Why are Line Search Methods Needed for Hydraulic DDM and PDM Solvers?

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ABSTRACT

It is common that non-convergence problems occur for simulations under normal or abnormal operations. Among the main causes, there are the use of sublinear functions for calculation of the hydraulic steady-state, some derivative issues and an ill-conditioned iteration matrix in the solution method. The objective of this paper is to specify non-convergence cases for existing hydraulic software solutions. The damped Newton solution together with regularization techniques are proposed for ensuring global convergence, whatever the initial solution. Failures of convergence are shown to exist even on small case studies.

Keywords: Steady state modelling; Convergence; Inexact line search method

1 BACKGROUND

Hydraulic solvers have been used for least-cost design [1-2], sampling design [3-5], calibration, state estimation, sensitivity and uncertainty analysis [6-8], monitoring and security [9-11], operation management and optimisation [12-13], vulnerability and resilience analysis [14-15] of water distribution networks amongst other applications. It is common that non-convergence problems occur for simulations under normal or abnormal operations, especially in the case of insufficient water supply resources, loss of connectivity, small and large diameter pipes, any of which may lead to fully inconsistent hydraulic predictions and may bias decision-making. The objective of this paper is to characterize some non-convergence cases for existing hydraulic software solutions. It is important for an understanding of how to overcome the problem and how to improve solution software toward attaining global convergence. Firstly, a convergence analysis of existing demand-driven modelling (DDM) and pressure-driven modelling (PDM) solvers is provided. Failures of convergence are shown to exist even on small case studies. Then, the damped Newton solution is recommended for the minimization of a suitably framed optimisation problem. Finally, the advantages of the proposed method are illustrated on small case studies

2 CHARACTERIZATION OF NON-CONVERGENCE CASES

Let $\mathbf{x}$ be the hydraulic steady-state satisfying the mass and energy balance equations for a given network model and under some known energy and water demand conditions. The problem of calculating the n hydraulic state variables, x_i consists of finding the zeros of a nonlinear function $\mathbf{F}$:

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}_n \tag{1}$$

The Global Gradient Algorithm (GGA) by Todini and Pilati (1988) is an example of Newton method that is implemented in EPANET [16] and the Newton method has been found to be one of the most efficient solution methods to solve Eq. (1) [17]. The main reasons are that the derivatives exist almost everywhere (it depends on network component head loss equations used), the Jacobian matrix involved in the linear systems to solve at each iteration is particularly sparse, and in most of the cases the convergence is at least quadratic in a neighbourhood of the zero, which, roughly speaking, means that the number of correct digits at least doubles in every step [18]. Nevertheless, several cases of non-convergence or slow convergence can occur in the hydraulic solution process. The main causes are reported below.

2.1 Sublinear functions

When the hydraulic Eq. (1) involves some sublinear functions of the hydraulic state, the Newton method tends to overshoot. Examples of sublinear functions are the inverse pipe head loss equation involved in the nodal head equations, the orifice equation for leakage outflow prediction or even the inverse power equation with an exponent greater than one. This was observed by several authors and the introduction of an under-relaxation factor in the Newton iteration was found to solve the problem in most circumstances [17,19-22].

2.2 Derivative issues

If the derivative is not defined or even not continuous near or at the solution, the Newton method may fail or the rate of convergence may not be longer quadratic. The convergence may also drop to linear if the function zero has multiplicity higher than one in some dimensions. The first condition arises for the zero flow solutions with the Hazen-Williams head-loss formula and the GGA algorithm [23]. It also occurs with the Wagner function as a Pressure Outflow Relationship (POR) in the pressure-driven model formulation [24]. Regularisation techniques have been used and appear very efficient [23-24].

2.3 Ill-conditioned Jacobian matrix

The Newton method performs a scaling of the equations; therefore, in most model configurations it is robust. But, if there are several orders of magnitude difference in coefficients in Eq. (1), the problem is ill-conditioned. Tank regulation and valves being partially closed may generate very large friction coefficients, which in presence of small diameter pipes makes the problem difficult to solve if the initial solution is far from the exact solution. To improve the condition of the Jacobian, one strategy is to remove closed valves in the network graph (it is used in EPANET). The latter has the disadvantage of changing the topology of the network and it does not necessarily adequately deal with all the network configurations (there exist networks without valves and with large and small resistance coefficients).

