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Dynamic Simulation of Chemical Kinetics in Microcontroller

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ABSTRACT
Arduino boards are interesting computational tools due to low cost and power consumption, as well as I/O ports, both analogs and digitals. Yet, small memory and clock frequency with truncation errors may disrupt numerical processing. This study aimed to design and evaluate the performance of a dynamic simulation based on ODEs in the Arduino, with three evaluated microprocessors; ATMEGA 328P and 2560, both 8 bits, and SAM3X8E Atmel ARM CORTEX – 32 bits. The study case was a batch reactor dynamic simulation. The Runge-Kutta 4th order algorithm was written in C++ and compiled for EPROM utilization. The output was a 115000bit/s serial connection. Processing time was almost identical for 8 bits architectures, while 32 bits was 25% faster. Without the serial connection the 8 bits architectures were 16 times faster and the 32 bits was 42 times faster. Error truncation was similar, since the floating points are done through software. The Arduino platform, despite its modest hardware, allows simple chemical systems simulation.
Keywords – Arduino, Chemical Reactions, Microcontrollers, Runge-Kutta

I. INTRODUCTION

Mathematical modeling of chemical processes and digital simulation are useful tools when dealing with daily chemical engineering situations. Enabling not only to describe, analyze, evaluate and optimize plant operations, but also to conceive new process technologies and/or new industrial unities.

As microcomputers prices decreased and miniaturization occurred, their popularization began. This fact has enabled the use of chemical system simulations analysis as a tool to a broader spectrum of institutions.

In a similar manner to microcomputers popularization during the 70's, the current dissemination of microcontrollers, due to low cost and energy consumption, as well as, processing power comparable to earlier full microcomputers, allows digital simulation in smaller hardware. It generated a wider range of chemical engineering simulation platforms for classes, research and technological development.

However, memory limitations for data and coding, as well as limitations in numerical precision due to faulty floating point operations, in these platforms, such as the Arduino Free Hardware Platform, may pose as a treat for numerical methods, inherent to most simulation algorithms.

The objective of this paper is to evaluate the computational performance of Arduino Boards regarding processing time, precision and accuracy for implementations of Runge-Kutta 4th order numerical solutions to ordinary differential equations from simple systems with concentrated parameters. More specifically, the first order reaction kinetics of a batch reactor. Three Arduino platforms were evaluated: ATMEGA 328P and 2560, both 8 bits, and SAM3X8E Atmel 32 bits ARM CORTEX – M3.

The Arduino microcontroller is an open hardware tool design to be easily integrated to sensors and actuators. One of its most important characteristics is how user friendly the coding is to even non advance developers in hardware development areas [1].

The platform was conceived in 2005 in the Ivrea Institute by Barragan, Banzi, Cuartielles, Mellis, Marino e Zambeti [2]. All moved by the necessity of teaching basic electronics, in a short period of time, to design students at the institute [3].

The board gained popularity among hobbyists, hackers and scientists in small to medium projects. This resulted in several extension boards (shields) to enhance the Arduino capabilities [4].

Recently the platform has been applied in several projects, encompassing fields such as biomedicine, automation, robotics and engineering [5,6,7]. A large number of applications are registered, such as datalogging [8,9,10,11], and bioprocess automation [12]. Also in a mechanical engineering application, where Zeno [13] designed and built a self-leveling platform utilizing low cost hardware. By using Arduinos, the total cost was less than US$ 100,00.

The cited applications main focuses are monitoring, automation and development of standalone devices, not in simulation. One point that may explain this behavior is that the board is

optimized to deal with standalone applications, and does not possess a I/O interface. Such visual output must be programmed by the user for each application. Thus, the utilization of microcontrollers in digital simulation of chemical processes is restricted. Especially when compared to other computational hardware platforms.

The digital simulation field generally demands a great computational effort, not only forced by the mathematical system, but also due to the requirement of running computational packages and toolboxes alongside the algorithm. One example is the necessity of running an Artificial Neural Network Model toolbox with MatLab, such as in the work of Khaouane et al. [14]. The toolbox provides faster developments within the computational application, since the packages are usually well documented and user friendly, enabling its utilization by an intermediate user. However, loading the entire toolbox, even when all its features are not applied, impairs computational speed.

Gödeke et al. [15] reports that computational solutions based on ARM (Advanced Reduced instructions set computer Machine) architectures are more efficient under an energy utilization point of view when compared with x86 platforms.

