

Scientific computing over the Web

CPQ Centro de Processos Químicos
Centre for Chemical Processes



IST DEQ
DEPARTAMENTO
DE ENGENHARIA QUÍMICA
TÉCNICO LISBOA

U LISBOA | UNIVERSIDADE
DE LISBOA

Miguel CASQUILHO

Assist. Prof. (retired)

CERENA “Centro de Recursos Naturais e Ambiente” (*Centre for Natural Resources and the Environment*) & CPQ

DEQ Department of Chemical Eng.^{ing}

IST *Instituto Superior Técnico*

UL *University of Lisbon*

<http://web.tecnico.ulisboa.pt/mcasquilho/>

CERENA's Seminars

Lisboa, IST, 19 March 2014

19-Mar-2014

Scientific computing over the Web

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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:

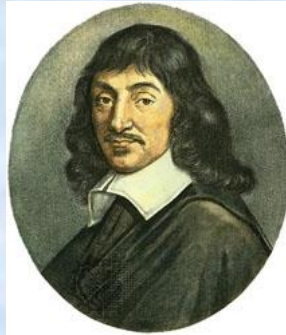
1. Antecedents;
2. Examples;
3. *Producer-consumer* communication (of SCW); and
4. Conclusions — and the Web offers a link between Academia and Industry.

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



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

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Scientific computing over the Web

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



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

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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.

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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)

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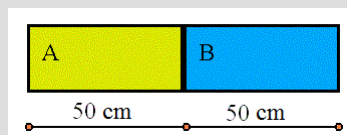
Software that exists in our organization (A parenthesis)

▪ *One of us* (technical staff, professor, etc.)

- *can use* the software (Matlab \Rightarrow), 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 \Rightarrow **You also can do it !**

1. 2. 3. 4. Antecedents

Webpages on **science** and...

- Wolfram *Mathworld*, by Eric Weisstein
<http://mathworld.wolfram.com/>
- Springer *Encyclopaedia of Mathematics*
<http://eom.springer.de/>
- Wikipedia (part)
<http://en.wikipedia.org/>
- NIST/SEMATECH e-Handbook of Statistical Methods
(Statistical Eng.^{ing} Division \leftarrow Information Technology Laboratory \leftarrow
Nat'l Inst. of Standards and Technology, 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)

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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



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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 ?)

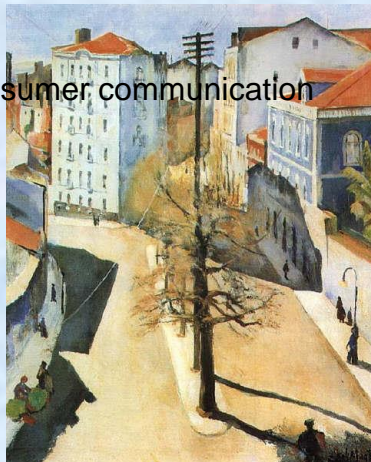
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1. Antecedents
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Abel Manta
(1888-1982)
“Rua de São Bernardo”
(St. Bernard Str.)

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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>



Chi-square

Calculates and draws a graph of a chi-square[†] distribution.

Execute

2013.May.27 13:50:43

n	10		Degrees of freedom.
x or P	0.5	variable tol: 1-6	Value of variable, x, or probability, P, and (in this case) tolerance.
ymax	0		Max. y (automatic iff 0).
Show values	No		Show the values of the graph coordinates.



Calculates, for given degrees of freedom, n: a) the chi-square (χ^2) distribution ('cdf'), $P = \chi^2(x; n)$, of a given value of the variable, x; or b) the inverse function, $x(P)$ ('tol' being the tolerance in the numerical procedure).
 Draws a graph of the 'pdf', from 0 to twice the mean ($\mu = n$) of the distribution.

For this distribution it is: $f_{\chi^2}(x; n) = \frac{1}{2^{\frac{n}{2}} \Gamma(\frac{n}{2})} e^{-\frac{x}{2}} \left(\frac{x}{2}\right)^{\frac{n}{2}-1}$ The mean is $\mu = n$, the mode $n - 2$ ($n \geq 2$), and the variance $2n$.

† Google: "chi-square" or "chi-squared"

References:

- WEISSTEIN, Eric, W., "Chi-Squared Distribution". From MathWorld—A Wolfram Web Resource.
- Craig, R. J. (.pdf), 1984, "Normal family distribution functions: Fortran and Basic programs", *Journal of Quality Technology*, pp 232–236.
- 1862-01-23: [Hilbert](#), David, birthday.

