



UNIVERSITY OF ICELAND
SCHOOL OF ENGINEERING AND NATURAL SCIENCES

FACULTY OF INDUSTRIAL ENGINEERING,
MECHANICAL ENGINEERING AND COMPUTER SCIENCE

RAISE
Center of Excellence



HPC Systems Engineering with the Interaction Room

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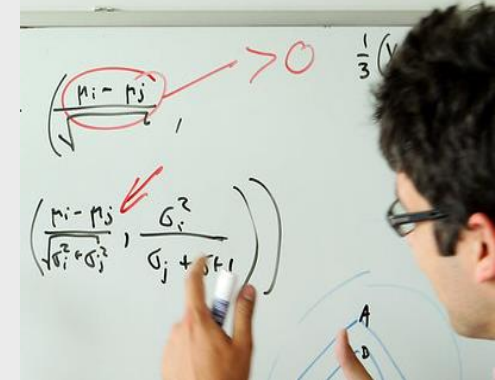
Interaction Room Might Work Well for Business Applications... ...but HPC Is Not a Business Application

- In fact, similar considerations apply as well, e.g.:
different implicit assumptions/knowledge between stakeholders:
- HPC projects often start with a domain expert writing HPC code.
 - E.g. Science/Engineering PhD student with no formal education in HPC nor Computer Science.
- The same problems at different occasions:
 - Code survives often academic scientists with temporary contracts:
Code needs to be handed over to new scientists.
⇒ **Implicit assumptions and knowledge lost.**
 - Domain expert sooner or later struggles with HPC problems: code needs to be handed to HPC experts, e.g.
at a supercomputing centre.
⇒ **Implicit assumptions and knowledge need to be transferred.**

Same within the CoE RAISE: Experts
with different knowledge working
together.

Interaction Room for HPC?

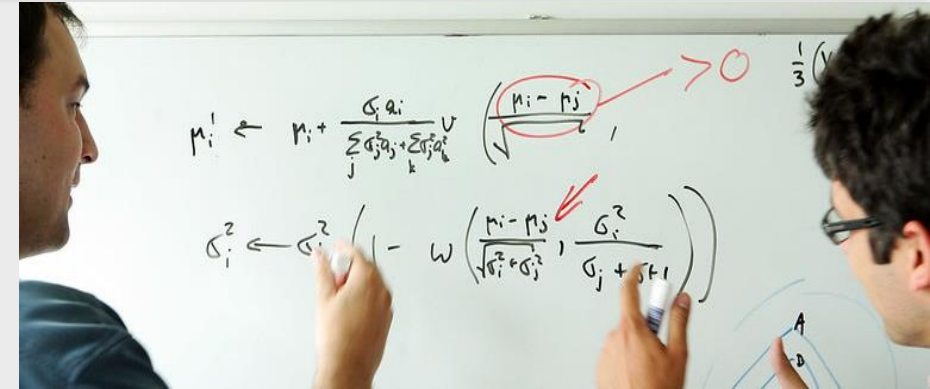
- Goal: Facilitate collaboration of experts from
 - the natural science/engineering domain,
 - the HPC domain,
 - the AI/ML domain,
 - the computer science/software engineering domain.
- Adapt proven Interaction Room concepts:
 - But: canvases needed that are specific to HPC/AI/ML needs.



Public domain <https://www.piqsels.com>

Interaction Room for HPC!

- HPC/AI-specific canvases that address:
 - Crucial interdisciplinary discussion points,
 - Typical HPC/AI software development phases.
- Different domains needing different canvas types, e.g.:
 - Simulation sciences (“classic” HPC),
 - Data sciences (HPDA) / AI/ML.
- So far: Interaction Room canvases developed for HPC simulation sciences...
- ...to foster **collaboration within CoE RAISE**:
go beyond \Rightarrow canvases for **HPC combined with AI**.