The damped Newton method is a Newton method that considers a damping or relaxation parameter that presents the following advantages: under- and over- relaxations are possible and some sufficient conditions exist that guarantee the global convergence no matter what the value of the initial solution is.

3 THE DAMPED NEWTON METHOD

Starting from an initial guess $\mathbf{x}^0$, the method solves a linear system to obtain the Newton direction, then an inexact line search is carried out until some condition holds true. Let $\mathbf{x}^k$ be the k^{th}-estimate and $\boldsymbol{\delta}_x\mathbf{F}^k$ be the Jacobian of $\mathbf{F}$ at $\mathbf{x}^k$. At iteration k, the following linear system is solved for the Newton direction:

$$(\boldsymbol{\delta}_x\mathbf{F}^{k-1})[\mathbf{d}^k] = -\mathbf{F}(\mathbf{x}^{k-1}) \tag{2}$$

Then the Newton direction $\mathbf{d}^k$ is used with some choice of a damping factor $\rho_{k,m}$, where m is the number of attempts at the line search:

$$\mathbf{x}^{k,m} = \mathbf{x}^{k-1} + \rho_{k,m}\mathbf{d}^k, k \in \mathbb{N}^*, m \in \mathbb{N}^* \tag{3}$$

The $\rho_{k,m}$ helps reduce sufficiently a suitable criterion *f* in the Newton direction (*e.g.* the weighted sum of the mass and energy residuals squared). The strategy introduced by Goldstein for inexact line search may be adopted as in [25] as long as $\mathbf{d}^k$ is a direction of descent for *f*. The tangent line to the curve $f(\mathbf{x}^{k-1} + \rho\mathbf{d}^k)$ at $\rho = 0$ is given by $\tau(\rho) = f(\mathbf{x}^{k-1}) + \rho\boldsymbol{\nabla} f(\mathbf{x}^{k-1})^T\mathbf{d}^k$. Let us define the family of lines:

$$L_\mu(\rho) = f(\mathbf{x}^{k-1}) + \mu\rho\boldsymbol{\nabla} f(\mathbf{x}^{k-1})^T\mathbf{d}^k, \text{ with } 0 \le \mu \le 1 \tag{4}$$

The Goldstein principle (see Figure 1) states that ρ should be chosen such that the point $(\rho; f(\mathbf{x}^{k,m}))$ lies between the two lines $L_\sigma(\rho)$ *and* $L_{1-\sigma}(\rho)$ for a fixed $\sigma > 0$. This ensures that there is sufficient descent and that it departs significantly from zero.

