Political Vision on e-Infrastructures for Science & Innovation

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informed through membership of
PRACE Scientific Steering Committee
UK e-Infrastructure Leadership Council

The words are coded

Political Vision on e-Infrastructures for Science & **Economic Growth**

Visions?

Politician

- visible socio-economic impact during my term?
- (EC) Europe wide cooperation and benefit
- (exceptionally) legacy to science and innovation

Provider = Centres + Suppliers

- scientific and political agendas justify large budgets
- technology is complex, expensive and changing fast
- (increasingly) money is in services not hardware

New hardware = photo opportunity

Visions?

Scientist

- provided by others for free
- (so) modify research to what is possible
- (exceptionally) drive technology and engage with e-infrastructure

Industry User

- never heard of it, can't see the benefits, no time to engage
- (increasingly) core to my business
- (clouds?) can't get enough expert people, or buy the services I need

The case … is made

PRACE – The Scientific Case for HPC in Europe 2012 - 2020

"Molecular simulation is a key tool for computer-aided drug design … ***Biomedical Simulation*** *will reduce costs, time to market and animal experimentation. In the medium to long term, simulation will have a major impact on public health, providing insights into the cause of diseases and allowing the development of new diagnostic tools and treatments. It is expected that understanding the basic mechanisms of cognition, memory, perception etc. will allow the development of completely new forms of energy efficient computation and robotics. The potential long-term social and economic impact is immense."*

"The ***automotive industry*** *is actively pursuing important goals that need exaflop computing capability or greater. Examples include (i) vehicles that will operate for 250,000 kilometres on average without the need for repair; … and (ii) Insurance companies require full-body crash analysis that includes simulation of soft tissue damage"*

"The impact of ***computer simulation in aircraft design*** *has been significant … Boeing, for example, exploited HPC in order to reduce drastically the number of real prototypes from 77 physical prototype wings for the 757 aircraft, to only 11 prototype wings for the 787 "Dreamliner" plane. HPC usage saved the company billions of dollars"*

*"***Computational materials science, chemistry and nanoscience** *is concerned with the complex interplay of the myriads of atoms in a solid or a liquid, thereby producing a continuous stream of new and unexpected phenomena and forms of matter, characterised by an extreme range of length, time, energy, entropy and entanglement scales. The target of this science is to design materials ranging from level of a single atom up to the macroscopic scale, and unravel phenomena and design processes from electronic reaction times in the femtosecond range up to geological periods."*

Communication from the Commission to the European Parliament

"High-Performance Computing: Europe's place in a Global Race", Brussels, 15.2.2012

"The race for leadership in HPC systems is driven both by the need to address societal and scientific grand challenges more effectively … and by the needs of industry to innovate in products and services."

"Access to rapid simulations carried out by ever-improving super computers can be the difference between life and death; between new jobs and profits or bankruptcy."

"… whilst there is great confidence in the fact that ***climate change*** *is happening, there remain uncertainties … Increasing the capability and comprehensiveness of 'whole Earth system' models that represent in ever-increasing realism and detail, scenarios for our future climate is the only way to reduce these latter uncertainties."*

In ***Astrophysics*** *determination of the nature of dark energy and dark matter requires a detailed comparison of predictions from large classes of cosmological models with data from the new satellites and ground based detectors which will be deployed until 2020.*
In ***high-energy physics****, one of the tasks is to explore many possible extensions of the Standard Model to such a degree, that even minute deviations between experimental data and Standard Model predictions can serve as smoking guns for a specific realization of New Physics.*
In ***plasma physics****, one of the tasks is to understand the physics observed at ITER at such a high level that substantially more efficient fusion reactors could be reliably designed based on theoretical simulations which explore a large range of options."*

But … what is the value proposition?

- (electricity myth) 20MW politico-economic pain barrier can be crossed
  - proxy for how much we value the results

- (truth) computational models are not commensurate with the importance of their results
  - uncertainty quantification, validation, verification
- (screams) big data!
  - data deluge is driving demand
- (politics) no obvious limit when the stakes are high
  - global and scientific challenges
  - emergencies
  - quality of our lives
- (threat) errors will waste €Ms and wrong results could be catastrophic

Recommendations from scientists

1 The need for HPC infrastructure at the European level

The scientific progress that has been achieved using HPC since the "Scientific Case for Advanced Computing in Europe" was published in 2007, the growing range of disciplines that now depend on HPC, and the technical challenges of exascale architectures make a compelling case for continued investment in HPC at the European level.

