Computational Science & HPC

Scientific Paradigm, Adequate Technology and Organizational Strength

Dr. S. Bieri, CEO Bieri IP Partner

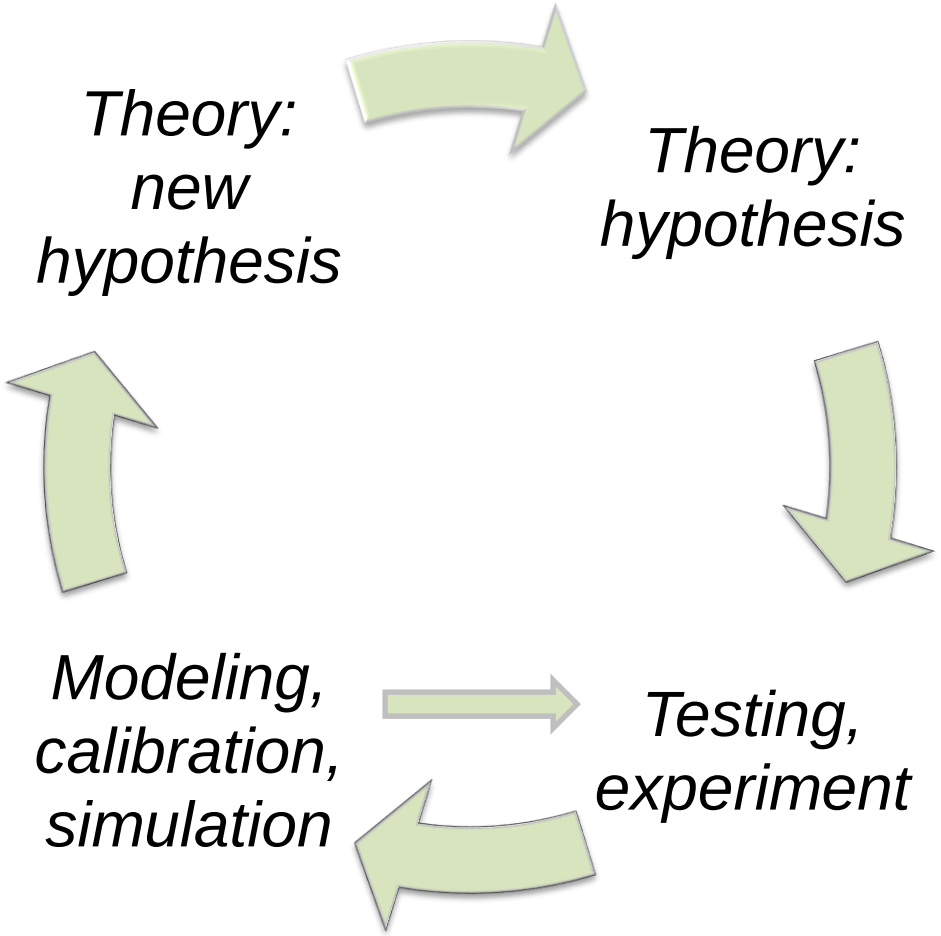
1. Bottom-line
2. The meaning of Computational Science
3. The data problem
4. A new distribution of tasks?
5. Functions of a HPC center
6. How to proceed

