Aspects of High Performance Computing, the underlying national e-infrastructures and the international dimension

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Three talks in one

• Computational Science and technology

<intermezzo>

• Building e-infrastructure, given SC, grids, data

<intermezzo>

• About organisation at national level and Europe
Chapter 1: About the exiting world of computing

• The development of a new science: computational research

• About the interaction of research and computing technology
• Born in 1918 in The Netherlands,
• Worked at Philips, University of Chicago
• PhD in 1950:

Prof. dr. Clemens J.J. Roothaan

• In 1951 Roothaan published an article in Reviews of Modern Physics
• About solving the many-electron equations of motion for atoms and molecules

PART I: The pioneering development of a new science
The pioneering development of a new science (2)

- The “SCF-MO-LCAO” equations were so elegantly and expressive that they just had to be programmed in computer code.

From one of the PH.D. Committee members: “Never mind all those beautiful formalities – what can you really calculate?”
“Computational Science”

- The idea that equations could be solved not only *qualitatively* but also *quantitatively*
- The feeling (or vision) that computers could play an essential role in doing so.

- From $H\Psi=i\hbar\frac{\partial}{\partial t}\Psi$ to (photo-excitation processes in biomolecules)
Calculated, but how?

• On a 1953 computer!

For example on an IBM 701

0.016 Mflop/s
0.00128 MB memory
100m2 floor
75 KW

But still 100,000x faster than by hand…
Meanwhile in Turkey…

- A little later, in 1960, the first electronic computer appeared in Turkey.
- It was an IBM 650 Data Processing Machine.
- Taken into use by the General Directorate of Highways (Kara Yolları Genel Müdürlüğü) in 1960 and used until approximately 1972.
- Completed with an IBM 355 disk unit it was known as the IBM RAMAC 650.
Did the vision become true?

- Can we really calculate the result of complex processes, multi-particle interactions, multi-scale processes?
- Can we do so accurately enough?
- Can we do so fast enough to be relevant?
Complexity increased

• Physical problem size in chemistry ~ related to the number of electrons, n, according to $n^4 - n^6$, depending on the quality of the approximation.
• 1951: small and simple, 10 electrons, problem size $\sim 10^4$
• 2009: large and robust, >1000 electrons, problem size $\sim 1000^6 (=10^{18})$!

• Ergo $> 10^{14}$ more computational power required today than in 1951.
• (or a little less due to increased methodological insights and programming skills)

• $\rightarrow 1.6 \times 10^{18}$ Flop/s would be required, we are at about $10^{15}$ max (1 Petaflop)

• *Only increased computational power (+ intelligence) enabled this progress*
• But do we just do more of the same or is it about essentially more than that?
I think we do essentially more

- Biochemistry, large proteins, elements of life
- Catalysis, large macromolecules help us save energy (washing at low temperature)
- Chemistry in climate, green house-chemistry
- Relativistic chemistry, for heavy elements
- Molecules “on demand”-nanochemistry
- Increased interaction with experimental chemistry
- Applied computational chemistry plays a large role in daily life.

And chemistry is only one of many application fields.
Methods come in different flavours and styles

- For large proteins
- For relativistic chemistry (Dirac)
- Or Electron density-based
- For Molecular Dynamics
- For systematic higher order improvements

There exists a large diversity in software for different purposes. Not only researchers but also companies develop codes.
What’s more to come? (1)

- Bio-medical:
  - Simulation of the complete cell;
  - Simulation of the complete heart beat, with 3D EM field
  - Simulation of the 3D vascular deformation at heart beat
  - Brain functionality, 3D complete neuron network
What’s more to come? (2)

- Methodological improvements:
  - Relativistic chemistry: the chemistry of heavy elements, 4-component Dirac-based
  - Carr-Parrinello (electronic and nuclear motion in one model)
- The domain of nanochemistry
- Ab initio chips (grow chips from atom to computer chip)
- New materials
- New medicines
PART II: The other large domain in computing: computational fluid dynamics

- In 1759: equations of motion for fluids by Leonhard Euler. Expressed as partial differential equations this was revolutionary.
- In 1822: the general equations (incl. friction) for non-compressible fluids by Claude Navier
- In 1845: the general equations by George Stokes also for compressible fluids
- Presently known as the Navier-Stokes equations

\[
\begin{align*}
\partial_\alpha u_\alpha &= 0, \\
\partial_t u_\alpha + u_\beta \cdot \partial_\beta u_\alpha &= -\frac{1}{\rho} \partial_\alpha p + \nu \partial^2_\alpha u_\alpha.
\end{align*}
\]
CFD in three lines

• Easy for fluids
• Difficult for people
• Impossible for computers*

*by: Phil Gresho: Incompressible Flow and the Finite Element Method
John Wiley & Sons, 2000
However...

