Scientific computing over the Web

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CERENA's Seminars

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Scientific computing over the Web

ABSTRACT ▪ In our technological era, **scientific computing over the Web** (SCW) has been overlooked: by Academia, by Industry. Besides its value to both, it can provide an easy link between them.

SCW: the user (in a website) supplies his data, executes an available program, and gets his results. ***(No software installation.)***

Based on cases that I use in teaching (***via the Web***), the talk will follow these points:

1. Antecedents;
2. Examples;
3. *Producer-consumer* communication (of SCW); and
4. Conclusions — and the Web offers a link between Academia and Industry.

- ***Cogito, ergo sum***.

- ***In Interrete non existo, ergo non sum.***

Scientific computing over the Web

1. Antecedents
2. Examples
3. Producer-consumer communication
4. Conclusions

Raphael
(1483–1520)
Scuola di Atene
(School of Athens)

1. 2. 3. 4. Antecedents

- Scientific computing is laboriously taken to Industry…

- …But Industry often does not take advantage from SC:
  - Lack of *structure* — no "surplus" technical personnel for it
  - Lack of *stimulus* — no disposition; fear

We don't use *those things that you taught us… (*sic*)**

* **One of my former students, about Operational Research.**

1. 2. 3. 4. Antecedents

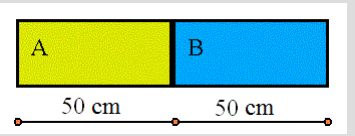
- We talk to: **Industry**, but also other **academic institutions**.
- Yet:
- The Web* itself **has not paid attention** to **SC** (either with free or paid software).
- **Many** webpages and applications deal with **science**, but tend to the novelty of the medium (images, video, etc.).
- Among innumerable webpages, there are:
  - ***many*** (didactic) for consultation, study
  - ***few*** for dynamic use, *i.e.*: data → results
- Scarce ***applicable*** **material** is found on
  - Mathematics, Physics, Engineering, industrial applications
- ***What about solving problems (academic, industrial) ?***

* http://en.wikipedia.org/wiki/Internet#Services (about: Web ∈ Internet)

Software that exists in our organization
(A parenthesis)

- ***One of us*** **(technical staff, professor, etc.)**
  - ***can use*** the software (Matlab ⇨), **to which he can access remotely,**
  - to solve this simple problem (via Monte Carlo simulation):

What is the total length of these 2 (similar) bars, each with ~50 cm ? (Perhaps 1 m !)
Suppose *uniform* distributions in 49–51 cm.



- On the Web: sum of uniforms ⇨ ***You also can do it !***

1. 2. 3. 4. Antecedents

Webpages on **science** and…

- Wolfram *Mathworld*, by Eric Weisstein
  http://mathworld.wolfram.com/
- Springer ***E****ncyclopaedia* ***o****f* ***M****athematics*
  http://eom.springer.de/
- Wikipedia (part)
  http://en.wikipedia.org/
- NIST/SEMATECH e-Handbook of Statistical Methods
  (Statistical Eng.[ing] Division ← **I**nformation **T**echnology **L**aboratory ← **N**at'l **I**nst. of **S**tandards and **T**echnology, USA)
  http://www.itl.nist.gov/div898/handbook/
- Etc., etc.

1. 2. 3. 4. Antecedents

…webpages on **scientific computing**

- Emphasis on images, interactivity
  - **"Atractor"** (.pt) http://atractor.pt/ (but needs "our" Java !) (in WebMathematica) Example (polyhedra, etc.):

    http://atractor.pt/webM/exemplos/poliedros.htm
- **Academic SCW:** scarce ***working*** material on Mathematics, Physics, Industry. **Exception:**

  - **Prof. V. M. Ponce,** San Diego St. U. (in Fortran: remarkable, although without default data)

    http://ponce.sdsu.edu/onlinewaterbalance.php
- **"scientific computing on the internet"** ←←←
  - **~6** results (sources of software, university courses)

1. 2. 3. 4. Antecedents

FROM MY EXPERIENCE

- **Computer Science engineers** (informatics engineers), generally:
  - Are not enthusiastic about (this) Scientific Computing
  - Are not inclined to Mathematics

- The **other engineers**, generally:
  - Leave Information Technology (Informatics) to the former
  - Fear (justifiably…) the Internet environment

1. 2. 3. 4. Antecedents

- In my academic work:
  - *"Computing"* ◆ *"Operational Research"* ◆ "*Quality Control"*
  - I have adopted SC **over the Web**
  - since 1998
- 1.st example:
  - Area of a triangle by Heron's* formula (year AD 60)

$$A = \sqrt{s(s-a)(s-b)(s-c)}$$

  - Program in Fortran (5 lines) (*a*, *b*, *c*, sides; *s*, semiperimeter)
  - About 1 year to put it on the Internet

http://web.tecnico.ulisboa.pt/mcasquilho/compute/misc/F-triang.html

* Heron of Alexandria (AD 10 ?–75 ?)