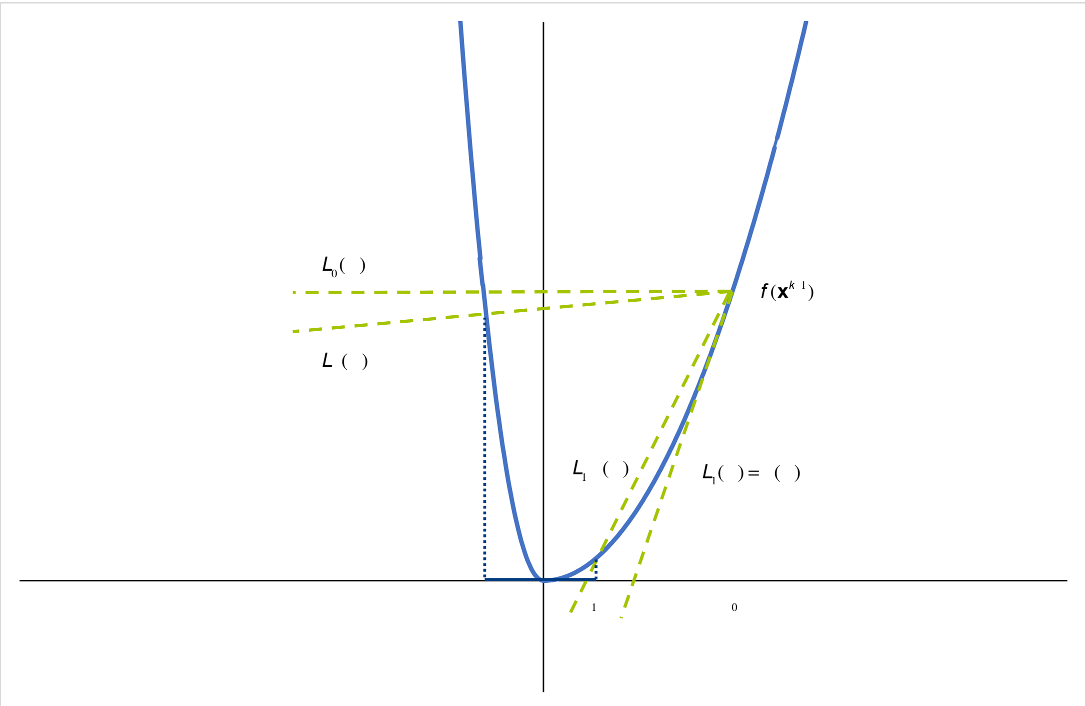

Figure 1. Illustration of the Goldstein principle – the x-axis is ρ; the blue curve is the f criterion to minimize along the line search.

For that purpose, the Goldstein index is calculated and $\rho_{k,m}$ is adjusted repeatedly until it falls in the range $[\sigma, 1-\sigma]$:

$$0 < \sigma \le \frac{f(\mathbf{x}^{k-1}) - f\left(\mathbf{x}^{k-1} + \rho_{k,m}\mathbf{d}^k\right)}{\rho_{k,m}\boldsymbol{\nabla} f(\mathbf{x}^{k-1})^T\mathbf{d}^k} \le 1 - \sigma \tag{5}$$

The Goldstein rule Eq. (5) includes the Armijo rule and a simpler curvature condition than is in the Wolfe conditions for performing an inexact line search. Ideally, this index is 0.5 and f does not need to be convex. One possible implementation is to start with $\rho_{k,1} = 1$ and to increase or decrease the value until the Goldstein condition Eq. (5) holds.

4 ILLUSTRATION OF THE CONVERGENCE

In the context of the ResiWater project [26], we are pushing further the limits of existing hydraulic solutions, because we must deal with fully or partially disconnected components following critical events such as a natural disaster or a terrorist attack. PDM models are used with the Wagner function and the failure mode is likely to occur at nodes with negative pressures. The first example closely examines the interest of regularisation of the Wagner function. The second example demonstrates that in the case of insufficient water supply resources, the undamped Newton method does not converge while the damped version does.

4.1 Interest of regularization techniques

The example network one (see Fig. 2) consists of one single pipe of length 500 m, diameter 150 mm and HW C-factor 100 (the resistance coefficient for the flow rate in L/s is r_q = 0.03023). The tank node R1 is empty and the head at this source node is 120 m.

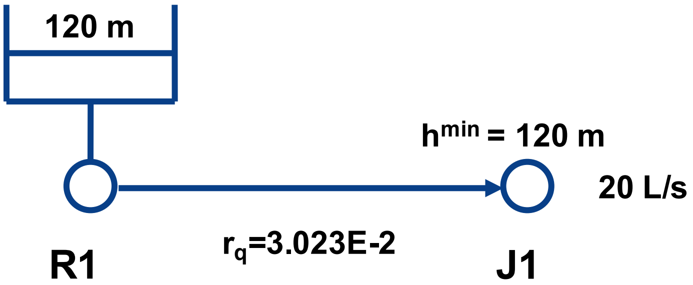

Figure 2. Network #1; one single pipe supplying the junction J1 with demand at d = 20 L/s from tank node R1; the tank is low and there is not enough pressure at J1.