Book, Riedel, Neukirchen, Goetz: *Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room*.
4th ACM SIGPLAN International Workshop on Software Engineering for Parallel Systems (SEPS 2017)

Crucial Interdisciplinary Communication Points in HPC Simulation Science Projects

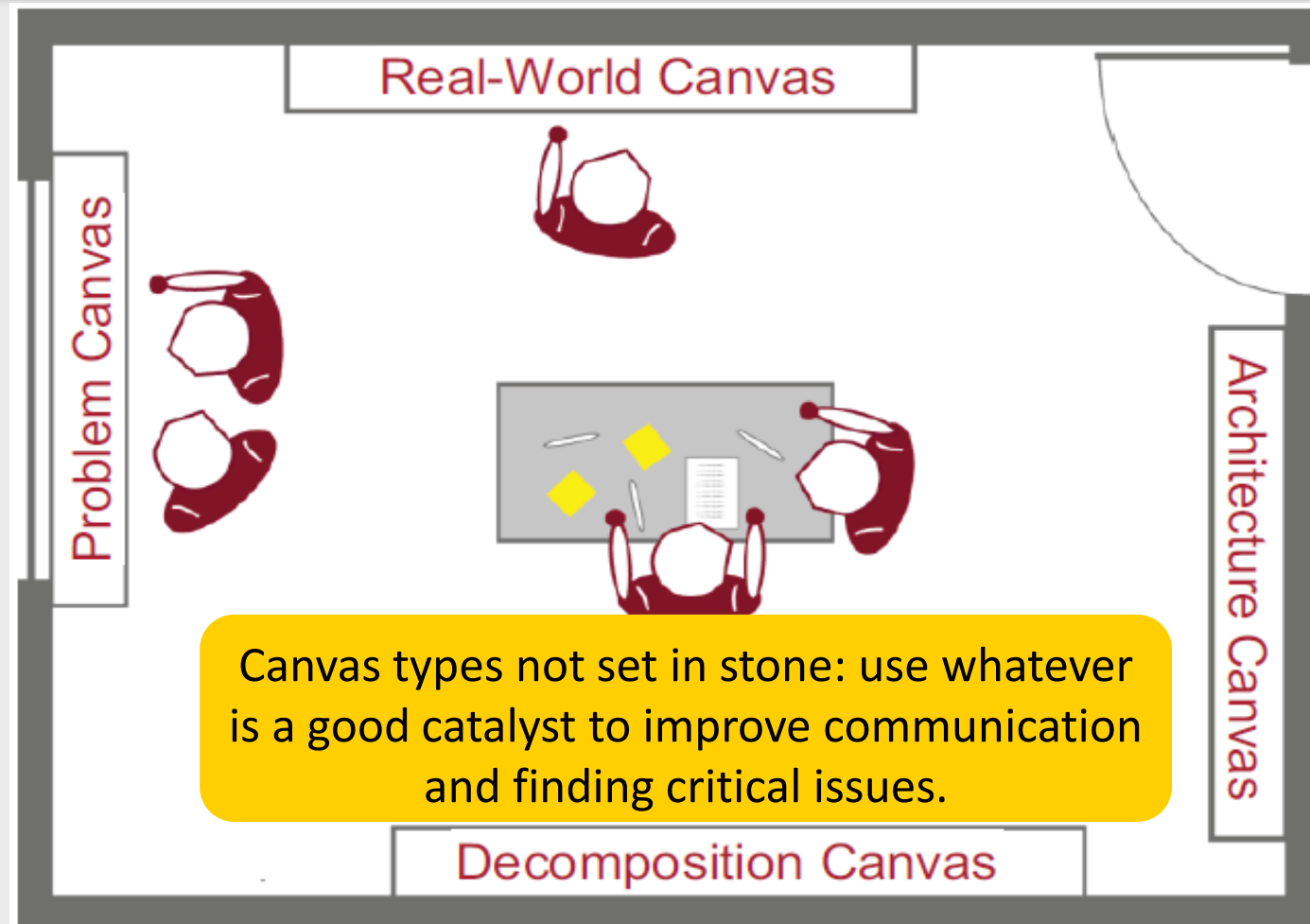
- Science/Engineering domain experts need to help HPC experts **understand**, e.g.:
 - Research question we trying to answer?
 - What assumptions/simplifications are made?
 - What parameters and variables are there?
 - How do they affect each other? How do they evolve over time?
- HPC experts need to **validate** technical decisions with domain experts, e.g.:
 - Domain decomposition (How to map the problem most efficiently to the HPC cluster?),
 - HPC cluster HW architecture? (CPU or GPU? Memory-intensive or compute-intensive?),
 - Memory model (Distributed memory? Shared memory? Hybrid?),
 - Communication patterns (Choice of communication type? Ghosts/halos?).