- According to Van den Herik and Postma:

At the University of Tilburg 27 March 2009, a dual inaugural lecture was held by Prof. Jaap van den Herik (Computer Science) and Prof. Eric Postma (Artificial Intelligence) about "faith in computers".

Van den Herik deals with the question can computers believe (have faith) and shows that mankind can keep on believing in computers. Postma sketches the future perspective of the friendly computer (the companion).
John von Neumann forecasted in 1946 that ‘automatic calculating machines' would replace the analytical solution of the simplified fluid equations by a ‘numerical' solution of the complete, non-linear equations for general geometries. This marked the start of conceiving Computational Fluid Dynamics (CFD)*.

Today there are many derivations of the formal theory, but there are main lines:

- **DNS (Direct Numerical Simulation)**
- **LES (Large Eddy Simulation)**

DNS is what it says, just brute force

LES stems from the late sixties in, to simulate atmospheric air currents. After that it became in use in engineering.

*After: “geschiedenis van de stromingsleer, CWI”.

An eddy is a turbulence such as arises after passing an object and the back stream to the virtual hole behind the object.
A pallet of specific applications

Computational problem size grows with $Re^{(11/4)}$!

Reynolds number $Re$ is a dimensionless number that can be used as a measure for the balance between the powers of inertia and viscosity.

$Re \ll 1$ \hspace{1cm} $Re \gg 1$

- creeping
- inviscid

<table>
<thead>
<tr>
<th>Object</th>
<th>medium</th>
<th>speed in km/h</th>
<th>Reynolds</th>
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<tbody>
<tr>
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<td>air</td>
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<tr>
<td>Skater</td>
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<td>air</td>
<td>80</td>
<td>$2.10^6$</td>
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<td>Shark</td>
<td>water</td>
<td>20</td>
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<tr>
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<td>air</td>
<td>900</td>
<td>$2.10^7$</td>
</tr>
<tr>
<td>Ship</td>
<td>water</td>
<td>20</td>
<td>$2.10^8$</td>
</tr>
</tbody>
</table>

Veldman & Verstappen NAW 5/2 nr. 4 december 2001
From: http://www.cyclone.nl/rekenen/rekenen.htm
CFD, a super domain for supercomputing

- Straight flow
- Turbulence
- Rheology, “like ketchup”
- Liquid and gas phase
- According to Newton, or with QM interacties

- Moving objects
- Flow along objects
- Fluids with spec. properties (blood, oil)
- Bubble formation

- Interaction with other phenomena
  - Chemistry, in combustion
  - Chemistry in pollution
  - Chemistry in chemical reactions (in a pipe)
  - +finite elements
  - ....
CFD

- CFD in water
  - Integral national water management
  - Sea, coastal protection, artificial island
  - Rivers, estuaries
- CFD in technology, cars, planes, factories, processes
- CFD in air, weather and climate
  - Pollution spreading
  - Consequences climate change
  - Climate influencing
  - Interaction between air, water and land (+bio)
CFD in weather and climate

• Were collapses of the Atlantic MOC responsible for the rapid temperature fluctuations on Greenland over the last 100,000 years?
  • repeated inflow of freshwater due to massive iceberg releases
• What is the probability that a collapse will occur before the year 2100?
  • possible freshwater input due to melting of the Greenland ice cap
• What is the impact of such a collapse on the weather in Europe?
  -> Need for Climate Models!

Few scientific creations have had greater impact on public opinion and policy than computer models of Earth’s climate (Nature, March 15, 2008)

10 Gflop/s Ocean Model

1 Tflop/s + Carbon cycle + aerosols + circulation

15 Tflop/s + vegetation + chemistry

400 x 400 km, L12, 100 yr, #1

200 km x 200 km, L18, 1000 yr, #1

50 km x 100 km, L24, 1000 yr, #5-10

Date: 1996

Date: 2001

Date: 2007

Volcanic activity

Carbon cycle

Atmospheric chemistry

Vegetation interaction
Are you prepared for Copenhagen? Do you want to know for yourself? Compute your future!