1. Bottom-line

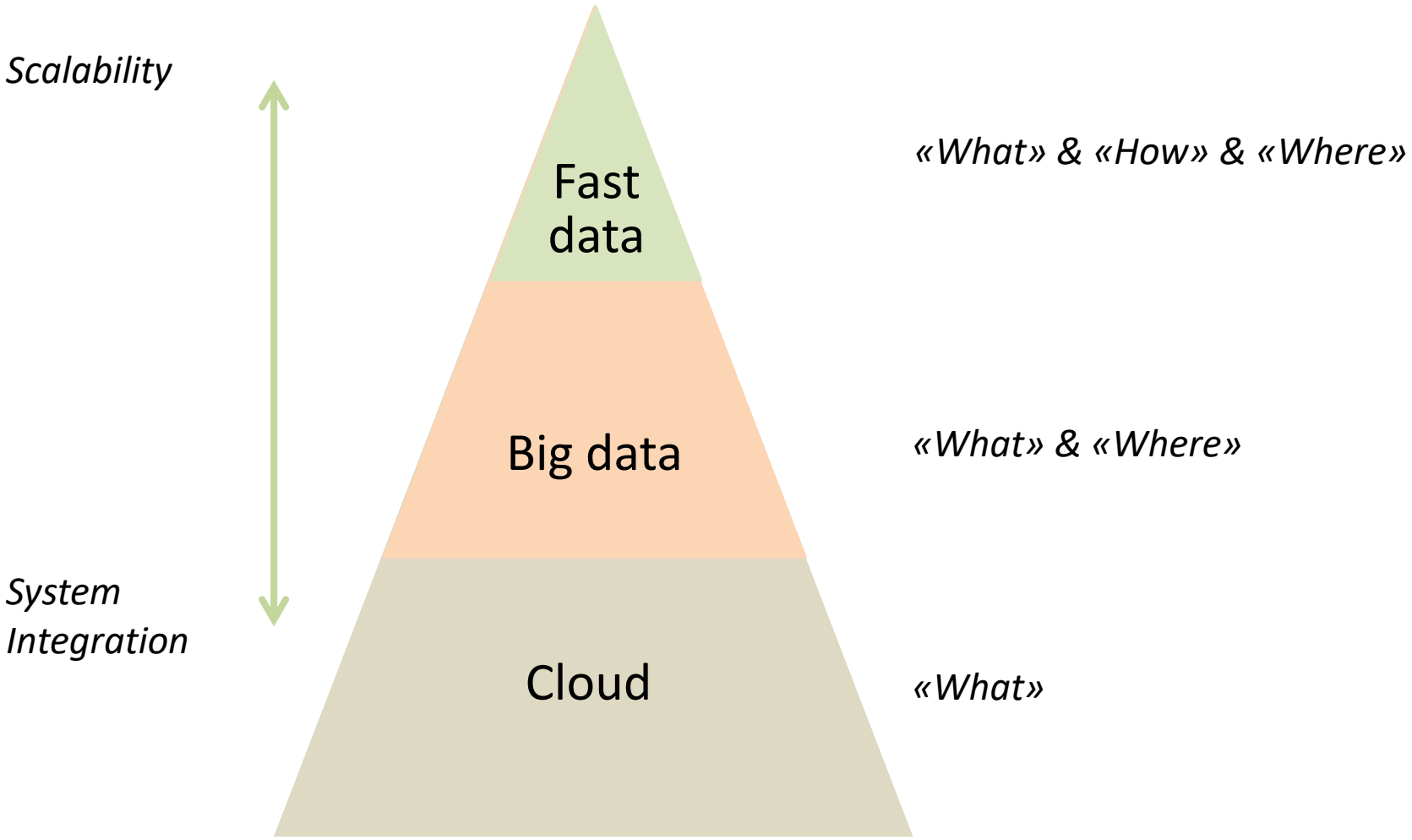
- Computational Science is a novel way of doing scientific work by using the power of computers – HPC is a prerequisite for it.
- HPC should be understood as holistic approach, combining technological with task driven interfaces and pushed by outstanding R&D.
- So hardware, software, and support are parts of one system.
- The cost-side dictates minimum scales and specialisation within a given scientific institution or network, but there is no everlasting hierarchy.
- The idea of a “HPC centre” implies four main qualities:
  a) a joint architectural concept of capacities,
  b) an integrated communication network including data storage,
  c) a congenial understanding of the scientific topics and the models used,
  d) a flexible service *and* knowledge base covering especially imaging and data mining.

