hold safeguards against accepting an inaccurate solution. It should be noted, however, that a small residual does not guarantee an accurate solution.

By comparison with (7) the EPANET program (the widely used open source network modeling package developed by Rossman (2000)) is designed to stop iterating when the *relative flow* is smaller than a preset stopping parameter, δ_{stop},

$$\phi^E(\boldsymbol{q}^{(m)}) \stackrel{\text{def}}{=} \frac{\sum_{k=1}^{n_p}\left|Q_k^{(m)} - Q_k^{(m-1)}\right|}{\sum_{k=1}^{n_p}\left|Q^{(m)}\right|} \le \delta_{stop}. \quad (9)$$

Modelers using an iterative procedure are sometimes tempted, where the iteration process has signaled a failure to converge, to relax the stopping test by increasing the stopping tolerance (e.g. from the EPANET minimum value of $\delta_{stop} = 10^{-5}$ to, say, $\delta_{stop} = 10^{-2}$). This is a dangerous practice and without the residual check (8) can lead to an inaccurate solution being accepted as satisfactory.

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THE GLOBAL GRADIENT ALGORITHM

The Newton system to solve for the heads and flows (Simpson & Elhay 2010) is

$$\begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m+1)} \\ \boldsymbol{h}^{(m+1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F}-\boldsymbol{G} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{A}_2\boldsymbol{e}_\ell \\ \boldsymbol{d}_m \end{pmatrix}, \qquad (10)$$

where $\boldsymbol{o}$ is an $n_p \times n_j$ zero matrix. The (1,1) block of the Jacobian here should be written $\boldsymbol{F}^{(m)}$ to indicate that it depends on $\boldsymbol{q}^{(m)}$ and so changes every iteration but, in the interests of clarity, we omit the superscript except where necessary.

Denote the n_j–square matrix $\boldsymbol{V} = \boldsymbol{A}_1^T\boldsymbol{F}^{-1}\boldsymbol{A}_1$. Provided $\boldsymbol{F}$ and $\boldsymbol{V}$ are invertible, the two stage GGA equations are

$$\boldsymbol{h}^{(m+1)} = -\boldsymbol{V}^{-1}\left[\boldsymbol{d}_m + \boldsymbol{A}_1^T\boldsymbol{F}^{-1}\left((\boldsymbol{F}-\boldsymbol{G})\boldsymbol{q}^{(m)} + \boldsymbol{A}_2\boldsymbol{e}_\ell\right)\right] \qquad (11)$$

and

$$\boldsymbol{q}^{(m+1)} = \boldsymbol{q}^{(m)} + \boldsymbol{F}^{-1}\left(\boldsymbol{A}_1\boldsymbol{h}^{(m+1)} - \boldsymbol{G}\boldsymbol{q}^{(m)} + \boldsymbol{A}_2\boldsymbol{e}_\ell\right). \qquad (12)$$

A NEW REGULARIZATION METHOD FOR THE CASE OF ZERO FLOWS

Consider the case of a network in which the head loss is modeled by the Hazen-Williams formula. If, as a result of zero flows, any of the diagonal elements of $\boldsymbol{F}$ given by (6) become zero then neither the diagonal matrix $\boldsymbol{F}^{-1}$ (with terms $1/(nr_j|Q_j|^{n-1})$) nor the matrix $\boldsymbol{V} = \boldsymbol{A}_1^T\boldsymbol{F}^{-1}\boldsymbol{A}_1$ exist. When the steady state solution being sought has one or more zero flows the method fails catastrophically.

We now introduce a regularization technique for the GGA which allows computation to continue even when some zero flows cause the diagonal elements of the $\boldsymbol{F}$ matrix to become zero (provided the Jacobian remains invertible - see Appendix A for a discussion of the conditions for the invertibility of the Jacobian when there are zero flows). The regularization is applied at each iteration by identifying those elements on the diagonal of the $\boldsymbol{F}$ matrix that present a difficulty and then defining a corrective element which counteracts the problem.

Define a n_p–square matrix

$$\boldsymbol{T} = \operatorname{diag}\left\{t_1, t_2, \ldots, t_{n_p}\right\} \text{ where } \begin{cases} t_i = 0 & \text{if } Q_i \neq 0, \\ t_i > 0 & \text{if } Q_i = 0. \end{cases} \tag{13}$$

(Small non-zero flows can also cause problems. These are discussed later.) The iterative scheme (10) seeks the exact $\boldsymbol{q}$ and $\boldsymbol{h}$ which satisfy the equation

$$\begin{pmatrix} \boldsymbol{F} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F}-\boldsymbol{G} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} + \begin{pmatrix} \boldsymbol{A}_2\boldsymbol{e}_\ell \\ \boldsymbol{d}_m \end{pmatrix}. \tag{14}$$

Adding the term $\begin{pmatrix} \boldsymbol{T} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix}$ to both sides of equation (14) gives

$$\begin{pmatrix} \boldsymbol{F}+\boldsymbol{T} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix} + \begin{pmatrix} \boldsymbol{A}_2\boldsymbol{e}_\ell \\ \boldsymbol{d}_m \end{pmatrix}, \tag{15}$$

which has the same solution as (14). This suggests the iteration

$$\begin{pmatrix} \boldsymbol{F}+\boldsymbol{T} & -\boldsymbol{A}_1 \\ -\boldsymbol{A}_1^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m+1)} \\ \boldsymbol{h}^{(m+1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T} & \boldsymbol{o} \\ \boldsymbol{o}^T & \boldsymbol{O} \end{pmatrix} \begin{pmatrix} \boldsymbol{q}^{(m)} \\ \boldsymbol{h}^{(m)} \end{pmatrix} + \begin{pmatrix} \boldsymbol{A}_2\boldsymbol{e}_\ell \\ \boldsymbol{d}_m \end{pmatrix}, \tag{16}$$

which leads to the following two-stage iterative scheme:

$$\boldsymbol{h}^{(m+1)} = -\boldsymbol{W}^{-1}\left(\boldsymbol{d}_m + \boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\left[(\boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T})\,\boldsymbol{q}^{(m)} + \boldsymbol{A}_2\boldsymbol{e}_\ell\right]\right), \tag{17}$$

where $\boldsymbol{W} = \boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1$, and

$$\boldsymbol{q}^{(m+1)} = (\boldsymbol{F}+\boldsymbol{T})^{-1}\left(\boldsymbol{A}_1\boldsymbol{h}^{(m+1)} + \left[(\boldsymbol{F}-\boldsymbol{G}+\boldsymbol{T})\boldsymbol{q}^{(m)} + \boldsymbol{A}_2\boldsymbol{e}_\ell\right]\right). \tag{18}$$

Provided $\boldsymbol{J}$ in (5) remains invertible, relations (17) and (18) can be used even if some of the flows are zero because, with the elements of the diagonal matrix $\boldsymbol{T}$ chosen as in (13), the submatrix $\boldsymbol{F}+\boldsymbol{T}$ is always invertible. We now propose a bound minimization strategy for choosing the elements of $\boldsymbol{T}$.