For a Pressure Dependent Modelling (PDM), several pressure outflow relationship functions can be defined [25]. The most commonly used is perhaps the Wagner function (the dark blue curve in Figure 3). The derivative is not defined at z = 0. When using the damped Newton algorithm from [25] on the example network #1, it converges in 44 iterations to (q = 0 L/s; h_{J1} = 120 and the actual delivered demand of c = 0.0 L/s). The convergence rate is merely linear. Adopting a regularization technique around the z = 0 value to avoid the derivative not being defined (such as in [24]), leads to a quadratic rate of convergence and only 8 iterations are needed. Only a small loss of accuracy is suffered: when the regularized Wagner is used, the final solution is q = 0 L/s; h_{J1} = 120 and the actual delivered demand is c = 0.2 L/s. It should be noted here that a regularized Hazen-Williams function was used as well.

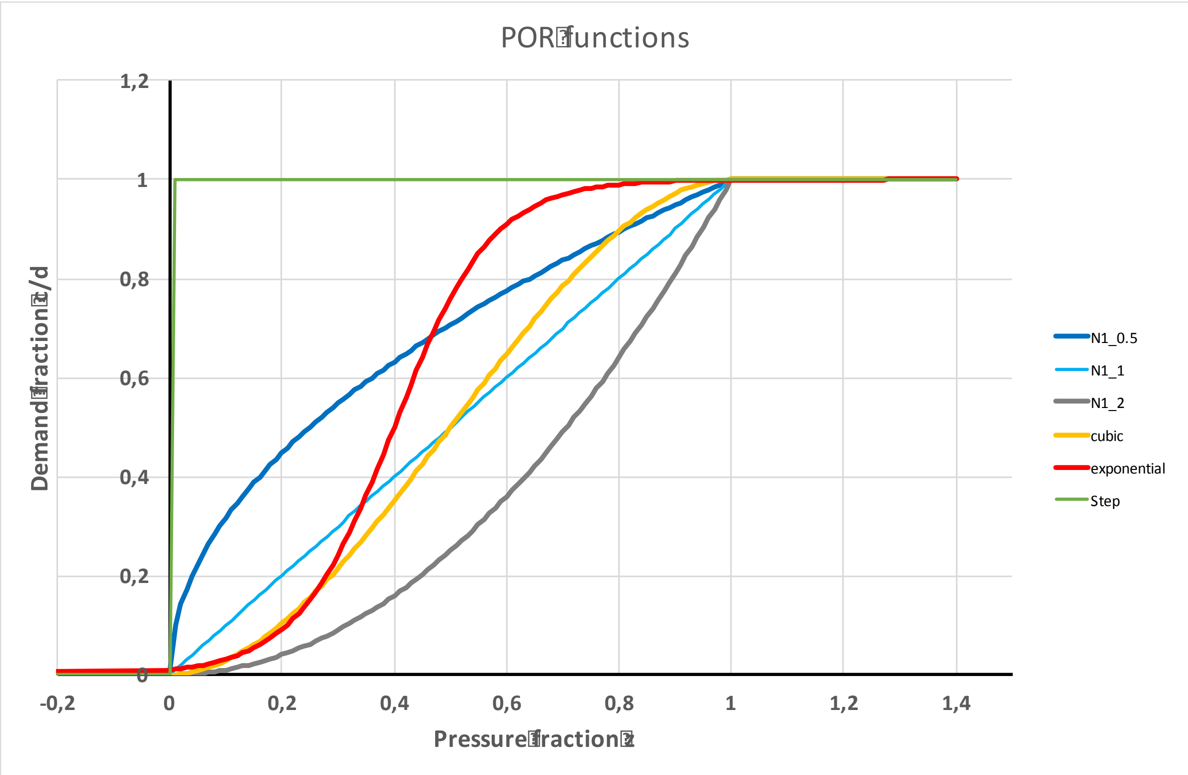

Figure 3. Examples of POR functions; the dark blue curve is the Wagner function; red is exponential; light blue and grey are power equations; yellow is cubic; and green is the step Heaviside function.

4.2 Interest of the Damping factor

The second network example was taken from [25] and is shown in Figure 4. The pipe and node characteristics are as in [25] except for the reservoir head and the demands. The Darcy-Weisbach formula was used for the head loss calculation. It has a single reservoir at elevation 7.62 m, which is insufficient to supply all the demand nodes, and all nodal demands were magnified by a factor 20 to change the problem into a dramatic PDM problem. The original non-regularized Wagner POR and the cubic functions (see Figure 3) have been used with the original PDM Newton method of [25] without the damping factor. The first one is not continuously differentiable in $z = 0$ and $z = 1$ but the cubic is.