<http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-chisquare.php>
 Created: 2008-01-23 — Last modified: 2011-11-07

(Images are hyperlinks)

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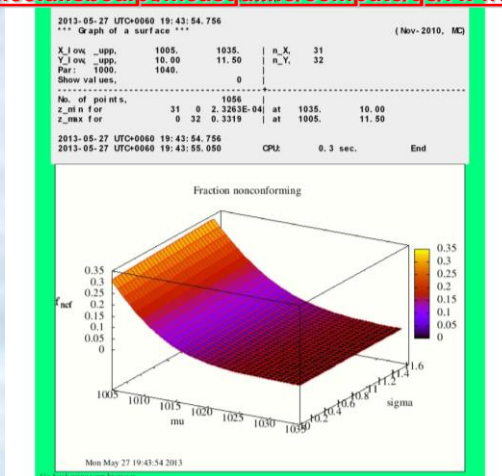
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1. 2. 3. 4. Examples

- **Fraction defective (Quality Control)** ⇨ Try $\sigma_{low} = 10$, 1.

<http://web.tecnico.ulisboa.pt/mcasquilho/compute/qc/Fx-fracdefective.php>



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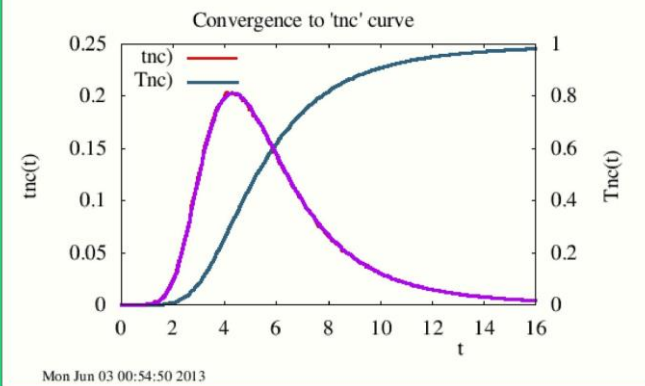
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- Conver

<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			
Crit. (min) values:			Simul.	Theo.	Sigma,	
Critical t:	3.12	3.14			(simulated vs. theoretical values)	3.48
Crit. Q i.e., k:	1.396	1.403			Q = t / sqrt(n)	sqrt(n) = 2.236
					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

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Go back using your browser

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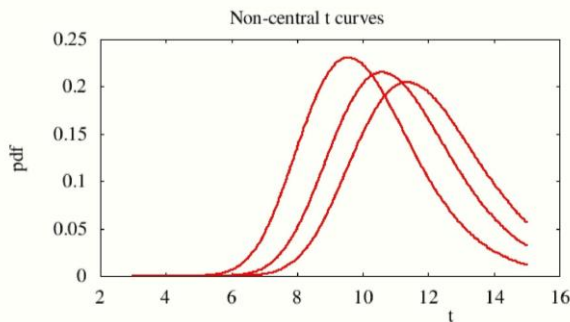
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1. 2. 3. 4. Examples

- Sequence of non-central t curves \Rightarrow Try AQL = 1, 1.5, 6.5 (%).

<http://web.tecnico.ulisboa.pt/mcasquilho/compute/gc/F-tncseq.php>

Qleft, _right,	0.6000	3.000		11.63
omega, L', delta:	1.00 %	-2.326		10.85
omega, L', delta:	1.50 %	-2.170		9.800
omega, L', delta:	2.50 %	-1.960		
2013-05-27 UTC+0060	21:56:57.612		CPU:	0.1 sec.
2013-05-27 UTC+0060	21:56:57.704			End



Mon May 27 21:56:57 2013

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1. 2. 3. 4. Examples

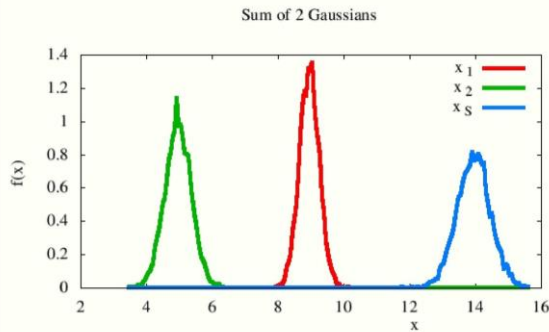
- **Sum of 2 Gaussians** \Rightarrow Try $(\mu_1, \sigma_1) = (5, 0.1)$. $(5+9=14)$