An important number in the solution of the system of linear equations $\boldsymbol{Ax} = \boldsymbol{b}$ is the *2–norm condition number* of $\boldsymbol{A}$, $\operatorname{cond}_2(\boldsymbol{A}) = \|\boldsymbol{A}\|_2 \left\|\boldsymbol{A}^{-1}\right\|_2$ where $\|\cdot\|_2$ is the matrix 2–norm (see (B-1) in Appendix B). A useful rule of thumb is that 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 increase in the condition number. The computed solutions of matrix systems with large condition numbers are unreliable. Thus, we should

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choose $\boldsymbol{T}$ so that the condition of the matrix $\boldsymbol{W}$, in (17), is kept small relative to the arithmetic precision.

In Appendix B we show that

$$\mathrm{cond}_2\left(\boldsymbol{A}_1^{\mathrm{T}}(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1\right) \leq \mathrm{cond}_2(\boldsymbol{F}+\boldsymbol{T})\mathrm{cond}_2(\boldsymbol{A}_1)^2. \tag{19}$$

The best we can achieve therefore is to limit the bound on $\mathrm{cond}_2\left(\boldsymbol{A}_1^{\mathrm{T}}(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1\right)$ at each iteration by choosing $\boldsymbol{T}$ to limit the size of $\mathrm{cond}_2(\boldsymbol{F}+\boldsymbol{T})$.

For the special case of the diagonal matrix $\boldsymbol{F}+\boldsymbol{T}$, which has only positive elements on the diagonal, the 2–norm condition number is given by the ratio of the largest to the smallest diagonal element,

$$\mathrm{cond}_2(\boldsymbol{F}+\boldsymbol{T}) = \frac{\max_{\mathrm{j}}\left([\boldsymbol{F}]_{\mathrm{jj}}+[\boldsymbol{T}]_{\mathrm{jj}}\right)}{\min_{\mathrm{j}}\left([\boldsymbol{F}]_{\mathrm{jj}}+[\boldsymbol{T}]_{\mathrm{jj}}\right)}.$$

The algorithm we discuss below, which chooses the elements of the regularization matrix $\boldsymbol{T}$ to limit the size of $\mathrm{cond}_2(\boldsymbol{F}+\boldsymbol{T})$ to some predetermined value, is intended to clearly illustrate the method rather than to compute $\boldsymbol{T}$ efficiently.

Before starting the first iteration, we select a threshold value, κ, above which we will not allow the condition number $\mathrm{cond}_2(\boldsymbol{F}^{(\mathrm{m})}+\boldsymbol{T}^{(\mathrm{m})})$ to grow throughout the iteration process (e.g. $\kappa = 1000$). Suppose that for the m–th iteration $\boldsymbol{F}^{(m)} = \mathrm{diag}\left\{\sigma_1^{(m)}, \sigma_2^{(m)}, \ldots, \sigma_{n_p}^{(m)}\right\}, \sigma_j^{(m)} \geq 0$. Assume, for simplicity, that the $\sigma_j^{(m)}$ are in non-decreasing order along the main diagonal from top to bottom. This makes $\sigma_1^{(m)} = \sigma_{max}^{(m)}$ and $\sigma_{n_p}^{(m)} = \sigma_{min}^{(m)}$.

The algorithm is:

(1) Set all the elements of the regularization matrix $\boldsymbol{T}^{(m)}$ to zero.

(2) At the m-th iteration identify the minimum diagonal element of the $\boldsymbol{F}+\boldsymbol{T}$ matrix $\sigma_{min}^{(m)}$. (The first time through $\sigma_{min}^{(m)} = \sigma_{n_p}^{(m)}$.)

(3) If the condition number for the matrix, $\sigma_{max}^{(m)}/\sigma_{min}^{(m)}$, is smaller than κ, no regularization is necessary. Exit. Otherwise choose the regularization parameter $t_{n_p}^{(m)}$ such that

$$\frac{\sigma_{max}^{(m)}}{\sigma_{n_p}^{(m)} + t_{n_p}^{(m)}} = \kappa.$$

This ensures that $\sigma_{n_p}^{(m)}$ does not cause the condition of the $\boldsymbol{F}+\boldsymbol{T}$ matrix at the m–th iteration to be greater than κ. Thus,

$$t_{n_p}^{(m)} = \frac{\sigma_{max}^{(m)}}{\kappa} - \sigma_{n_p}^{(m)}$$

and the regularized value of the last element in the matrix is now

$$\sigma_{n_p}^{(m)} + t_{n_p}^{(m)} = \frac{\sigma_{max}^{(m)}}{\kappa}.$$

Repeat steps (2) and (3) with $\sigma_{min}^{(m)}$ set in turn to $\sigma_{n_p-1}^{(m)}, \sigma_{n_p-2}^{(m)}, \ldots$ until exit occurs at step (3). If more than n_j of the $\sigma_j^{(m)}$ values are zero then the Jacobian is singular and the system has no unique solution. Cease execution.

This algorithm can be described more succinctly by

$$\sigma_j^{(m)} = \max\left(\sigma_j^{(m)}, \frac{\sigma_{max}^{(m)}}{\kappa}\right), \quad j = 1, 2, \ldots, n_p,$$

but, of course, the number of $\sigma_j^{(m)}$ which are too small still need to be counted.

The regularization method of (17) and (18) is no longer a true Newton scheme. However, we have found the rate of convergence to be close to quadratic when $\kappa = 1000$ was used on the example networks we tested.

The strategy of replacing a zero diagonal element of $\boldsymbol{F}$ by a small non-zero number to avoid singularity (thereby changing $\text{cond}_2(\boldsymbol{F})$ from a value of ∞ to a large finite number) actually solves the wrong set of equations while the proposed regularization method avoids this.

EXAMPLE NETWORKS

All the calculations in this paper were performed using two programs: one written by the authors in Matlab (Mathworks 2008), and the other the package EPANET V2.00.12. Both codes use IEEE standard double precision arithmetic with precision, measured by machine epsilon (Forsythe & Moler 1967), of

$$\epsilon_{mach} \approx 2 \times 10^{-16}. \tag{20}$$

The EPANET program was (slightly) modified and verified as described in Simpson & Elhay (2010).