Turkish Climate policy plans

CO₂ Emissions
- 1990-1995 %23.1
- 1990-2000 %60.3
- 1990-2004 %72.6

Policy Proposal: Research
- Scientific and Technological Research Council of Turkey (TUBITAK)
- Attract other public and private research institutions
  - Develop and submit requests for funding from the World Bank, UNDP, and the EU

1st National Conference on High Performance Computing

UNIVERSITIES
NATIONAL CENSUS FOUNDATION

BAŞARI'09
I. Ulusal Yüksek Başarı ve Grid Konferansı
15-18 Nisan 2009, ODTÜ KKM, Ankara

TEMA
EVDE SUYU KURTARMANIN 10 YOLLAR
NE KADAR SU HARÇADIĞINI HESAPLA
NASIL TASARRUF EDERSİN?
EVİN İÇİNDE SAMAL TUR

COPI5
COPENHAGEN
UNIVERSITY
CLIMATE CHANGE
CONFERENCE
DEC 7-DEC 18
2009
Interaction between computational science and technology

- Computational science is (still) the driver for e-technology innovation;
- Innovations descent quickly to mass-user level;
- e-Technology drives Computational Science methodology innovations.

Research

Computational Science (e-science)

New methods
New insights

New customers
New requirements

Manufacturers

e-Technology

Customers

Users
From the past to the present…

- Radio tubes,
- No RAM
- (mercury line sequential memories, few words)
- Mflop/s:
  - 0.005 (ENIAC, 1946)
  - 0.016 (IBM 701, 1953)
- The size of present supercomputers

Turkish first Electronic computer

IBM 3090 1987
IBM Blue Pacific 1998
Cray Jaguar XT3 2008
IBM Roadrunner 2008
IBM POWERparallel Systems SP2, 1994

- Chips
- Caches
- Solid state memory
- Disk
- Pflop/s >1
- The size of soccer fields
But there is nothing called “enough”

• Time for PRACE
• Time for EGI
• Towards EXAﬂops
Interaction between computational science and economy

Four lines from CS to economy:

- Research results, such as climate-friendly/low-energy consumer products
- Spin-off from the software development scene
- Boosting the country profile (compare Spain with BSC!!!)
- Focus on national interests: earthquake, stable building, harbor and coastal research, education
Computing and science

• Engineers develop computers
  – But for drafting Petaflop or Exaflop computers and their software the knowledge of the full scientific ICT-field is necessary
  – Researchers in the disciplines conceive their methods, but computer scientists and mathematicians are necessary to implement these efficiently on modern HPC-systems

• More importantly: applied computing (computational science) has established itself as fundamental research methodology (like the reproducible experiment and the forming of theory)

• Called the third methodology

• And that did not happen overnight…
<Time for an intermezzo>

• Some historical perspective…
• Let’s assume, for convenience, that in between 1900-1910 electricity became publicly available
• In homes electrical wires were installed gas light replaced, etc.
Some serious fun

- “Tit-for-tat”
- Laurel & Hardy
- Issued 1935
- In the US already shops for electrical appliances
  - Lamps,
  - Toasters,
  - Clocks
  - Mixers,
  - Hair curlers,
  - ... 
  - In NL: Irons!
The perspective

• This is the perspective:
  – 35 years after the introduction of a fundamental technology (electricity) already many products have been developed (like in the US). But we know now what has come to follow that…
  – We live now <20 years after the public introduction of the internet (www). With respect to the internet we still can expect a lot to come
  – We live now 50 years after the introduction of the computer in science/research. Are we mature?
Chapter 2: about HPC, grids, data, e-infrastructures

Two questions relevant for building an e-infrastructure:

1. What do you want to accomplish?
   - Who are the clients?
   - What is the ideal future situation (one transparent eco-system for the user?)

1. Which parameters define the character and dimensions of an e-infrastructure?
e-Infra parameters

- Parameters for the dimensions of an e-infrastructure
  a) Research and user profile;
  b) Latency, at various levels;
  c) Bandwidth;
  d) CPU capacity;
  e) Data: storage density and capacity, meaning (content) and curative requirements, addressability.
a) Research and user Profile

• Research topics, scientific and social profile determine what an e-infrastructure should deliver;

• Themes of interest determined by Universities, Research centers, Research councils, Public/Ministries/parliament
b1) Latencies in e-INFRA

Latencies are the major determining factor in communication (but often underrated)

- Latency can not be overcome, it only can be minimized!
- While we near nano and pico scales in chip design, the speed of light comes uncomfortably close (0.3 mm per picosecond)
b2) Latencies in e-INFRA