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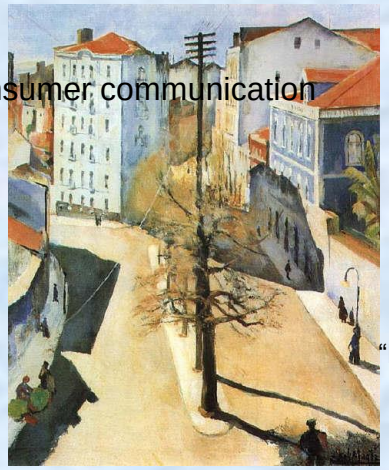
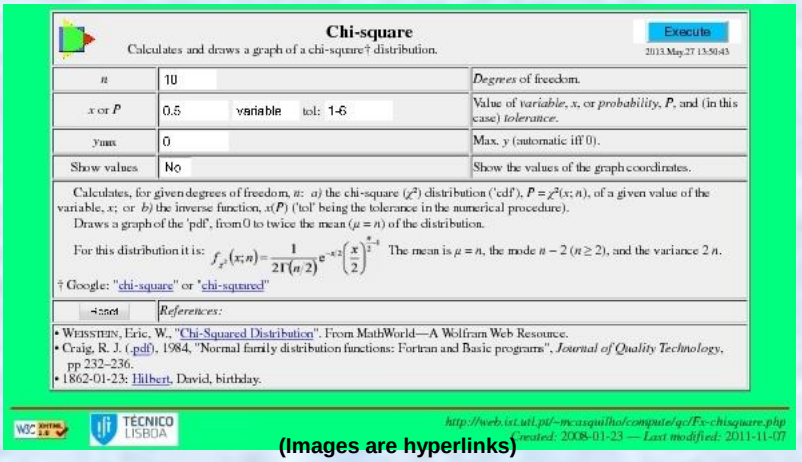


Abel Manta
(1888-1982)
"Rua de São Bernardo"
(*St. Bernard Str.*)

1. **2.** 3. 4. Examples

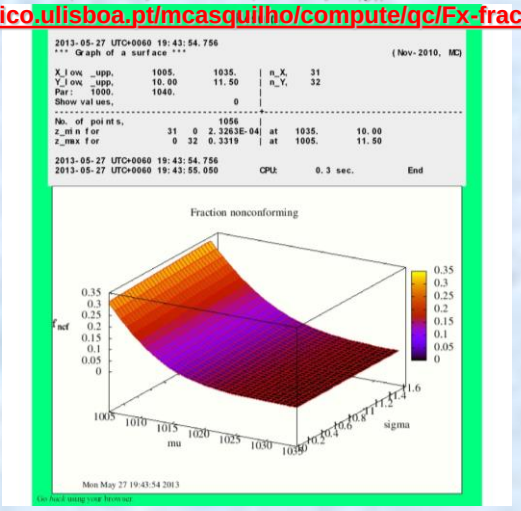
- **Chi-square** ➲ Try $\nu = 3$, $\nu = 50$ (nearly Gaussian)
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-chisquare.php



(Images are hyperlinks)

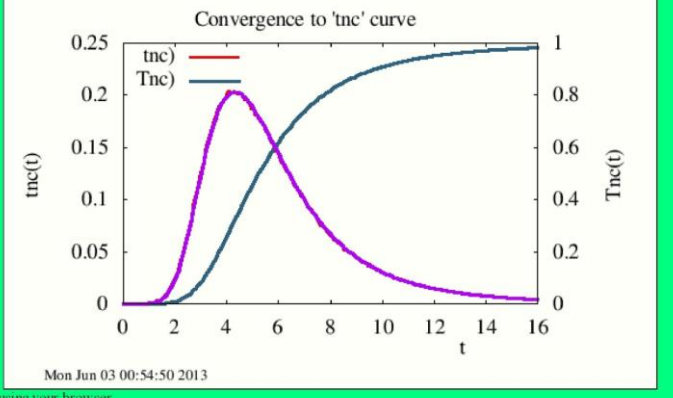
1. **2.** 3. 4. Examples

- **Fraction defective** (Quality Control) ➲ Try σ_{low} = 10, 1.
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-fracdefective.php



