Automatic generation of a symbolic Jacobian of non-linear equations

C. Garneau[1], Claeys F.H.A[2], Vanrolleghem P.A.[1*]

[1]modelEAU, Département de génie civil et de génie des eaux, Université Laval, 1060 Avenue de la Médecine, Québec, QC, G1V 0A6, Canada

[2]DHI, Guldensporenpark 104 block K, B-9820 Merelbeke, Belgium

* peter.vanrolleghem@gci.ulaval.ca

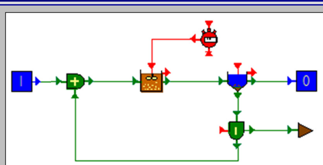
Introduction

Large and stiff water and wastewater quality models require important computing power. Using symbolic manipulation to compute the Jacobian of these models offers more accurate and faster computations at small cost.

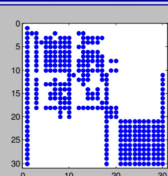
Objectives

- Implement a symbolic tool to compute symbolic partial derivatives
- Compare the performance of the symbolic approach with the finite difference approximation

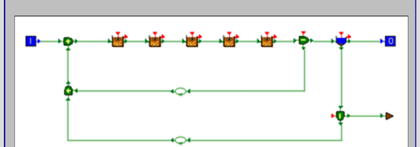
Three test models and their Jacobian



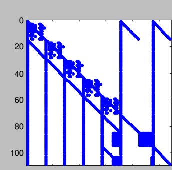
Single ASU: An ASM2d activated sludge unit with intermittent aeration and a secondary settler. This model contains **30 state functions and state variables**.



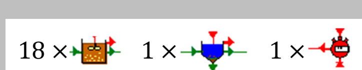
30 state variables
334 non-zero elements
Filling ratio = 0.37



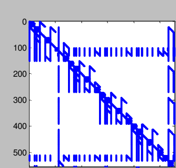
Benchmark Simulation Model (BSM): This model uses 5 ASM1 activated sludge units and a secondary settler. It contains **108 state functions and state variables**.



108 state variables
1227 non-zero elements
Filling ratio = 0.11



Full scale WWTP model: (unpublished) containing 18 ASM2d units, one secondary settler and one controller, for a total of **554 state functions and state variables**.



554 state variables
9638 non-zero elements
Filling ratio = 0.03

What is the Jacobian?

- In a system of Ordinary Differential Equations (ODE), it is the matrix of the first order partial derivatives of the state functions with respect to the state variables.

$$J = \begin{bmatrix} \partial f_1/\partial x_1 & \dots & \partial f_1/\partial x_n \\ \vdots & \ddots & \vdots \\ \partial f_n/\partial x_1 & \dots & \partial f_n/\partial x_n \end{bmatrix}$$

- The Jacobian matrix computed at a point $\hat{x}$ is also the best linear approximation of the model around this point.
- The partial derivative is usually estimated through the **finite differences approximation** and requires $n+1$ evaluations of the model

$$\frac{\partial f_i}{\partial x_j} \approx \frac{f_i(x_j + \Delta x_j) - f_i(x_j)}{\Delta x_j}$$

Observed speed-up

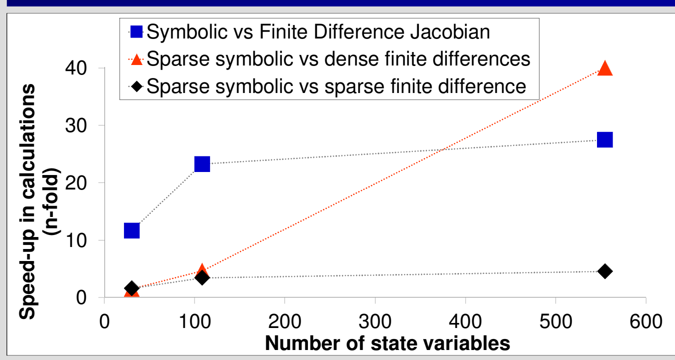


Figure: The n-fold speed-up of computation made with symbolic jacobian is shown in three cases. Computation of one symbolic jacobian versus one finite difference approximation (**Squares**). Simulation of 60 days with symbolic jacobian and sparse matrix tools versus finite difference jacobian and dense matrix operations (**Triangle**) or sparse matrix operations (**Diamond**).

Key findings

- The generation of a symbolic Jacobian provides insight into the sparsity pattern of the matrix and favours the use of sparse matrix tools.
- Benefits of symbolic manipulation increase with increasing complexity of test models.
- A simulation less than 15 simulated days suffices to compensate for the time needed for the generation of the symbolic jacobian generation

http://modelEAU.fsg.ulaval.ca

cyrilgarneau@gmail.com