The Arduino platform has also been utilized in entry level Chemical Engineering classes for datalogging or small scale automation during practical lectures [16].

The computing power, associated with the flexibility of a multipurpose computational system and standard interface, makes the general architecture of microcomputers more attractive to simulations. However, microcontrollers are far more inexpensive and more robust [4].

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II. MATERIALS AND METHODS

During the simulations, the performance of three boards were evaluates; Arduinos Nano (Provider: Funduino), Mega (Provider: Funduino) e Due (Provider: Arduino Store). The three boards are displayed in Fig. 1.

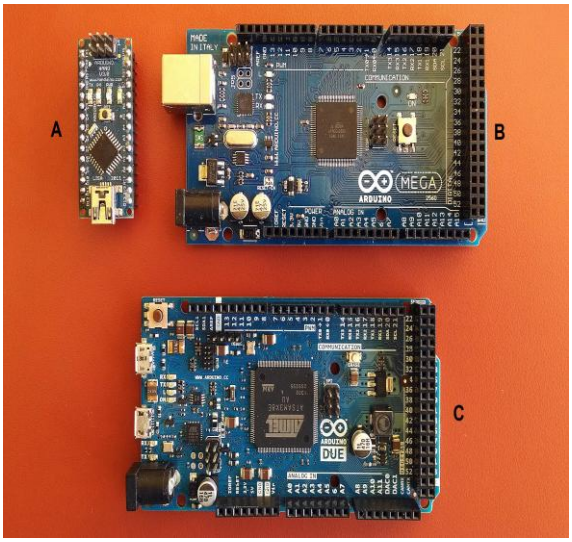

Figure 1 – (A) Arduino Nano, (B) Arduino Mega e (C) Arduino Due.

The main characteristics of each board are described on Table 1. The Nano board, is the smallest of the three, and thus, the one with the least hardware resources and also the most inexpensive. The Mega board is an extension of the Arduino Uno concept, with extra serial ports, more input/output ports and approximately 8 times more memory than a Nano board. The most recent board architecture, among the evaluated, is the Due board. It has a 32 bit processor, more memory, and a clock speed 5 times higher than the 8 bit processors.

The interface was made through a serial communication, by USB port in 115,000 bit/s. A notebook was used solely as an output for the numerical results developed by the Arduino boards.

Table 1 – Main Characteristics from the Evaluated Arduino Boards

Board	Arduino Nano	Arduino Mega	Arduino Due
Microcontroller	ATmega328	ATmega2560	AT91SAM3X8E
Clock Speed (MHz)	16	16	84
Flash Memory (KB)	32 (2 used by boot loader)	256 (8 used by bootloader)	512
SRAM (KB)	2	8	96
EEPROM (KB)	1	4	-
Price (Brazilian Market - US$)	20,00	40,00	100,00
Architecture	8 bit	8 bit	32 bit - Cortex

The study case was based in modeling an elementary first-order reaction occurring in an ideal batch reactor isothermal example [17], following Equation 1.

$$A \rightarrow B \quad (1)$$

The case is the first order differential equation that describes the concentration behavior of a generic chemical specie "A", according to Equation 2.

$$dC_A = -k \cdot C_A \quad (2)$$

Subject to the initial condition represented by Equation 3.

$$t = 0 \rightarrow C_A = C_{A_0} \quad (3)$$

The exact solution to the problem was calculated, according to Equation 4, in order to evaluate the precision of the numerical solution.

$$C_A = C_{A_0} \cdot e^{-k \cdot t} \quad (4)$$

The numerical method was a Runge-Kutta 4th order method, according to Balsa [18], displayed in Equation 5.

$$y_{k+1} = y_k + \frac{h_k}{6}(K_1 + 2 \cdot K_2 + 2 \cdot K_3 + K_4) \quad (5)$$

Where the four increments are calculated by Equations 6 through 9.

$$K_1 = f(t_k, y_k) \quad (6)$$

$$K_2 = f\left(t_k + \frac{h_k}{2}, y_k + \left(\frac{h_k}{2}\right) \cdot K_1\right) \quad (7)$$

$$K_3 = f\left(t_k + \frac{h_k}{2}, y_k + \left(\frac{h_k}{2}\right) \cdot K_2\right) \quad (8)$$

$$K_4 = f(t_k + h_k, y_k + h_k \cdot K_3) \quad (9)$$

The coding was constructed using the Arduino interface, version 1.5.4, according to Figure 2.