- **Conver**
  http://we

```
Descriptive measures:   pdf       cdf     |
  Mode        4.38      0.203     0.330   |
  Median      5.27      0.176     0.500   |
  Mean        6.08      0.137     0.628   | Sigma,                          3.48
Crit. (min) values:   Simul.      Theo.    | (simulated vs. theoretical values)
  Critical t:           3.12      3.14     | Q = t / sqrt(n)     sqrt(n) =  2.236
  Crit. Q ie., k:       1.396     1.403    | Verify Tnc(theo. k): alpha', 10.00 %

2013-06-03 UTC+0060   0:54:49.714
2013-06-03 UTC+0060   0:54:50.912          CPU:        1.2 sec.          End
```

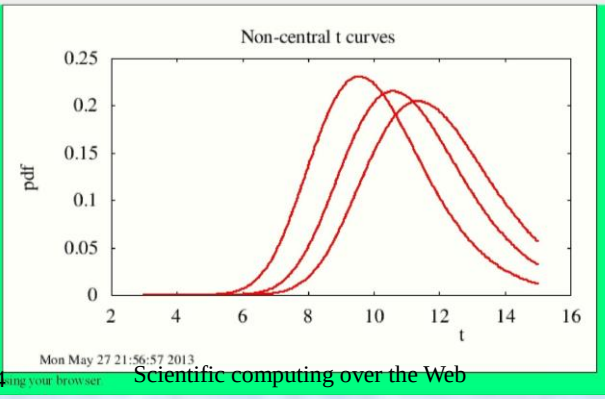


Go *back* using your browser.

1. **2.** 3. 4. Examples

- **Sequence of non-central *t* curves** ➲ Try AQL = 1,1.5, 6.5 (%).
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/F-tncseq.php

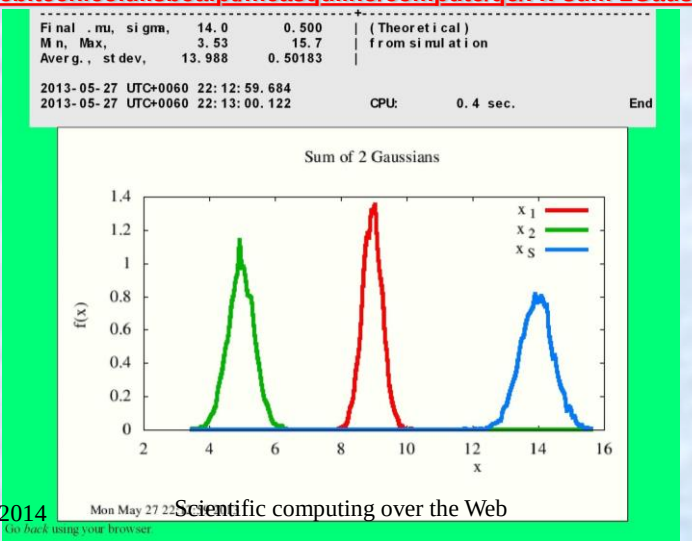
```
Q_left, _right,    0.6000        3.000    |
omega, L', delta:   1.00 %      -2.326       11.63
omega, L', delta:   1.50 %      -2.170       10.85
omega, L', delta:   2.50 %      -1.960        9.800

2013-05-27 UTC+0060 21:56:57.612
2013-05-27 UTC+0060 21:56:57.704          CPU:        0.1 sec.          End
```



Go *back* using your browser.