2 Leadership and management

The development of Europe's HPC infrastructure, its operation and access mechanisms must be driven by the needs of science and industry to conduct world-leading research.

3 A long-term committment to Europe-level HPC

Major experiments depend on HPC for analysis and interpretation of data, including simulation of models to try to match observation to theory, and support research programmes extending over 10-20 year timeframes.

4 Algorithms, software and tools

Most applications targeting Tier-0 machines require some degree of rewriting to expose more parallelism and many face severe strong-scaling challenges

5 Integrated environment for compute and data

Most application areas foresee the need to run long jobs (for months or years) at sustained performances around 100 Pflop/s to generate core data sets and very many shorter jobs (for hours or days) at lower performances for pre- and post-processing, model searches and uncertainty quantification. A major challenge is the end-to-end management of, and fast access to, large and diverse datasets, vertically through the infrastructure hierarchy.

6 People and training

There is grave concern about HPC skills shortages across all research areas and, particularly, in industry.

7 Thematic centres

Organisational structure is needed to support large long-term research programmes, bringing together competences to share expertise. This could take the form of virtual or physical Thematic Centres which might support community codes and data, operate dedicated facilities, focus on co-design, or have a cross-cutting role in the development and support for algorithms, software, or tools

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investment in software

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ISV codes

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cloud

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Competence Centres

make it accessible and cheap

The political process

"So here is Industrial Strategy 101. You set up a leadership council probably co-chaired by a BIS minister and a senior industry figure in which researchers, businesses, perhaps regulators a purchasers come together. You use it to get them talking to each other confidently that group might commission a trusted expert to prepare a technology road map w e the relevant technologies are heading over the next five years or so, where publicl s going, and what business is likely to do. Just this exercise, before any increase in pu transform behaviour.

ETP 4 HPC

- Member States are invited to carry out joint procurement activities and to use PCP to stimulate the development of advanced HPC systems and services. Each Member State should actively encourage the use of PCP and devote in the order of 10% of its annual HPC procurement budget to it.
- The Commission should contribute to the funding provided collectively by Member States for PCP of R&D on HPC systems services with an EU-level mission and with EU-wide availability.
- HPC e-Infrastructure projects receiving funding from the Commission should be encouraged to use PCP where relevant.
- EU Industry is encouraged to actively engage in advanced HPC and application development efforts in response to PCP.

neans their managers here and nore investment here. It can w it fits in alongside investment government puts some money

s the opposite and some need ely be adopted.

ore and more willing to go for an But crucially you have a vehicle

The quality of links between business, the research community and government is itself a source of comparative advantage in the modern world."

The Rt Hon David Willetts (UK Minister for Universities & Science, 24 Jan 2013)