<http://web.tecnico.ulisboa.pt/mcasquilho/compute/gc/Fx-sum-2Gauss.php>

```

Final . mu, si gm, 14.0 0.500 (Theoret ical)
M n, Mbx, 3.53 15.7 from si mulat ion
Averg., st dev, 13.988 0.50183

2013-05-27 UTC+0060 22: 12: 59. 684
2013-05-27 UTC+0060 22: 13: 00. 122 CPU: 0.4 sec. End
    
```



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Mon May 27 22: Scientific computing over the Web

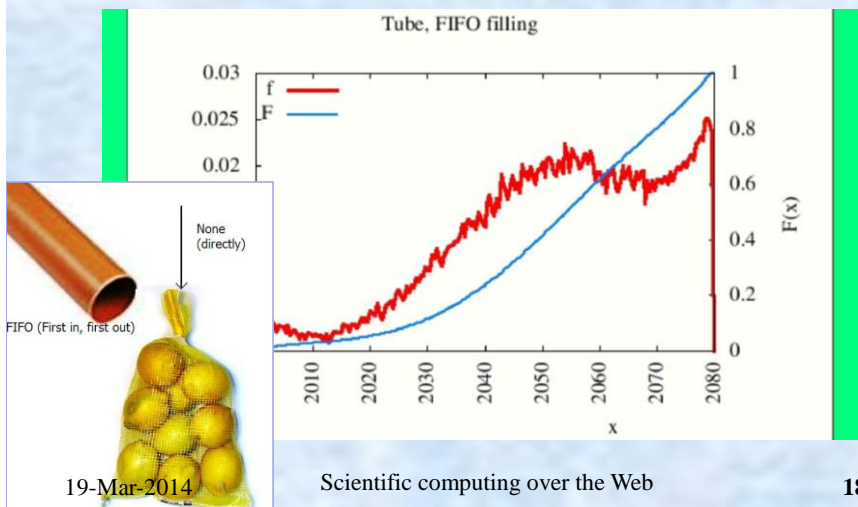
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[Go back using your browser](#)

1. 2. 3. 4. Examples

- **Packet filling, as tubes (FIFO)** \Rightarrow Result FIFO. Try: none, FIFO.

<http://web.tecnico.ulisboa.pt/mcasquilho/compute/gc/Fx-3tubefill.php>



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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>

```
Optimal order size (replenishment),  
.s*, 3  
z*, 290.2
```

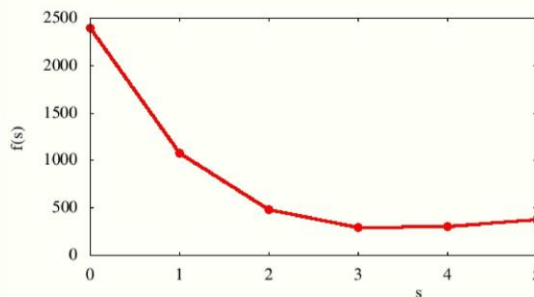
```
2013-05-27 UTC+0060 22:36:44.477
```

```
2013-05-27 UTC+0060 22:36:45.658
```

```
CPU: 1.2 sec.
```

```
End
```

EOQ: random demand with holding and shortage costs



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Mon May 27 22:36:45 2013

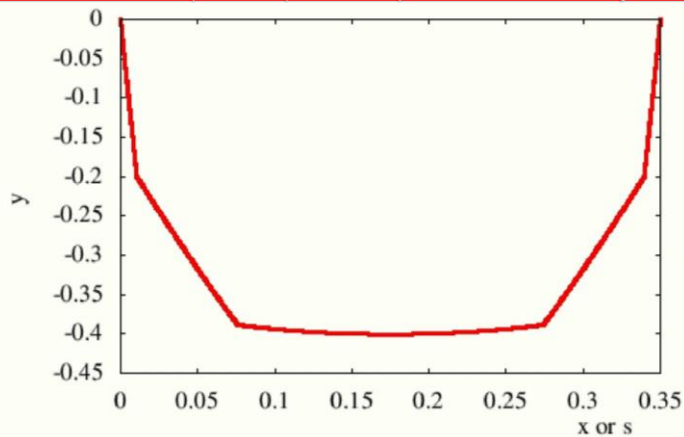
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1. 2. 3. 4. Examples

- **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

Mon May 27 22:46:56 2013

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Results

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

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	
T0,	313.0		K	
CP, DeltATR,	1.18	500.	kJ/L-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) ?		1	Temperature or conversion	
Show values (0) ?		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 CPU: 0.4 sec. End
 2013-05-27 UTC+0060 23:13:58.238