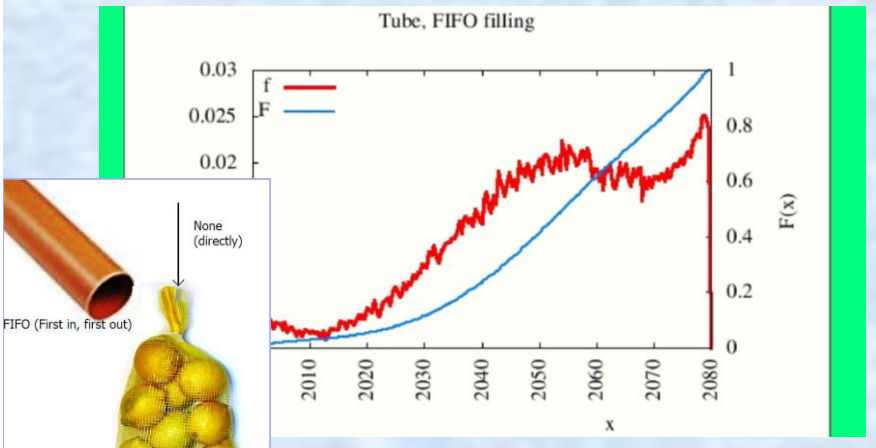
1. **2.** 3. 4. Examples

- **Sum of 2 Gaussians** ➲ Try (μ_1, σ_1) = (5, 0.1). $\left(5+9\overset{?}{=}14\right)$
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-sum-2Gauss.php



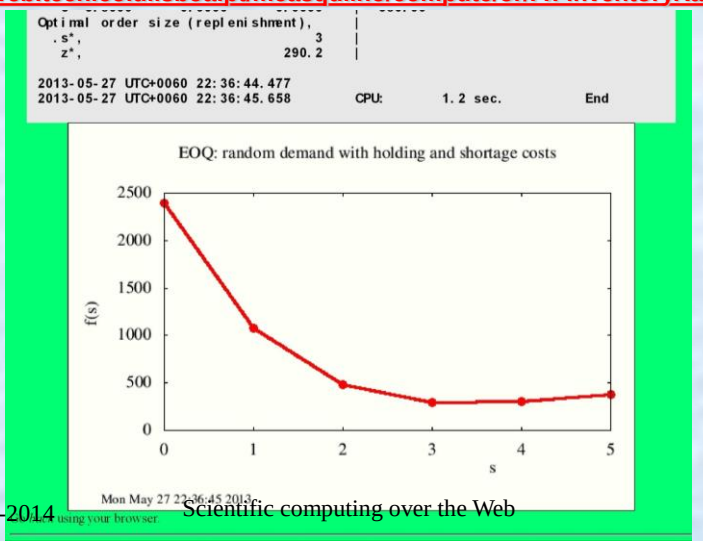
1. **2.** 3. 4. Examples

- **Packet filling, as tubes (FIFO)** ➲ Result FIFO. Try: none, FIFO.
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-3tubefill.php



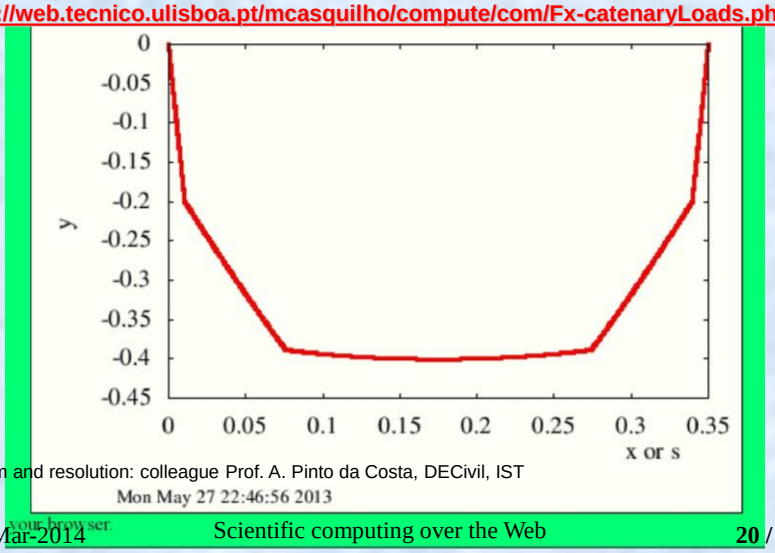
1. **2.** 3. 4. Examples

- **EOQ (economic order q.) with random demand** ➲ Try c_p = 2000, 150.
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/or/Fx-inventoryRand.php



1. **2.** 3. 4. Examples

- **Catenary with concentrated loads*** ➲ Try 3.rd load -1, -1.9.
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/com/Fx-catenaryLoads.php

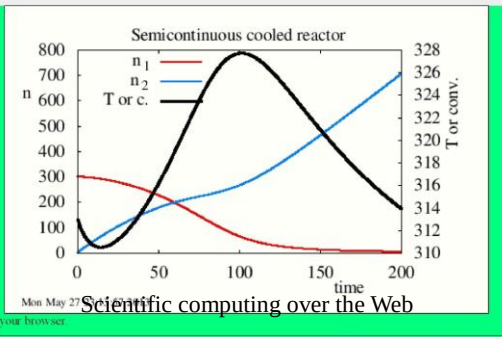


* Problem and resolution: colleague Prof. A. Pinto da Costa, DECivil, IST

- **Semicontinuous cooled reactor** ➲ Try T = 298, 348 K (25, 75 °C).
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/com/Fx-scoolreactor.php