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Example 1 We consider the symmetric network shown in Figure 1. It has eleven pipes, seven junctions at which the head is unknown and one fixed head node reservoir at 40 m elevation and all other nodes are at zero elevation. All pipes have diameters, D_j, of 250 mm and lengths, L_j of 1000 m. Node 8 has a demand of 80 L/s and all other nodes have zero demands. In the steady state this network has zero flow in Pipes 2, 6, 9 because of symmetry.

The head loss is modeled by the Hazen-Williams equation and each pipe has a Hazen-Williams coefficient $C_j = 120$. The computation was set to use the stopping test defined by (7). The iteration was run until $\phi^\infty(\boldsymbol{h}^{(m)}) < 10^{-10}$. We use a smaller than practical tolerance in order to better illustrate the points discussed.

When the GGA of (11) and (12) is applied to this network the iterates trend towards the solution and the flows in Pipes 2, 6, 9 approach zero. As this happens, the condition number of the matrix $\boldsymbol{F}$ grows larger (the matrix approaches singularity more and more closely), the matrix $\boldsymbol{V} = \boldsymbol{A}_1^T \boldsymbol{F}^{-1} \boldsymbol{A}_1$ becomes more and more badly conditioned and the solution computed with (11) becomes less and less reliable. This in turn takes the iterates away from the solution and as a result the flows which are near zero are replaced by larger flows which improve the condition of $\boldsymbol{F}$. Thus, as shown clearly in Column 2 of Table 1, the iterates move, alternately, towards and away from the solution but never converge to it. The last two columns of Table 1 show the condition numbers for the matrices $\boldsymbol{F}$ and $\boldsymbol{V}$. At each iteration the accuracy achieved in the heads is entirely consistent, for IEEE standard double precision arithmetic (20), with the size of the condition number of $\boldsymbol{V}$.

Now, using instead the regularized method of (17) and (18) and choosing $\boldsymbol{T}$ so that the condition of $\boldsymbol{F} + \boldsymbol{T}$ does not exceed 1000 we get rapid convergence as shown in Table 2. Even though the condition of $\boldsymbol{F}$ becomes very large and eventually may become infinite, the method finds the solution rapidly because the matrix $\boldsymbol{F} + \boldsymbol{T}$ is guaranteed to be well conditioned by the appropriate choice of $\boldsymbol{T}$. The order of convergence of the regularized method appears to be close to quadratic. Limiting the growth of $\text{cond}_2(\boldsymbol{F}+\boldsymbol{T})$ constrains $\text{cond}_2(\boldsymbol{W})$ at convergence to 1.3×10^4. The energy and continuity residuals for the regularized solution are, respectively, $1 \times 10^{-13}\ m$, and $5 \times 10^{-14}\ m^3/s$ while those of the EPANET solution are larger at $5 \times 10^{-13}\ m$ and $2 \times 10^{-8}\ m^3/s$. We therefore conclude that

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the Matlab solution is the more accurate.

Computing the steady state solution directly for the network in Figure 1 using the full matrix formulation of the Newton method (10), i.e. solving the matrix equation directly rather than using the GGA, produces quadratic convergence to the correct solution because the Jacobian matrix in this particular case is invertible even when there are zero flows in Pipes 2, 6, 9. Table 3 shows this case. Note that the full matrix formulation and the GGA give almost identical results when both the matrices $\boldsymbol{F}$ and $\boldsymbol{V}$ are well conditioned. Note also that when using the full Newton system as it stands we invert an 18×18 $(n_p + n_j \times n_p + n_j)$ matrix in contrast to the GGA in which the matrix to be inverted has dimension 7×7 $(n_j \times n_j)$.

Applied to the same problem EPANET V2.00.12, modified to allow a stopping tolerance of $\delta_{stop} = 10^{-10}$, as defined in (9) fails to converge after 71 iterations when the EPANET parameter controlling the maximum number of iterations allowed is set to 50. Although the EPANET stopping test (9) differs from that used by our implementation the failure of both the Matlab code without regularization and the EPANET code to find a solution to the required accuracy illustrates the problem we wish to address. It can be seen from the fifth column of Table 1 that using a stopping tolerance of 10^{-5}, the smallest allowed in EPANET, the program signals convergence after four iterations. The energy and continuity residuals for this EPANET solution are well within practical engineering requirements.

The steady-state flows and heads/pressure heads (all elevations for this network are zero) for this case are shown in Table 4.

Example 2 We also considered a network based on the network shown in Figure 1 but with pipes 5 and 8 removed. Pipe 6 then has zero flow because Node 5 has zero demand. Dead–end pipe configurations such as this are of interest because they occur frequently in the modeling of water distribution systems. The results for this example are similar to the results for the previous example: the unregularized method fails because of the ill–condition of $\boldsymbol{V}$ and the regularized method, with parameters chosen as in the previous example, rapidly finds the solution.

ZERO FLOWS IN SYSTEMS WITH THE DARCY-WEISBACH HEAD LOSS MODEL

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In this section we consider the second issue of the effect of zero flows when the GGA is applied to networks in which the Darcy-Weisbach head loss model is used.

Simpson & Elhay (2010) give formulae for the diagonal elements of the $\boldsymbol{G}$ and $\boldsymbol{F}$ matrices when the Darcy-Weisbach head loss model is used in the GGA of (11) and (12). From those formulae it is immediately clear that zero flows can occur only when the Reynolds number lies in the laminar flow range. However, an important observation is that, in this range, the corresponding term on diagonal of the matrix $\boldsymbol{F}$ is actually a constant value independent of Q_j.

To see this consider the case of a pipe in which the head loss is modeled by the Darcy-Weisbach formula. The head loss for this pipe is given, for friction factor f, by

$$h_f = f\frac{LV^2}{2gD} = f\frac{LQ^2}{2gDA^2} = f\frac{8LQ^2}{\pi^2 gD^5}. \tag{21}$$

Now, for laminar flow, with $\mathcal{R} < 2000$,

$$f = \frac{64}{\mathcal{R}} = \frac{64\nu}{VD} = \frac{16\pi\nu D}{Q} \tag{22}$$

and so, substituting (22) into (21) gives the head loss for laminar flow as

$$h_L = \left(\frac{128\nu}{\pi g}\right)\frac{L}{D^4}Q = r_L Q \tag{23}$$

where the *laminar flow resistance factor*

$$r_L = \left(\frac{128\nu}{\pi g}\right)\frac{L}{D^4}. \tag{24}$$

is seen to be independent of the flow Q. Thus, it is important to use (23) rather than (21) when dealing with laminar flows which are very small or zero.