Semicontinuous cooled reactor

Mon May 27 23:13:58 2013

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1. 2. 3. 4. Examples

• **Minimum distance “within an angle”** \Rightarrow Try $\gamma = 50^\circ, 5^\circ$
<http://web.tecnico.ulisboa.pt/mcasquilho/compute/com/Fx-angdistlmg.php>

If x_2 = x_1:	0.41318	0.49240	(absolute minimum d0)	d0 = x_1 cos^2 = x_P = 0.41318
x_P, y_P,				
If x2 = infinity:	0.82635	0.98481	x_P = 2 d0	
x_P, y_P,				

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
Mn. distance,		3.3229	A-P-B

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

Distance within an angle

Mon Jun 03 02:11:55 2013

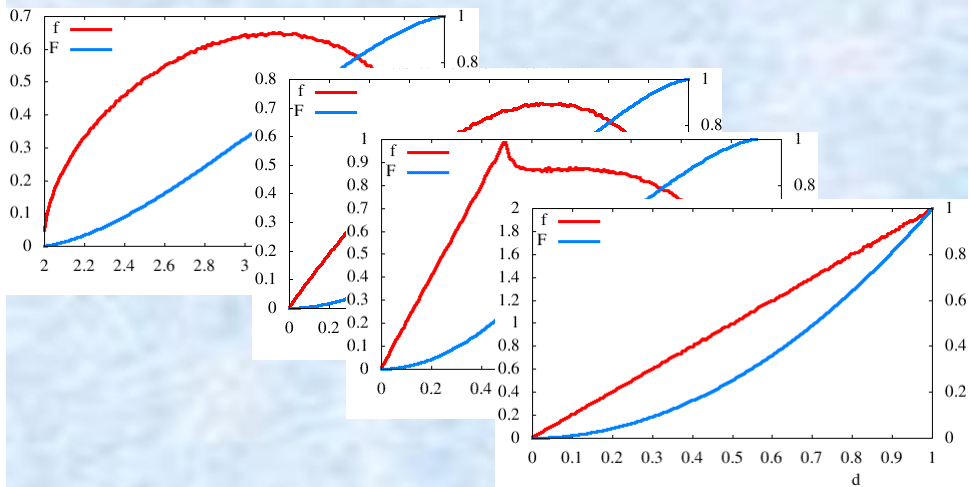
(Casquilho & Buescu [2011])

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1. 2. 3. 4. Examples

- Distance to points in a circle \Rightarrow 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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Henrique Medina
(1901–1988)
“A rapariga da
galinha branca”
(The girl with the white hen)

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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**

Minimum distance "within an angle" Execute

Calculates a minimum distance within the sides of an angle, showing the solution image. 2013.May.28.00:00:34

7	50	degrees (driven to $0 \leq \gamma < 90^\circ$)	Angle (see Figure).
			Abscissa of B (end point), not < 0 for easier graph.

sides of an angle^o (see Figure). $D = d_1 + d_2$, to go from A, with (fixed) $x_1 = 1$, to B, with x_2 , both on the x axis, passing by P, to be determined, on the half-line s, given the angle γ and x_2 . [$\gamma := \text{MOD}(\gamma, 90)^\circ$]
 Point $P = (x, y)$, with radial coordinate ρ , is found by differentiation
 $r \cdot x^{-1} = \frac{1}{2} (x_1^{-1} + x_2^{-1}) \sec^2 \gamma$. In polar γ (R below) and $\theta \equiv \gamma$. Counterintuitively, *mic* (not the arithmetic) mean.
 and y are, thus: $0 \leq x \leq 2 x_1 \cos^2 \gamma \leq 2 x_1$. Thus, the graph would not need to exceed P describes a circle with radius R centred
 in the Figure.

Plate: angdistRemote

2011, "A minimum distance: arithmetic and harmonic means in a geometric dispute", *Mathematical Education in Science and Technology*, **142**(3), 399–405
[10.526253](https://doi.org/10.526253) (250 kB)
<http://www.mathworld.com>, from MathWorld — a Wolfram Web Resource (2008-01-01).
 Wilhelm (1944-12-25).

<http://webpages.fc.ul.pt/~macasquilho/compute/Fx-angdistRemote.php>
 Created: 2012-11-03 — Last modified: 2013-03-05

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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”

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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).

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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
- **Milipeia** (Lab. of Advanced Computation), University of Coimbra
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Keywords

- Scientific computing; Web; Internet; academia, industry

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- **Hughes**, Alan [2006] “University-industry linkages and UK science and innovation policy”, Working Paper No. 326, Centre for Business Research, University of Cambridge, Cambridge (UK)
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