Results

```
2013-05-27 UTC+0060 23:13:57.870
*** Semicontinuous cooled reactor ***                    (May-2005, MC)

t_f,  h,  (min.)          200.      5.000E-02|  nsteps,                    4000
. k0,  E_A,               4.000E+12  85.0     |  M-1 min-1,  kJ/mol
V0,                                  300.     |  L
                                     [illegible]|  M/min
                                     298.     |  K
                                     [illegible]|  kJ/m2-min-K
U,  A,                    30.0       0.624    |  kJ/m2-min-K,  m2
. n_A0,  . n_B0,          300.       0.00     |
T_0,                                 313.     |  K
Plot {1|2} ?                           1      |  Temperature or conversion
Show values (0|1) ?                    0      |
-------------------------------------------------+-----------------------------
Final T,                             313.9    |
Final . n,                4.553      704.6    |
Conversion of A,                     0.9848   |

2013-05-27 UTC+0060 23:13:57.870
2013-05-27 UTC+0060 23:13:58.238          CPU:        0.4 sec.          End
```



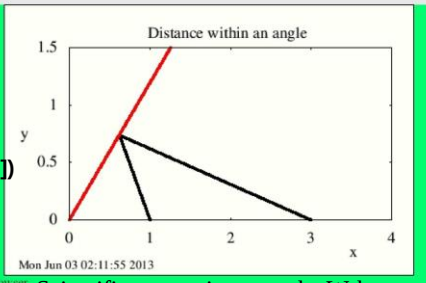
Mon May 27 [illegible]
Go back using your browser

1. **2.** 3. 4. Examples

- **Minimum distance "within an angle"** ➲ Try γ = 50°, 5°
  http://web.tecnico.ulisboa.pt/mcasquilho/compute/com/Fx-angdistImg.php

(Casquilho & Buescu [2011])

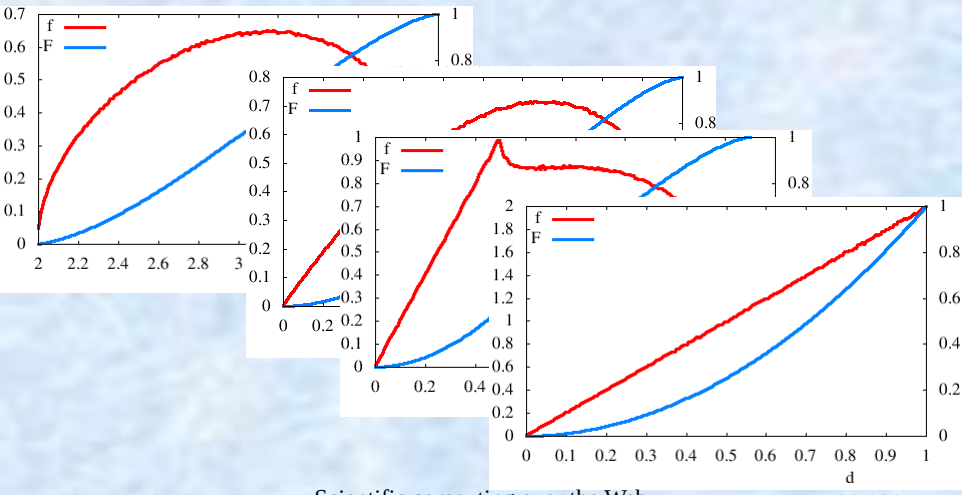
```
If x_2 = x_1:                                |
  x_P,  y_P,        0.41318     0.49240      |  (absolute minimum  d0)
If x2 = infinity:                            |  d0 = x_1 cos^2 = x_P =   0.41318
  x_P,  y_P,        0.82635     0.98481      |
                                             |  x_P = 2 d0
MINIMUM DISTANCE for given x_2               |
x_P,  y_P,          0.61976     0.73861      |  Cartesian coordinates
rho_P,                          0.96418      |  (Polar) radial coordinate
d_1,  d_2,           0.8307       2.492      |  A--P,  P--B
Min. distance,                   3.3229      |  A--P--B

2013-06-03 UTC+0060  2:11:55.207
2013-06-03 UTC+0060  2:11:55.729          CPU:        0.5 sec.          End
```