In the computation of the Jacobian elements for pipes in which the flow is laminar, we are required to differentiate terms which are of the form $r_L Q$ with respect to Q. Hence, the term r_L is exactly the term on the diagonal of the matrix $\boldsymbol{F}$ for those pipes. It follows that when the Darcy-Weisbach formula, (23), is used to model head loss in a network the matrix $\boldsymbol{F}$ cannot be singular as a result of flows being zero. Thus, the GGA applied to this system will not fail if the correct Darcy-Weisbach formula, (23), is used. But in practice it may still be that case that, for certain networks, the condition of the matrix $\boldsymbol{F}$, and so the condition of the whole Jacobian, is too large for the precision of the arithmetic

Journal of Hydraulic Engineering. Submitted October 27, 2009; accepted February 23, 2011;
posted ahead of print February 25, 2011. doi:10.1061/(ASCE)HY.1943-7900.0000411

engine that is being used. In such a case the regularization strategy we have proposed can still be used to avoid a degradation of accuracy in the calculation.

To make the point that the matrix $\boldsymbol{F}$ can be ill–conditioned even though no flows are zero, we show that realistic ranges of network parameters can lead to an ill–conditioned $\boldsymbol{F}$. Recall that the condition of a diagonal matrix with positive elements is the ratio of its largest to its smallest element. Suppose a network with head loss modeled by the Darcy-Weisbach formula contains two pipes with the parameters shown in Table 5. Suppose also that the water in these pipes has kinematic viscosity $\nu = 1.01 \times 10^{-6}$ (m^2/s) and that the gravitational constant g is $9.81 m/s^2$. If the two pipes under consideration have the parameters shown in Columns 2 to 7, of Table 5 then the associated elements on the diagonal of the $\boldsymbol{F}$ matrix for the two pipes are as shown in the eighth column of Table 5. The condition of the corresponding matrix $\boldsymbol{F}$ is therefore at least $4.1 \times 10^4 / 2.7 \times 10^{-7} \approx 1.5 \times 10^{11}$. The solution to such a system in IEEE Standard Single Precision arithmetic would have no reliable digits in it while in IEEE Standard Double Precision it would have lost at least 11 digits of reliability. Thus, we recommend that the regularization algorithm be included in the implementation of the GGA for the Darcy-Weisbach head loss formula to ensure it is robust since the additional (overhead) cost of computation is small.

CONCLUSIONS

This paper considers three issues concerning the iterative solution of the non-linear equations governing the flows and heads in a water distribution system network.

The first issue relates to dealing with zero flows in the iterative solution process for a network in which the Hazen-Williams head loss model is used. A regularization procedure for the GGA has been proposed in which we add a diagonal matrix $\boldsymbol{T}$ with carefully chosen elements into the Jacobian matrix (and to the right hand side) when the matrix to be inverted becomes ill–conditioned. This prevents failure of the solution process if a flow in the network is ultimately zero or near-zero. The condition number of the Jacobian matrix is controlled by the selection of $\boldsymbol{T}$ so that the matrix $\boldsymbol{W} = \boldsymbol{A}_1^T(\boldsymbol{F} + \boldsymbol{T})^{-1}\boldsymbol{A}_1$ always remains invertible when the Jacobian is invertible. The speed of convergence of the regularization process is relatively insensitive to the selection of $\boldsymbol{T}$ for all the examples tested by the authors. Examples which illustrate the application of the method have been given. The regularization procedure leads to the correct solution for a network with zero flows within a relatively small number of iterations.

The second issue concerns the fact that where the Darcy-Weisbach head loss model is used, zero flows do not cause the key matrices of the GGA to become singular if the laminar flow case is correctly handled. This is the second key finding of the paper. We nevertheless recommend that the regularization procedure of (17) and (18) be implemented for the solution of Darcy-Weisbach head loss networks to avoid loss of accuracy where the $\boldsymbol{F}$ matrix becomes ill–conditioned.

The third issue introduced concerns (i) a new convergence stopping criterion based on the infinity-norm of the nodal heads differences vector from one iteration to the next and (ii) testing of the norms of the energy and continuity residuals vectors after iteration has ceased. The new stopping criterion is recommended because the infinity-norm test is easier to interpret physically than the relative discharge stopping criterion that is currently used in EPANET. The residuals test of (ii) guards against the acceptance of an inaccurate solution.

ACKNOWLEDGMENTS

The authors wish to record their thanks to Tania Clees, Jaroslav Kautsky, David Knight, Angela Marchi, Lewis Rossman and Caren Tischendorf for their insightful discussions and suggestions regarding this work. The authors also wish to acknowledge the assistance of Matt Gibbs.

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APPENDIX A. CONDITIONS FOR THE INVERTIBILITY OF THE JACOBIAN WITH SOME ZERO FLOWS

The Jacobian $\boldsymbol{J}$ of (5) for the Hazen-Williams head loss formulation may be invertible even though the matrix $\boldsymbol{F}$ in (6) is singular. We briefly review here the theorem (Benzi, Golub & Liesen 2005) which underpins the discussion of how zero flows in the system affect the invertibility of the Jacobian matrix.

Provided that $\boldsymbol{F}$ is invertible, the matrix $\boldsymbol{J}$ of (5) admits the factoring

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

where $\boldsymbol{S} = -\boldsymbol{A}_1^T \boldsymbol{F}^{-1} \boldsymbol{A}_1$, and $\boldsymbol{I}_m$ is an m–square identity. Thus, $\det(\boldsymbol{J}) = \det(\boldsymbol{F})\det(\boldsymbol{S})$ and so provided $\boldsymbol{F}$ is invertible then $\boldsymbol{J}$ is invertible if and only if $\boldsymbol{S}$ is invertible.