The challenge we face

e-infrastructure is

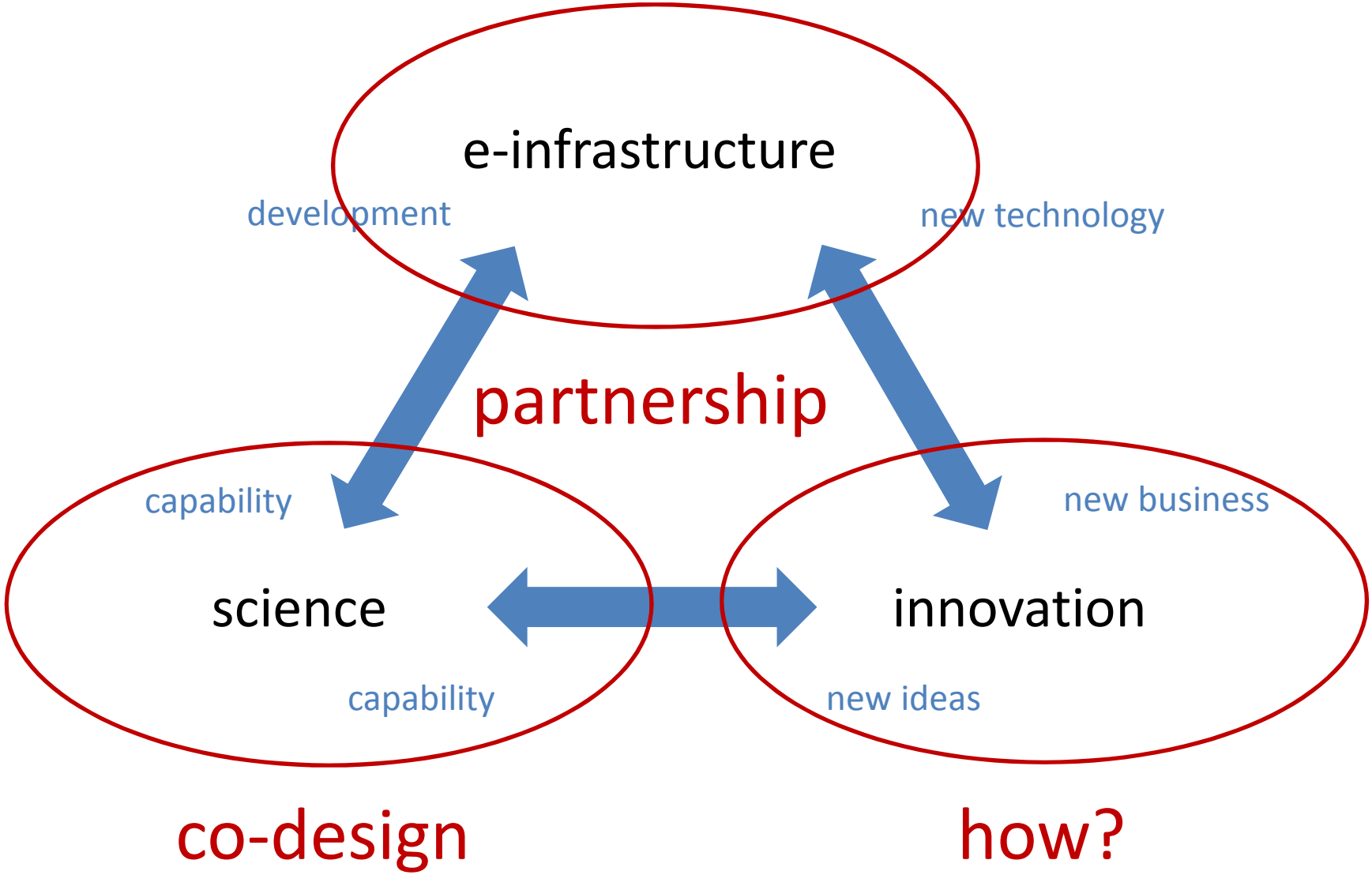
- seen as a vehicle for socio-economic strategy
  - "innovation" + "open data" = growth?
- complex, fast changing, driven by science and technology
  - owned by no one constituency
- increasingly pervasive
  - internet of things, mobiles, international facilities
- full of potential
  - not yet a service

Directions to 2020

- political reality
  - must address growth agenda
- technical reality
  - science and innovation are e-infrastructure limited (hardware + software + services)
  - public sector provision must extend beyond the commercial market (to lead it)
  - e-infrastructure extends beyond national capabilities (coordination + subsidiarity)
- many paths forward = many dead ends
  - co-design at all levels = users and providers in partnership
- who leads?

> *"Our partnership for advanced computing, PRACE, already makes supercomputer capacity available, for industry and academics to simulate and design. Why not make access to those platforms systematic, pervasive, available to every high-tech small company?"*
> Neelie Kroes, EC Vice-President for the Digital Agenda, 25 September 2012

interrelationships



How to promote innovation = growth?

- raise awareness
  - amongst SMEs of the business opportunities
  - amongst scientists and their funders of the need to share expertise
- increase openness + accessibility
  - reduce regulatory barriers
  - fund fast and easy access to expertise = “on-ramps”
- create stability + roadmap
  - software benefits accrue over 10-20 years
  - encourage investment and new businesses

Train many more people!!!

- new skill combinations
  - computing + mathematics + domain science
  - urgent = no short-term fix
  - technological evolution requires on-going training
- opportunity for coordinated action across Europe
  - shared expertise + training materials
- make more efficient use of the people we have
  - build on existing centres of expertise
  - promote community codes + open data
  - encourage industry investment
- prerequisite for solving any of the other technical challenges!