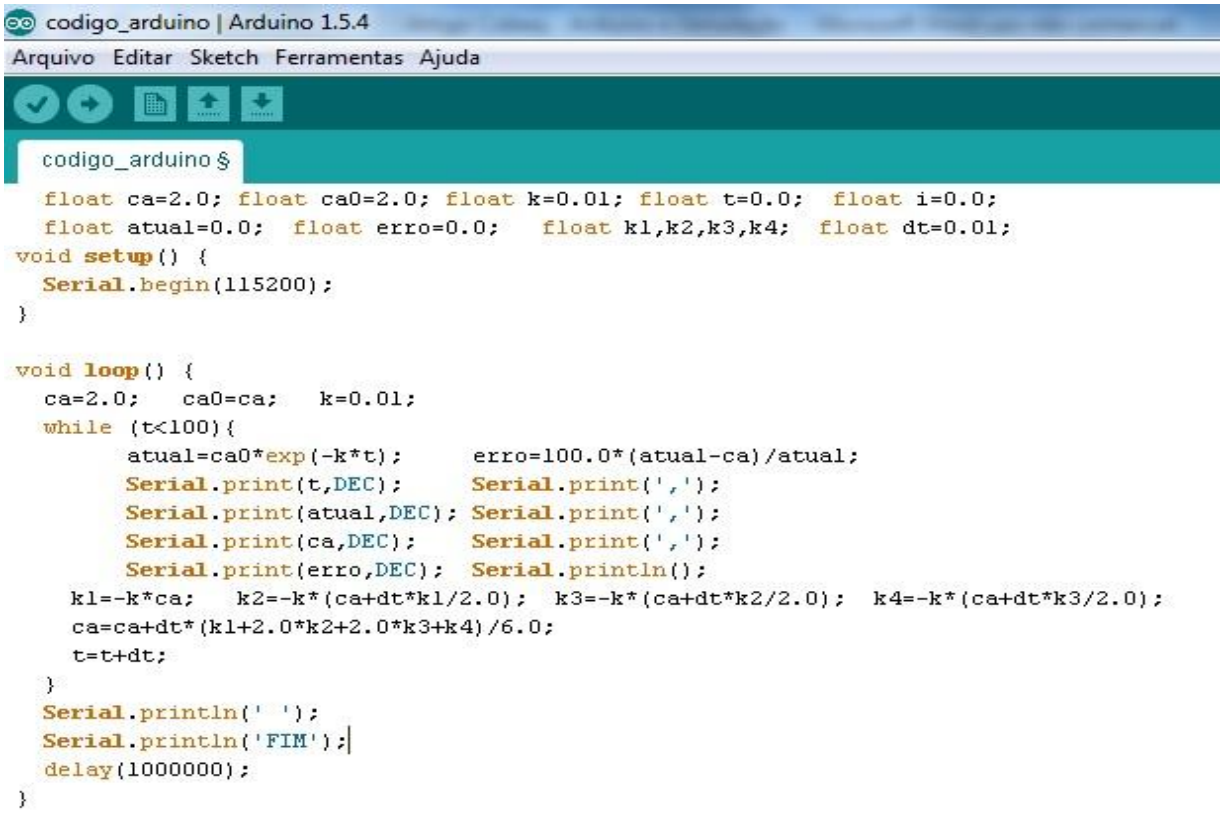

Figure 2 – Computational Experiment Dynamic Simulator Code

III. RESULTS AND DISCUSSION

Throughout the simulations, it was proven that the utilization of the Serial interface for results output greatly limits the processing capacities and speed. A summary of the simulation speeds are presented in Table 2. As it was expected, the Due board was approximately 25% faster when executing the code.

The memory allocation, even with the relative small capacity for code and data in the Nano board,

was not a limitation. The entire experiment code occupied 5572 bytes, with 240 bytes of memory representing the program global variables

The percentage minimal and maximum errors, respectively -2,2x10-3% e 5,1x10-3%, were identical in all three boards.

The numerical solution was very similar among the boards. The concentration profiles, as well as the error percentage, were identical in the 8 bits boards, but differed in the 32 bits board. The results shown in Figure 3 confirm that the behavior of the numerical solution in the ODE was very similar in all Arduino boards.