Recall that a matrix $\boldsymbol{M}$ is said to be

$$\left\{ \begin{array}{c} \text{Positive definite} \\ \text{Non–negative definite} \\ \text{Negative definite} \end{array} \right\} \text{ if } \boldsymbol{x}^T \boldsymbol{M} \boldsymbol{x} \left\{ \begin{array}{c} > 0 \\ \geq 0 \\ < 0 \end{array} \right\} \text{ for all } \boldsymbol{x} \neq \boldsymbol{0}.$$

It follows from these definitions that positive definite and negative definite matrices are invertible and that all the diagonal elements of a positive definite matrix are positive. It also follows that, if all the diagonal elements of $\boldsymbol{F}$ are positive, then $\boldsymbol{S} = -\boldsymbol{A}_1^T \boldsymbol{F}^{-1} \boldsymbol{A}_1$ is negative definite. 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 unknown head node incidence matrix $\boldsymbol{A}_1$ has full column rank (Welsh 1976) and, since $\boldsymbol{F}$ is positive

Journal of Hydraulic Engineering. Submitted October 27, 2009; accepted February 23, 2011;
posted ahead of print February 25, 2011. doi:10.1061/(ASCE)HY.1943-7900.0000411

definite then $\boldsymbol{S}$ 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 $\boldsymbol{S}$ exist and relations (11) and (12) cannot be used. But the singularity of the matrix $\boldsymbol{F}$ does not, of itself, imply the singularity of the Jacobian matrix (5). 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.

Denote by $\ker(\boldsymbol{X})$ the null space of the matrix $\boldsymbol{X}$: it is the space spanned by the set of all vectors $\boldsymbol{y}$ such that $\boldsymbol{X}\boldsymbol{y} = \boldsymbol{0}$.

Theorem 1 *(Benzi et al. 2005) Assume that the diagonal matrix $\boldsymbol{F}$ is non–negative definite and that $\boldsymbol{A}_1$ has full column rank. A necessary and sufficient condition for the matrix $\boldsymbol{J}$ of (5) to be invertible is* $\ker(\boldsymbol{F}) \cap \ker(\boldsymbol{A}_1^T) = \{0\}$.

The intersection of the two nullspaces $\ker(\boldsymbol{F})$ and $\ker(\boldsymbol{A}_1^T)$ is characterized by the nullspace of the $(n_p + n_j) \times n_p$ matrix $\boldsymbol{Z}^T = \begin{pmatrix} \boldsymbol{F}^T & \boldsymbol{A}_1 \end{pmatrix}$. If $\ker(\boldsymbol{Z})$ is empty then the Jacobian matrix is invertible. If more than n_j of the flows, and hence the diagonal elements of $\boldsymbol{F}$, are zero then the nullspace of $\boldsymbol{Z}$ cannot be empty and $\boldsymbol{J}$ is necessarily singular. However, the nullspace of $\boldsymbol{Z}$ may be non-empty (and hence $\boldsymbol{J}$ may be singular) for some particular combinations of incidence matrix $\boldsymbol{A}_1$ and zero flows even though there are fewer than n_j zero flows.

APPENDIX B. AN UPPER BOUND ON THE CONDITION OF $\boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1$

Before proving the bound given in (19) we briefly review some theory which is necessary for the sequel. For a detailed treatment of the theory see Golub & Van Loan (1989).

Let the full column–rank matrix $\boldsymbol{A} \in \mathbb{R}^{m\times k}$, $m > k$, have singular value decomposition (SVD) $\boldsymbol{A} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T$, $\boldsymbol{U} \in \mathbb{R}^{m\times m}$, orthogonal, $\boldsymbol{V} \in \mathbb{R}^{k\times k}$, orthogonal and $\boldsymbol{S} = \text{diag}\{\sigma_1, \sigma_2, \ldots, \sigma_k\} \in \mathbb{R}^{m\times k}$, $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_k > 0$. The σ_i are called the *singular values* of $\boldsymbol{A}$. Denote by $\sigma_{min}(\boldsymbol{A})$ the smallest singular value of $\boldsymbol{A}$ and by $\sigma_{max}(\boldsymbol{A})$ the largest singular value of $\boldsymbol{A}$.

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posted ahead of print February 25, 2011. doi:10.1061/(ASCE)HY.1943-7900.0000411

The matrix 2–norm, $\|\boldsymbol{A}\|_2$, induced by the vector 2–norm, $\|\boldsymbol{x}\|_2 = \sqrt{\boldsymbol{x}^T\boldsymbol{x}}$, is defined by

$$\|\boldsymbol{A}\|_2 \stackrel{\text{def}}{=} \sup_{\boldsymbol{x}\neq\boldsymbol{o}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} = \max_{\|\boldsymbol{x}\|_2=1} \|\boldsymbol{A}\boldsymbol{x}\|_2 = \sigma_1(\boldsymbol{A}) = \sigma_{max}(\boldsymbol{A}). \tag{B-1}$$

From this definition it follows that $\left\|\boldsymbol{A}^{-1}\right\|_2 = 1/\sigma_{min}$. It also holds that

$$\sigma_{min}(\boldsymbol{A}) = \sigma_k(\boldsymbol{A}) = \inf_{\boldsymbol{x}\neq\boldsymbol{o}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_2}{\|\boldsymbol{x}\|_2} = \min_{\|\boldsymbol{x}\|_2=1} \|\boldsymbol{A}\boldsymbol{x}\|_2 . \tag{B-2}$$

For square, invertible matrices we define $\text{cond}_2(\boldsymbol{A}) \stackrel{\text{def}}{=} \|\boldsymbol{A}\|_2 \left\|\boldsymbol{A}^{-1}\right\|_2$ and, in view of (B-1), we can write

$$\text{cond}_2(\boldsymbol{A}) = \sigma_1(\boldsymbol{A})/\sigma_{\text{k}}(\boldsymbol{A}) = \sigma_{\max}(\boldsymbol{A})/\sigma_{\min}(\boldsymbol{A}). \tag{B-3}$$

In fact, (B-3) is used to extend the definition of condition number to apply to non–square matrices (where standard inverses do not exist). Using the SVD of $\boldsymbol{A}$ we can write $\boldsymbol{A}^T\boldsymbol{A} = \boldsymbol{V}\boldsymbol{S}^T\boldsymbol{U}^T\boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^T = \boldsymbol{V}\boldsymbol{S}^T\boldsymbol{S}\boldsymbol{V}^T$ and immediately $\text{cond}_2(\boldsymbol{A}^{\text{T}}\boldsymbol{A}) = (\sigma_{\max}/\sigma_{\min})^2$.

Let us now return to the bound shown in (19). Since $\boldsymbol{F}+\boldsymbol{T}$ has only positive elements on the diagonal, there exists a matrix, $\boldsymbol{M}$, also with positive elements on the diagonal and such that $\boldsymbol{M}^2 = (\boldsymbol{F}+\boldsymbol{T})^{-1}$. Hence, $\boldsymbol{A}_1^T(\boldsymbol{F}+\boldsymbol{T})^{-1}\boldsymbol{A}_1 = (\boldsymbol{M}\boldsymbol{A}_1)^T\boldsymbol{M}\boldsymbol{A}_1$ and so $\text{cond}\left((\boldsymbol{M}\boldsymbol{A}_1)^{\text{T}}\boldsymbol{M}\boldsymbol{A}_1\right) = \text{cond}_2(\boldsymbol{M}\boldsymbol{A}_1)^2$ so let us consider the matrix $\boldsymbol{M}\boldsymbol{A}_1$ in isolation.