people → innovation → economic growth

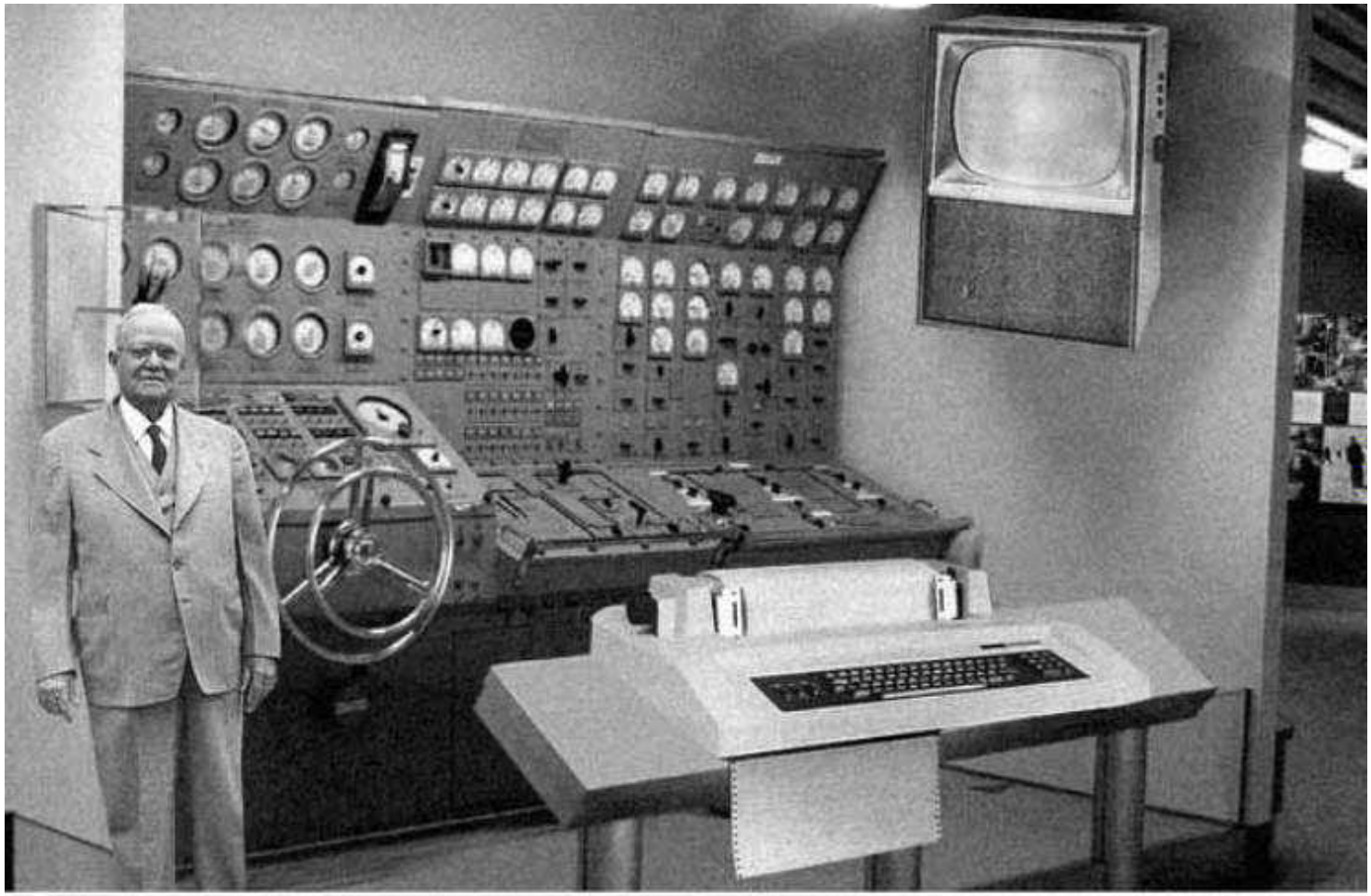
Co-work

- needed for the whole e-infrastructure
  - all components are interrelated and evolving
  - co-design is our only compass
- requirements are growing and changing
  - complex workflows + on-demand access + security + big data + open data → new knowledge
  - maintain a unified vision: divided we fall

BUT is “co-investment” a politician’s fantasy?

- or are we missing the value proposition?

If we fail …



Scientists from the RAND Corporation have created this model to illustrate how a "home computer" could look like in the year 2004. However the needed technology will not be economically feasible for the average home. Also the scientists readily admit that the computer will require not yet invented technology to actually work, but 50 years from now scientific progress is expected to solve these problems. With teletype interface and the Fortran language, the computer will be easy to use.

Take home messages

- e-infrastructure has a leadership deficit
  - unite
  - focus the vision
  - improve the value proposition

- users, providers, government must work together
  - expertise is in short supply
  - build on existing strengths

- transform education and training
  - mathematics + computing + data → knowledge