Typical HPC Simulation Science Software Process to be Supported by Interaction Room

1. Understand the problem domain:
 - a) In general (goal and scope),
 - b) In detail. (How would serial problem domain code look like?)
 2. Perform appropriate domain decomposition, choose appropriate communicators, etc.
 3. Implement communication between processes/threads; mix into code of problem domain.
 4. Test and validate simulation model and code.
 5. Optimize accuracy, tune performance (specific to HW architecture).
- Domain concepts to be supported by IR
- Domain concepts to be supported by IR
- HPC concepts to be supported by IR
- HPC concepts to be supported by IR

Interaction Room Canvases for HPC Simulation Science Projects

- **Problem canvas:**
 - Goal and scope of research question (=the science domain).
- **Real-world canvas:**
 - Description of the pertinent aspects of the science domain.
- **Decomposition canvas:**
 - Breakdown of scientific model into parallelizable units.
- **Architecture canvas:**
 - Implementation of simulation on suitable HPC technology/HW architecture.
- Not necessary sequential flow, but iterative refinement of canvas contents.



Problem Canvas

Goal and scope of research question about the domain

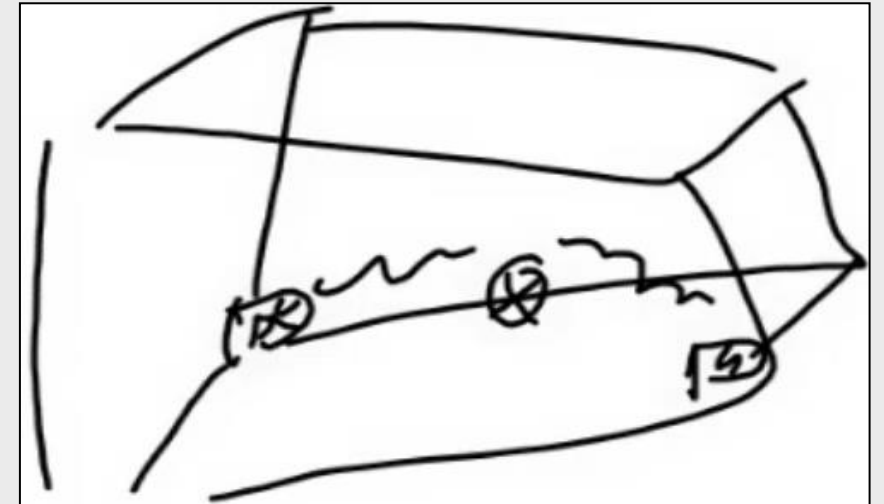
- Domain experts collect:
 - Research question,
 - Boundary conditions,
 - Assumptions,
 - Abstractions,
 - Quality requirements.
- Example: Heat dissipation problem
 - **Research Question:** “What will the temperature in a room after running an air conditioner on one side and a heater on the other for several hours?”
 - **Boundary conditions:** Starting temperature, A/C and heater setting.
 - **Abstractions:** Consider heat transfer by air flow / convection only, not by radiation.
 - **Assumptions:** No moving objects in the room, no windows/doors.
 - **Quality requirements:** Temperature must be determined as double precision float.