Mon Jun 03 02:11:55 2013
Go back using your browser

1. **2.** 3. 4. Examples

- **Distance to points in a circle** ➲ Try x_0 = 3, 1, 0.5, 0 (R = 1)
  http://web.tecnico.ulisboa.pt/~mcasquilho/compute/or/Fx-distInCircle.php



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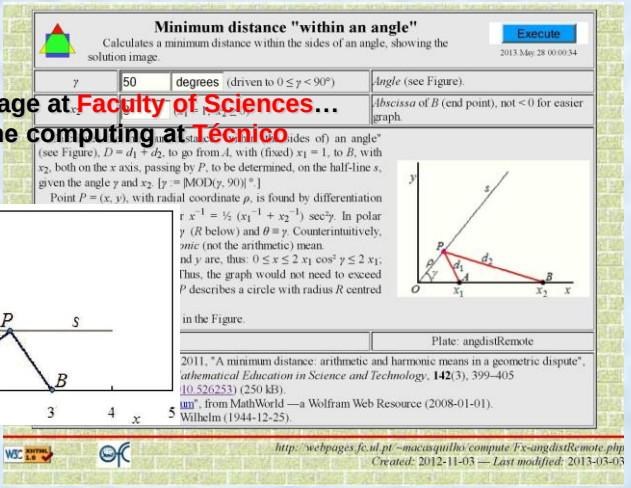
1. Antecedents
2. Examples
3. Producer-consumer communicaation
4. Conclusions

Henrique Medina
(1901–1988)
"A rapariga da galinha branca"
(*The girl with the white hen*)

1. 2. **3.** 4. Producer-consumer communication

- **Minimum distance "within an angle"** ➲ Compute: here at Técnico
  http://webpages.fc.ul.pt/~macasquilho/compute/Fx-angdistRemote.php



- **My webpage at Faculty of Sciences…**
- **…does the computing at Técnico**

1. 2. **3.** 4. Producer-consumer communication

- **For a company, the computing can be:**
  - Started on its website;
  - Executed on another site (University ?); and
  - Presented on the company's website.
- **The user does not even notice the circuit.**

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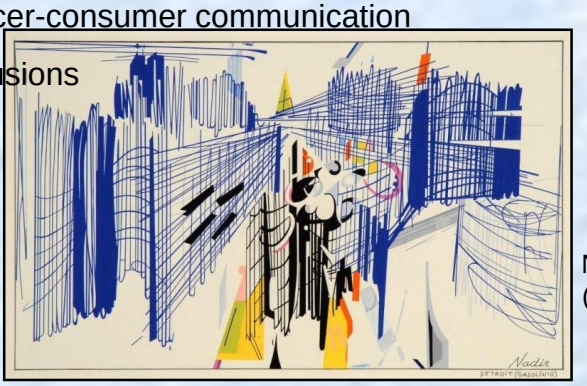

Nadir Afonso
(1920–2013)
"Detroit"

1. 2. 3. **4.** Conclusions…

- **Scientific computing over the World Wide Web** has been overlooked.
- It can provide an easy link — namely, with Industry.
- The "start" can be difficult, perhaps justifying the scarcity.
- Working on the Web
  - avoids platform incompatibilities (Windows, Mac, Linux)
  - obviates limitations of the user's terminal (PC, phone)
  - avoids software installation (uninstallation)
- Modern (scientific) languages (Mathematica, Matlab, etc.) favour productivity, but appear obsolete (!), as they aren't (yet) Web-friendly (licences, permissions).

1. 2. 3. **4.** …Conclusions

- Scientific computing over the Web benefits from
  - sharing — in team work
  - visibility — attracting connections, *e.g.*, with Industry
  - network computing — “grid”, “cloud”, parallel
  - easy access, just using a *browser*
- Problems: welcome !

■

Acknowledgements

- **CERENA:** “Centro de Recursos Naturais e Ambiente” (*Centre for Natural Resources and the Environment*), IST, ULisboa
- **CPQ:** “Centro de Processos Químicos” (*Centre for Chemical Processes*), IST, ULisboa (CPQ ∈ CERENA)
- **DEQ:** Department of Chemical Engineering, IST, ULisboa
- **CIIST:** “Centre of Informatics of IST”, Instituto Superior Técnico, University of Lisbon
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Keywords

- Scientific computing; Web; Internet; academia, industry

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