2. The meaning of Computational Science

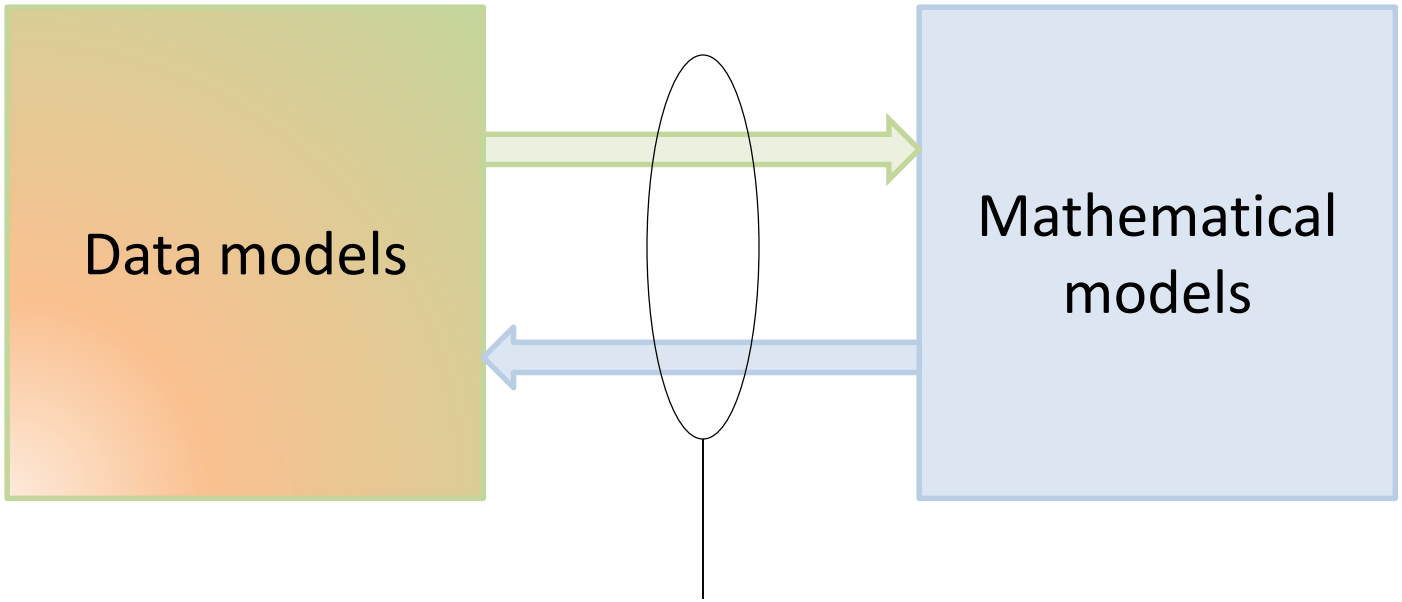
"Simulation is the synthesis of models and data!"



3. The data problem



4. A new distribution of tasks?



- Data intensive processing
- High throughput communication
- Sensoring

5. Functions of a HPC Centre (i)

	HPC Centre as institution wide *operator*	HPC Centre as *user lab*	HPC Centre as *research unit*
Goal	Providing integration & network	Offering capabilities & capacities	Autonomous R&D
Instruments	• Design of architecture • Operating hardware, software & network • „load management“	• HPC time • storage, software support & services (as package)	• Data models & codes • Technologies of shared computing, • R&D partnerships
Lead	Centre‘s management	Centre‘s SAB	Centre’s faculty

5. Function of a HPC Center (ii)

Front-end: Application of Simulation & Visualization

Zentrum für Visualisierung & Simulation *Portfolio: Modellierung,* ***Simulation, Visualisierung / Imaging****, Data Mining* *Aufgaben:* ***Support****, Hardware, Software,* ***Datenverwaltung***			
Teilnehmer	**Leading House**	**Interne Partner**	**Externe Partner**
Lehre & Forschung	• 1 Sonderprofessur mit Assistenz • 1 - 2 FuE-Gruppen	• Minimal 1 FuE-Gruppe pro Standort («Eintrittskarte»)	• Minimal 1 FuE-Gruppe pro Standort
Support & Administration	Koordinator mit 1 Supportteam		Vertragliche Zusammenarbeit
Infrastruktur	• Schneller Speicher in einer 2. Phase • Konzept Netzwerk • Software • Endgeräte • Reserveflächen	• Endgeräte	• Komplementäre Hard & Software • Endgeräte
Erstfinanzierung	• Eigenmittel • Sonderprofessur 6 Jahre • Projektförderung 4 Jahre • Investitionskredit in einer 2. Phase	• Projektförderung 4 Jahre	-

6. How to proceed

«Not money – the concept is the problem!»

- You need both leadership and organizational strength.
- Be aware that each user pretends to be a special case.
- Focus on synergies - enable forms of “joint modeling”.
- Proceed slowly and step by step, but keep milestones:

1. HPC Centre as institution wide operator	**2**. HPC Centre as user lab	**3.** HPC Centre as research unit
“Network & task distribution”	*“Resources”*	*“Ideas”*