Lemma 1 *(Kautsky) Suppose* $\boldsymbol{M} \in \mathbb{R}^{m\times m}$ *and* $\boldsymbol{A} \in \mathbb{R}^{m\times k}$ *both have full column–rank. Then*

$$\text{cond}_2(\boldsymbol{M}\boldsymbol{A}) \le \text{cond}_2(\boldsymbol{M})\text{cond}_2(\boldsymbol{A}).$$

Proof

We omit the subscripts on norms since only the 2–norm is used here.

From (B-2) we have $\sigma_{min}(\boldsymbol{M}\boldsymbol{A}) = \min_{\|\boldsymbol{y}\|=1}\|\boldsymbol{M}\boldsymbol{A}\boldsymbol{y}\|$. Suppose this minimum is achieved on the vector $\boldsymbol{y}_1$, $\|\boldsymbol{y}_1\| = 1$, ie. $\sigma_{min}(\boldsymbol{M}\boldsymbol{A}) = \|\boldsymbol{M}\boldsymbol{A}\boldsymbol{y}_1\|$. Also, $\sigma_{min}(\boldsymbol{A}) = \min_{\|\boldsymbol{y}\|=1}\|\boldsymbol{A}\boldsymbol{y}\| \le \|\boldsymbol{A}\boldsymbol{y}_1\|$. Now,

$$\sigma_{min}(\boldsymbol{M}) = \inf_{\boldsymbol{y}\neq\boldsymbol{o}} \frac{\|\boldsymbol{M}\boldsymbol{y}\|}{\|\boldsymbol{y}\|} \le \frac{\|\boldsymbol{M}\boldsymbol{A}\boldsymbol{y}_1\|}{\|\boldsymbol{A}\boldsymbol{y}_1\|} \le \frac{\sigma_{min}(\boldsymbol{M}\boldsymbol{A})}{\sigma_{min}(\boldsymbol{A})}.$$

Thus,

$$\sigma_{min}(\boldsymbol{M}\boldsymbol{A}) \ge \sigma_{min}(\boldsymbol{A})\,\sigma_{min}(\boldsymbol{M}). \tag{B-4}$$

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Turning to the largest singular values, we have $\sigma_{max}(\boldsymbol{MA}) = \max_{\|\boldsymbol{y}\|=1} \|\boldsymbol{MAy}\|$. Suppose this maximum is realized with the vector $\boldsymbol{y}_2$, $\sigma_{max}(\boldsymbol{MA}) = \|\boldsymbol{MAy}_2\|$. Similarly, $\sigma_{max}(\boldsymbol{A}) = \max_{\|\boldsymbol{y}\|=1} \|\boldsymbol{Ay}\| \geq \|\boldsymbol{Ay}_2\|$. Also,

$$\sigma_{max}(\boldsymbol{M}) = \sup_{\boldsymbol{y} \neq \boldsymbol{o}} \frac{\|\boldsymbol{My}\|}{\|\boldsymbol{y}\|} \geq \frac{\|\boldsymbol{MAy}_2\|}{\|\boldsymbol{Ay}_2\|} \geq \frac{\sigma_{max}(\boldsymbol{MA})}{\sigma_{max}(\boldsymbol{A})}$$

from which it follows that

$$\sigma_{max}(\boldsymbol{MA}) \leq \sigma_{max}(\boldsymbol{M})\, \sigma_{max}(\boldsymbol{A}) . \tag{B-5}$$

Putting together (B-4) and (B-5) we get

$$\frac{\sigma_{max}(\boldsymbol{MA})}{\sigma_{min}(\boldsymbol{MA})} \leq \frac{\sigma_{max}(\boldsymbol{M})\, \sigma_{max}(\boldsymbol{A})}{\sigma_{min}(\boldsymbol{M})\, \sigma_{min}(\boldsymbol{A})}$$

which is the statement of the lemma. This completes the proof.

Thus, we see, noting that $\boldsymbol{M}$ is diagonal, that

$$\begin{aligned} \text{cond}_2(\boldsymbol{MA})^2 &\leq \text{cond}_2(\boldsymbol{M})^2 \text{cond}_2(\boldsymbol{A})^2 \\ &= \text{cond}_2(\boldsymbol{M}^2) \text{cond}_2(\boldsymbol{A})^2 \\ &= \text{cond}_2((\boldsymbol{F}+\boldsymbol{T})^{-1}) \text{cond}_2(\boldsymbol{A})^2. \end{aligned}$$

In summary, we can write

$$\text{cond}_2(\boldsymbol{A}_1^{\mathrm{T}} (\boldsymbol{F}+\boldsymbol{T})^{-1} \boldsymbol{A}_1) \leq \text{cond}_2((\boldsymbol{F}+\boldsymbol{T})^{-1}) \text{cond}_2(\boldsymbol{A}_1)^2.$$

APPENDIX C. NOMENCLATURE

$\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \boldsymbol{D}$ = arbitrary matrices

$\|\boldsymbol{A}\|_2$ = matrix 2–norm

$\boldsymbol{A}_1$ = unknown head node incidence matrix

$\boldsymbol{A}_2$ = fixed head node incidence matrix

A_j = area of pipe j

C_j = the Hazen-Williams head loss coefficient of pipe j

$\text{cond}_2(\boldsymbol{A})$ = 2–norm condition number of matrix $\boldsymbol{A}$

D_j = diameter of pipe j

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$\boldsymbol{d}_m$ = vector of nodal demands