Real-World Canvas

Description of the pertinent aspects of the domain

- Domain experts sketch **static properties** of the simulation space:
 - Physical laws,
 - Spatial setup.
- Domain experts sketch **dynamic properties** of simulation process:
 - Forces,
 - Events.
- Example: Heat dissipation problem
 - Room geometry, heater & A/C location,
 - Working of convection forces/air flows,
 - Appropriate formulae for physical laws.



Decomposition Canvas

Breakdown of scientific model into parallelizable units

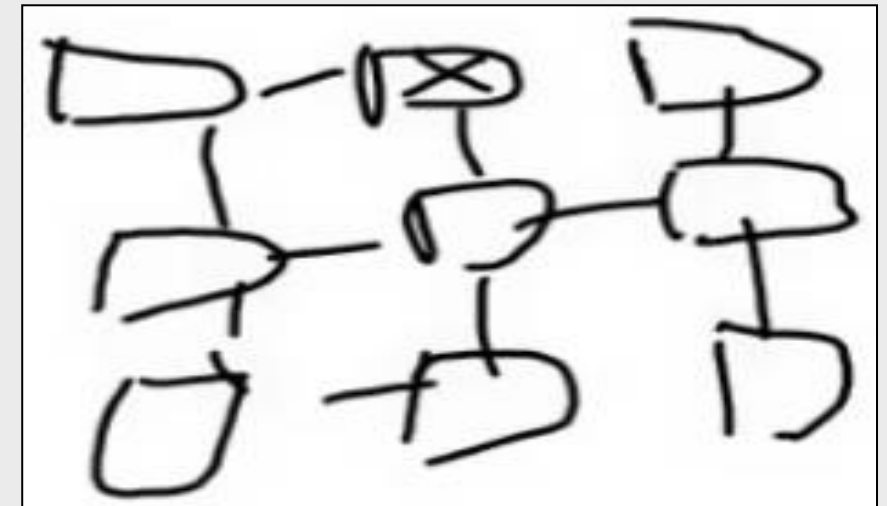
- HPC experts sketch parallel model reflecting real-world model:
 - **Static HPC aspects:** Domain decomposition, data structures.
 - **Dynamic HPC aspects:** Communication patterns, halos/ghosts, adaptive mesh refinements, iterative numerical methods.
- Example: Heat dissipation problem
 - Adaptive mesh refinement,
 - Halo creation & communication strategy,
 - Cartesian communicator,
 - Iterative method to solve formula of physical heat transfer law.





Architecture Canvas

Implementation of simulation on suitable HPC technology

- HPC experts sketch mapping of parallel model to actual cluster HW:
 - **Static aspects:** Cluster architecture, memory model, tools.
 - **Dynamic aspects:** Communication protocols, I/O operations, checkpointing.
- Example: Heat dissipation problem
 - 1024 CPU cores,
 - Hybrid MPI/OpenMP,
 - Jacobi solver,
 - Parallel I/O,
 - Checkpoints every 2.000 iterations.



- Interaction Room **facilitates collaboration of**
 - **domain experts (engineers/ scientists),**
 - **HPC experts,**
 - **AI/ML experts,**
 - **Computer science/software engineering experts.**
- Canvas topic types not set in stone. (Add what is a good catalyst.)
- Not only a tool within CoE RAISE WP2,
 - but also outcome of CoE RAISE itself,
 - reaching beyond CoE RAISE.

- To be developed during the CoE RAISE journey:
 - **Canvases for AI/ML.**
 - Including: combining HPC & AI, suitable annotations.  
- Virtual (due to COVID) Interaction Room sessions with individual RAISE CoE WP2 partners:
 - Collaborative whiteboard software,
 - Caveat: lots of interaction lost in video meeting, e.g. body language,
 - Participants need to talk.
 - If no one talks, the best Interaction Room does not help – but canvases are a good catalyst.

drive. enable. innovate.

Book, Riedel, Neukirchen, Goetz:

Facilitating Collaboration in High-Performance Computing Projects with an Interaction Room.

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