For both POR options the Newton method has not converged after 50 iterations. The relative difference in heads between iterates oscillates between 1 to 3 as illustrated in Figure 5.

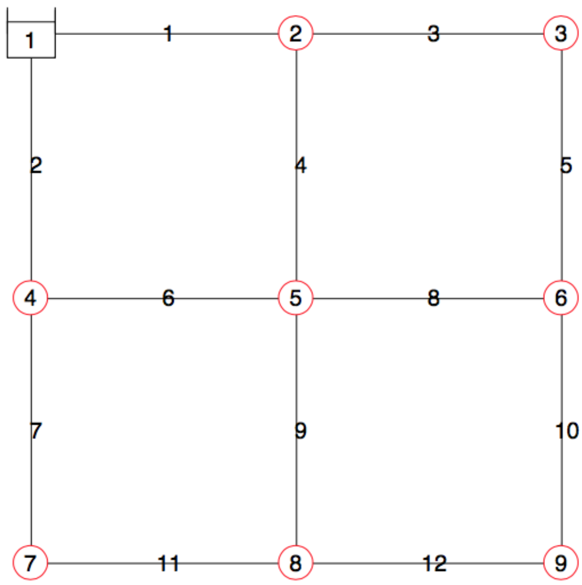

Figure 4. Network example #2 with a four-loop network. The pipe and node characteristic are similar to [25]; the reservoir node is changed to 7.62 m and the demand are magnified by 20.

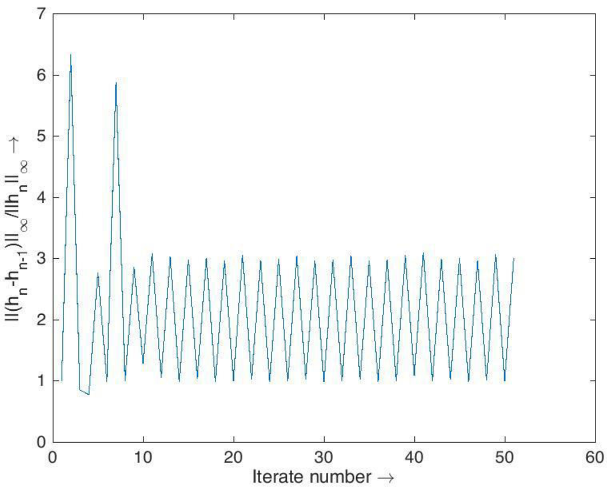

Figure 5. Non-convergent behaviour for the example network #2; the relative difference in the nodal heads between iterations is oscillating when using the Newton method.

The damped Newton converged in 20 iterations for the Wagner POR function. After 17 iterations, the relative difference in head is less than $1x10^{-4}$ and at iteration 20 it is $1.2x10^{14}$. For the three last iterations, the quadratic convergence behaviour is evident. Five of the seven nodes are in total failure mode (with $d>0$ and $c(h)=0$) and the other two nodes have a reduced consumption ($0<c(h)<d$). Similar results were obtained using the cubic POR function.

5 CONCLUSIONS

The objective of this presentation is to raise awareness about non-convergence cases for demand-driven and pressure-driven steady state simulations within normal and abnormal operations. The three following problematic cases have been identified:

- Use of sublinear hydraulic component functions (this is often a square-root-like function);

- The component functions are not differentiable at some points or the derivative is not continuous;
- The Jacobian of the system is ill-conditioned (large and small head loss coefficients involved).

The damped Newton method has been explained using the inexact linear search of the Goldstein principle.

Two small examples are provided to illustrate the impact of regularization techniques (that avoids the derivative issue) and of the damped Newton method (for global convergence).

This research work was led partially in the ResiWater project for which one of the main objectives is to develop robust hydraulic models even in the presence of large disconnected network sections. The research is ongoing with consideration of control valves and numerous hydraulic state constraints for such critical network operations.

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