$\boldsymbol{e}_\ell$ = vector of fixed head node elevations

$\boldsymbol{F}$ = diagonal matrix (1,1) block of the full Jacobian

f_j = Darcy-Weisbach friction factor for pipe j

$\boldsymbol{G}$ = diagonal matrix with elements r_L or $r_j|Q_j|^{n-1}$

GGA = Global Gradient Algorithm

g = gravitational acceleration constant

H_i = head at node i

$\boldsymbol{h} = (H_1, H_2, \ldots, H_{n_j})^T$ = vector of heads

$\boldsymbol{I}_k$ = k–square identity matrix

$\boldsymbol{J}$ = Jacobian matrix

L_j = length of pipe j

$\boldsymbol{M}$ = defined by $\boldsymbol{M}^2 = (\boldsymbol{F} + \boldsymbol{T})^{-1}$

n = head loss equation exponent

n_f = number of fixed–head nodes

n_j = number of variable–head nodes

n_p = number of pipes

$\boldsymbol{O}$ = n_j–square zero matrix

$\boldsymbol{o}$ = $n_p \times n_j$ zero matrix

$\boldsymbol{0}$ = an n_p–vector of zeros

p_j = pipe j

Q_j = flow in pipe j

$\boldsymbol{q} = (Q_1, Q_2, \ldots, Q_{n_p})^T$ = vector of flows

$\mathcal{R}$ = Reynolds number for pipe j, $\mathcal{R} = V_j D_j / \nu$

$\boldsymbol{r} = (r_1, r_2, \ldots, r_{n_p})^T$ = vector of resistance factors

r_j = resistance factor for pipe j with turbulent flow

r_L = resistance factor for pipe with laminar flow

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$\boldsymbol{S} = -\boldsymbol{A}_1^T \boldsymbol{F}^{-1} \boldsymbol{A}_1$ = Schur complement for the discussion of the invertibility of the Jacobian matrix

$\boldsymbol{T} = \text{diag}\left\{t_1, t_2, \ldots, t_{n_p}\right\}$ diagonal regularization matrix

$\boldsymbol{U}$ = orthogonal matrix in the singular value decomposition

u_1, u_2 = constants used in setting the residuals thresholds test

$\boldsymbol{V}$ = matrix for GGA ($= \boldsymbol{A}_1^T \boldsymbol{F}^{-1} \boldsymbol{A}_1$) or an orthogonal matrix in the singular value decomposition

V_j = average fluid velocity for pipe j

$\boldsymbol{W} = \boldsymbol{A}_1^T (\boldsymbol{F} + \boldsymbol{T})^{-1} \boldsymbol{A}_1$ = matrix used in the regularization method

$\boldsymbol{X}$ = arbitrary matrix

$\boldsymbol{x} = \begin{pmatrix} \boldsymbol{q} \\ \boldsymbol{h} \end{pmatrix}$

$\|\boldsymbol{x}\|_2$ = vector 2–norm = $\sqrt{\boldsymbol{x}^T \boldsymbol{x}}$

$\|\boldsymbol{x}\|_\infty$ = vector ∞–norm = $\max_j |x_j|$

$\boldsymbol{y}$ = arbitrary vector

$\boldsymbol{Z} = \begin{pmatrix} \boldsymbol{F} \\ \boldsymbol{A}_1^T \end{pmatrix}$

δ_{stop} = EPANET stopping tolerance

ϵ_j = roughness height of pipe j

ϵ_{mach} = machine epsilon

ϵ_{stop} = infinity norm stopping tolerance for heads in iterative solution termination test

k = maximum threshold condition number

ν = kinematic viscosity of water

ϕ^E = EPANET stopping test measure

ϕ^∞ = infinity–norm stopping test measure

$\rho_c(\boldsymbol{q}, \boldsymbol{h})$ the vector of continuity residuals

$\rho_e(\boldsymbol{q}, \boldsymbol{h})$ the vector of energy residuals

σ_i = diagonal element of matrix $\boldsymbol{F}$

σ_{max} = maximum diagonal element of matrix $\boldsymbol{F}$

σ_{min} = minimum diagonal element of matrix $\boldsymbol{F}$

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APPENDIX D. TABLES

Table 1: The convergence data for network shown in Figure 1 with the Hazen-Williams head loss model and no regularization ((11) and (12)). At each iteration the accuracy achieved in the heads is entirely consistent, for IEEE standard double precision arithmetic (20), with the size of the condition number of $\boldsymbol{V}$. Note that the residal norms in Columns 3 and 4 are displayed here for information but are not necessary at each iteration. Only the residuals of the final iteration need to be examined to exclude inaccurate solutions.

Hazen-Williams head loss model

m	$\phi^{\infty}(\boldsymbol{h}^{(m)})$	$\left\|\rho_e^{(m)}\right\|_\infty$	$\left\|\rho_c^{(m)}\right\|_\infty$	$\phi^E(\boldsymbol{q}^{(m)})$	$\mathrm{cond}_2(\boldsymbol{F}^{(\mathrm{m})})$	$\mathrm{cond}_2(\boldsymbol{V}^{(\mathrm{m})})$
1	$3.8e+001$	$3.3e+000$	$3.8e-016$	$7.4e-001$	$1.0e+000$	$3.6e+001$
2	$4.4e+000$	$2.4e-002$	$6.5e-016$	$5.2e-002$	$2.5e+001$	$3.2e+002$
3	$2.0e-002$	$2.2e-005$	$1.2e-014$	$1.2e-003$	$3.3e+002$	$4.4e+003$
4	$1.0e-005$	$3.5e-010$	$3.3e-012$	$2.7e-006$	$5.1e+004$	$6.6e+005$
5	$3.8e-006$	$6.1e-013$	$1.6e-008$	$1.5e-007$	$5.6e+008$	$7.3e+009$
6	$2.4e-005$	$1.7e-011$	$6.4e-008$	$1.1e-006$	$1.1e+009$	$1.4e+010$
7	$2.6e-005$	$1.8e-011$	$2.5e-008$	$1.1e-006$	$2.1e+009$	$2.7e+010$
8	$2.0e-005$	$1.4e-011$	$1.1e-007$	$8.1e-007$	$4.1e+009$	$5.3e+010$
9	$4.9e-005$	$9.6e-011$	$2.7e-007$	$2.0e-006$	$7.8e+009$	$1.0e+011$
10	$7.4e-005$	$2.0e-010$	$9.3e-009$	$3.0e-006$	$1.5e+010$	$2.0e+011$
11	$9.4e-005$	$5.0e-009$	$1.7e-006$	$8.0e-006$	$2.9e+010$	$3.9e+011$
12	$5.9e-005$	$4.2e-009$	$3.1e-007$	$6.6e-006$	$5.7e+010$	$7.5e+011$
13	$6.2e-004$	$2.1e-007$	$9.4e-006$	$4.1e-005$	$1.1e+011$	$1.5e+012$
14	$6.5e-004$	$1.8e-007$	$1.6e-008$	$4.3e-005$	$2.2e+008$	$2.9e+009$
15	$8.7e-006$	$1.5e-012$	$8.4e-009$	$3.6e-007$	$4.3e+008$	$5.6e+009$
16	$1.2e-005$	$2.7e-012$	$4.7e-008$	$4.8e-007$	$8.2e+008$	$1.1e+010$
17	$8.0e-006$	$2.8e-011$	$8.2e-008$	$4.8e-007$	$1.6e+009$	$2.1e+010$
18	$1.9e-005$	$7.9e-011$	$1.0e-007$	$1.1e-006$	$3.1e+009$	$4.1e+010$
19	$8.2e-006$	$6.4e-011$	$4.7e-008$	$6.0e-007$	$9.1e+008$	$1.2e+010$
20	$2.2e-005$	$1.2e-011$	$4.8e-008$	$9.1e-007$	$1.8e+009$	$2.3e+010$