- System level Latencies:
  - Memory-CPU
  - Internal network latencies
  - “MPI”/SW latencies
- Supercomputers defined to be machines to solve latency-bound codes
- SC’s change a CPU-bound problem into a latency bound problem
- Clusters are characterized by network latency to processor speed balance
- Intersystem latencies
  - Grid Middleware latencies
  - National network latencies
  - User access latencies: Peer review/administrative (!)
b3) Latencies in e-Infra

- Latencies in networking
  - May immobilize efficient grid usage
  - Use hybrid networks on fiber optics
  - Switched light paths!
  - Data propagation up to 1/3 of c
  - Distance Istanbul-Ankara is 350 km
  - Distance Istanbul-Van is 1644 km

\[ C = \text{“only” } 300.000 \text{ km/sec} \]

Roundtrip time:
- Istanbul-Ankara: > 2,3 msec
- Istanbul-Van: > 11 msec

1 msec ~ \(10^7\) cycles at 10 GHz

Prof. Gee-Kung Chang’s hybrid network
c) Bandwidth

- *Presently* bandwidth is not a severe issue
  - Not in computer systems, unless in the # paths to and from memory and in a far multi-core future;
  - Not in networking, in most cases.
  - (but this was different in the past)
- If bandwidth is short, replication is an easy remedy

The word broadband comes from the broadness of the data cables (one wire per bit) used in (older) computer systems.
d1) Pure processing power

- Science always requires more computational power than is available;
- Scientific requirements drive the demand for power, limited only by available funds
- (→ peer review)
d2) Pure processing power

- How does a code map onto a computer architecture?
- “One size fits all” is not true
- Different codes require different architectures
- How do you provide different architectures with a limited budget? (see chapter III)

- Vector $\leftrightarrow$ scalar
- Shared $\leftrightarrow$ distr. Mem.
- Latency $\leftrightarrow$ bandwidth
- Fastest single processor $\rightarrow x$ power/m$^3$
- Capability $\leftrightarrow$ capacity
Today it seems we produce more data every day than were produced and collected ever since the development of mankind.

e1) DATA

- Storage
- Services
- Replication for protection
- Transfer speeds
- Addressability
- Local or distributed
- ...
• The grid means different things for different people
  – The grid limited: like EGEE
  – The grid limited: defined by its middleware: glite, globus, unicore, boinc
• Basically modern grids are not used to solve problems over more than one system -> latency reduction
  – Modern grids provide a super-scheduler over the available resources (usually clusters) (this brings the latency-issue back into the systems)
  – Grids yield better return on investments for the resources in the grid
• Grids and HPC-resources are not mutually exclusive: HPC resources complement any grid infrastructure

*The broader vision on the grid: the co-carrier of the e-infrastructure (together with the network)*

Also consider sensor grids, like LOFAR for astronomy research, like for earth quake sensing, like for water management
Not the expert’s vision:

- Clouds are the non-transparent version of grids
- Less control
- Probably usable for very standardized applications (of which there are many)
- Offered as a pay-per-use commercial service
- Grid is rather about sharing
- Commercial clouds and shared grid can well coexist
Main events in Networking, grids and Supercomputing: (where one has to be - at least once)
- SC09 (SCxx series, since 1988, Portland OR, US)
- ISC09 (ISCxx series, since 1986, Hamburg, D).

SC08≈10.000 participants; well refereed scientific program
Chapter 3: How to organize e-Infra?

• At the national level
• At the European level (and beyond)
National e-Infra organisations
two examples

• The Swedish model
• The Dutch model
• Other models
The Swedish model (1)

- HPC2N (Umeå)
- UPPMAX (Uppsala)
- PDC (Stockholm)
- NSC (Linköping)
- C3SE (Göteborg)
- LUNARC (Lund)
The Swedish model (2)

- One organisation, SNIC
- Six independent well interconnected centers (universities)
- A collective, “democratic” approach
The Swedish model (3)

- SNIC is a well organised, (and managed) compact organisation
  - Board
  - Allocation committee (peer review), (SNAC)
  - User representatives in user group (SNUG)
  - Is the NGI for Sweden (NGI=National Grid Initiative)
  - The infrastructure had become fully grid-based
The Swedish model (4)

• Advantages:
  – Conceptually simple
  – Centralised organisation
  – Resources fully distributed
  – “conflict avoiding”
  – Flat infrastructure