Table 2 – Processing Times for the Simulations

Processing Time (s)	Arduino Nano	Arduino Mega	Arduino Due
Without Serial Output	4,060	4,190	1,072
2 digits precision display	21,060	21,580	19,148
8 digits precision display	57,886	58,952	42,269

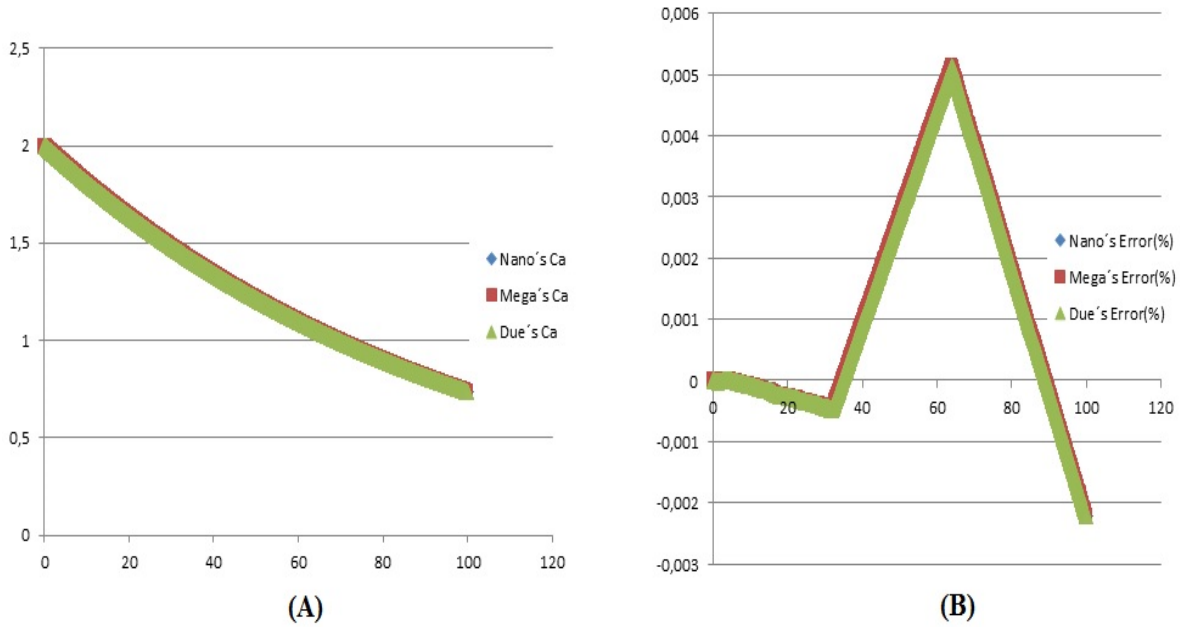

Figure 3 – (A) Concentration Profiles in Numeric Solution on Arduino Nano, Mega and Due; (B) Numeric Error (%) Profiles on Arduino Nano, Mega and Due.

IV. CONCLUSION

The utilization of boards in rapid prototyping is extremely welcome. Since its constructive characteristics are prone to easy utilization, low energy consumption, low cost, signal acquisition capacities, digital outputs and the capacity of emulating analog outputs, making the platform an excellent experimentation platform.

Regarding the field of dynamic simulation, even with small computing capacities, the use of Arduinos boards is a feasible option to emulate numerical solutions for ordinary differential equations with concentrated parameters systems. This is enabled since the deviation between the numerical and exact solution of the problem was acceptable, in spite of using simple precision and the way the floating point is handled.

Processing time was almost identical for 8 bits architectures, while 32 bits was 25% faster. Without the serial connection the 8 bits architectures were 16 times faster and the 32 bits was 42 times faster.

These characteristics may represent a step towards a new technology within process control. An industrial plant where microcontrollers may be responsible by not only controlling actuators, but also by evaluating current state and tuning future actuations based on predictions made by itself.

V – Nomenclature

A , B - Generic Species

C_A - Generic Species A Concentration

k - Kinetic Constant

C_{A_0} - Generic Species A Initial Concentration

y_{k+1} - Next Value

t_k - Current Time

t - Time

y_k - Current Value

h_k - Iteration Step

K_1, K_2, K_3, K_4 - Slope Increments

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