Journal of Hydraulic Engineering. Submitted October 27, 2009; accepted February 23, 2011;
posted ahead of print February 25, 2011. doi:10.1061/(ASCE)HY.1943-7900.0000411

Table 2: The convergence data for network shown in Figure 1 with the Hazen-Williams head loss model and the regularization method (17) and (18) applied. Rapid convergence is restored by the regularization. Note that the residal norms in Columns 3 and 4 are displayed here for information but are not necessary at each iteration. Only the residuals of the final iteration need to be examined to exclude inaccurate solutions.

Hazen-Williams head loss model

m	$\phi^\infty(\boldsymbol{h}^{(m)})$	$\left\|\rho_e^{(m)}\right\|_\infty$	$\left\|\rho_c^{(m)}\right\|_\infty$	$\phi^E(\boldsymbol{q}^{(m)})$	$\text{cond}_2(\boldsymbol{F}^{(\text{m})} + \boldsymbol{T}^{(\text{m})})$	$\text{cond}_2(\boldsymbol{W}^{(\text{m})})$
1	$3.8e+001$	$3.3e+000$	$3.8e-016$	$7.4e-001$	$1.0e+000$	$3.6e+001$
2	$4.4e+000$	$2.4e-002$	$6.5e-016$	$5.2e-002$	$2.5e+001$	$3.2e+002$
3	$2.0e-002$	$2.2e-005$	$1.2e-014$	$1.2e-003$	$3.3e+002$	$4.4e+003$
4	$1.0e-005$	$3.5e-008$	$5.6e-014$	$2.7e-006$	$1.0e+003$	$1.3e+004$
5	$1.1e-008$	$5.9e-011$	$4.7e-014$	$4.5e-009$	$1.0e+003$	$1.3e+004$
6	$2.1e-011$	$1.0e-013$	$5.0e-014$	$7.5e-012$	$1.0e+003$	$1.3e+004$

Table 3: The convergence data for the network shown in Figure 1 with the Hazen-Williams head loss model when the full matrix system (10) is solved directly at each iteration. Note that the residal norms in Columns 3 and 4 are displayed here for information but are not necessary at each iteration. Only the residuals of the final iteration need to be examined to exclude inaccurate solutions.

Hazen-Williams head loss model

m	$\phi^\infty(\boldsymbol{h}^{(m)})$	$\left\|\rho_e^{(m)}\right\|_\infty$	$\left\|\rho_c^{(m)}\right\|_\infty$	$\phi^E(\boldsymbol{q}^{(m)})$	$\text{cond}_2(\boldsymbol{J}^{(\text{m})})$
1	$3.8e+001$	$5.6e+001$	$6.2e-002$	$7.4e-001$	$2.9e+004$
2	$4.4e+000$	$3.3e+000$	$1.4e-017$	$5.2e-002$	$1.6e+005$
3	$2.0e-002$	$2.4e-002$	$1.7e-017$	$1.2e-003$	$1.6e+005$
4	$1.0e-005$	$2.2e-005$	$9.8e-018$	$2.7e-006$	$1.6e+005$
5	$1.4e-010$	$3.5e-010$	$1.4e-017$	$4.5e-011$	$1.6e+005$
6	$3.6e-015$	$6.2e-015$	$9.8e-018$	$2.2e-017$	$1.6e+005$

Table 4: The steady state flows and heads for the network shown in Figure 1 for the solution in Table 2.

Hazen-Williams head loss model

i/j	Flow (L/s) in pipe j	Head (m) at node i
1	$4.0000e-002$	40.0000
2	$1.9973e-014$	36.6813
3	$4.0000e-002$	36.6813
4	$4.0000e-002$	33.3626
5	$4.0000e-002$	33.3626
6	$3.0562e-014$	30.0440
7	$4.0000e-002$	30.0440
8	$4.0000e-002$	26.7253
9	$-1.9743e-014$	–
10	$4.0000e-002$	–
11	$4.0000e-002$	–

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Table 5: The elements $[\boldsymbol{F}]_{jj}$ on the diagonal of the $\boldsymbol{F}$ matrix for two pipes using the Darcy-Weisbach head loss model and with the parameters shown. Their ratio is a lower bound on the condition of the matrix $\boldsymbol{F}$.

Darcy-Weisbach head loss model

Pipe	$L(m)$	$D(m)$	$\epsilon(m)$	$Q(m^3/s)$	$V(m/s)$	$\mathcal{R}$	$[\boldsymbol{F}]_{jj}$
1	$1.0e+003$	$1.0e-001$	$2.5e-004$	$1.0e-001$	$1.3e+001$	$1.3e+006$	$4.1e+004$
2	$1.0e+000$	$3.0e+000$	$2.5e-004$	$1.0e-002$	$1.4e-003$	$4.2e+003$	$2.7e-007$

LIST OF CAPTIONS FOR TABLES AND FIGURES

Table 1. The convergence data for network shown in Figure 1 with the Hazen-Williams head loss model and no regularization ((11) and (12)). At each iteration the accuracy achieved in the heads is entirely consistent, for IEEE standard double precision arithmetic (20), with the size of the condition number of $\boldsymbol{V}$. Note that the residal norms in Columns 3 and 4 are displayed here for information but are not necessary at each iteration. Only the residuals of the final iteration need to be examined to exclude inaccurate solutions.

Table 2. The convergence data for network shown in Figure 1 with the Hazen-Williams head loss model and the regularization method (17) and (18) applied. Rapid convergence is restored by the regularization. Note that the residal norms in Columns 3 and 4 are displayed here for information but are not necessary at each iteration. Only the residuals of the final iteration need to be examined to exclude inaccurate solutions.

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Figure 1. The network discussed in Example 1 and Example 2. $n_p = 11$, $n_j = 7$ and $n_f = 1$. Pipes 5 and 8 are removed for Example 2.

Figure: zlad.pdf

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