• Disadvantages:
  – Flat infrastructure
  – Minimal variation in resources
  – No differentiation in architectures or system sizes

However, the model as such does not exclude differentiation
The Dutch model

- The Netherlands has a coordinated national e-infrastructures policy since 1985
  - It started with networking and supercomputing (1985)
  - Then an auxiliary policy followed (1994 onwards)
    - Additional systems co-financed by universities
    - Including CAVE and visualisation
    - Including massively parallel computing
  - National secure data storage (2000)
  - (Digital academic repositories by SURF 2002)
  - Grids (since 2004)
  - BiGGrid (since 2006)
- Population: 16.6 million
- GDP/Cap. €30,000
- (Dutch population is ¼ of Turkish population of 71.9)
Note that all such information can be obtained from knowledgebase.e-irg.eu!
Note how close The Netherlands and Turkey are!
The Dutch model - NCF

• National Computing Facilities Foundation (NCF)
  – Whenever resources become too big (expensive) for a single university (like supercomputers)
  – Long term policy setting
  – Funding by the national research council, NWO, (National Organisation for Scientific Research)
    • Fixed long term budget+extra’s
  – One national academic (super-)computing center (SARA)
    • With bi-location in Almere
    • And with University of Groningen CS as runner up
The Dutch model: elements of policy

- National research profile
  - Universities
  - NWO (Research Councils)
  - KNAW (Royal academy of Sciences)
  - Government
  - EC
- Technological developments
- European neighbor policies
- Available funding
The Dutch model: variety

• System variety
  – National cluster (Dell)
  – IBM Blue Gene for LOFAR-project
  – “DAS-cluster” (for computer science experiments)
  – GPU-test clusters

• One national supercomputer (IBM Power-6)

• PRACE Principal partner
The Dutch model: organisation

- **Organisation**
  - NCF is a foundation
  - Board, 5 members
    - 2 researchers
    - 2 university board members
    - 1 researcher/external with links to business
  - Bureau (+/- 4 fte fixed, 2 EU-funded)
  - Scientific Committee=peer review committee
The Dutch model: conditions

- Boundary conditions
  - Basis funding structural
  - Solid peer review
    - Absolutely independent referees
    - Referees from the Netherlands and international
    - Committee: Declaration of non-involvement
  - Computing time allocations for one year
  - Fast turn around for the access process
    - Pilot projects, by return mail, no referees, limited budget
    - Normal projects and programs
    - Institute budgets
    - Dutch Computing Challenge Projects
  - Single application form/digital form for all resources
The Dutch model: more conditions

• A good relationship between network innovation, grid and resources management and policy is essential
  – This relation has been good since 1987
  – Further integration of networking, grid and resources policies is being investigated

• Governments do not (always) want to choose between different e-infra components to fund:
  Make the choices for the government
The Dutch model: acquisition

Supercomputer acquisitions
- Requires visible and tangible involvement of users
- Inquiries of present usage and plans
- Inquiries on technology, planned vendor portfolio’s
- Request for proposals
  - European tender for scientific research equipment
- Benchmark suite
- Selection, final negotiations, acceptance test
Other models

• Many countries, many solutions
• Germany, France, UK have no central organisations, just combinations of entities that may act on behalf of the country (Genci, Gauss centre, (EPSRC))
• Overall management and interaction between e-infra organisations and users is preferable.
From national to European e-Infrastructures

- Scientists were never bound by borders
- And the same should be true for e-infrastructures
  - Fortunately this is often the case
- Most countries can’t host the required variety of resources
- Most countries are willing to share
- The EC strongly supports collaborative efforts in e-infrastructures
- Turkey is involved in many of those efforts
Examples of cooperative efforts:

- Géant, the European backbone network
- EGEE, the prototype pan-European grid project
- EGI, the formal organisation that builds on these efforts
- DEISA, that connects existing major national computing resources
- PRACE, the project and formal organisation that builds on these efforts and goes even further (Petaflop computing)
Just an observation...

Be sure to connect to the European e-infrastructure at all levels:

– Networking
– Gridding
– Supercomputing
– Data storage and services
– Repositories and curation

Shaping Europe’s digital future
From European to world scale e-Infrastructures

• e-Infrastructures are to be connected worldwide
  – Europe, Asia, Africa, The Americas, Australia
• e-Technology developments require world scale efforts
  – From networks to grids to supercomputers

*Turkey can play a pivoting role!*
Davetiniz, ilgi ve dikkatiniz için teşekkür ederim.