

Taxonomy of multiscale communities

Derek Groen, Stefan Zasada, Peter Coveney

University College London

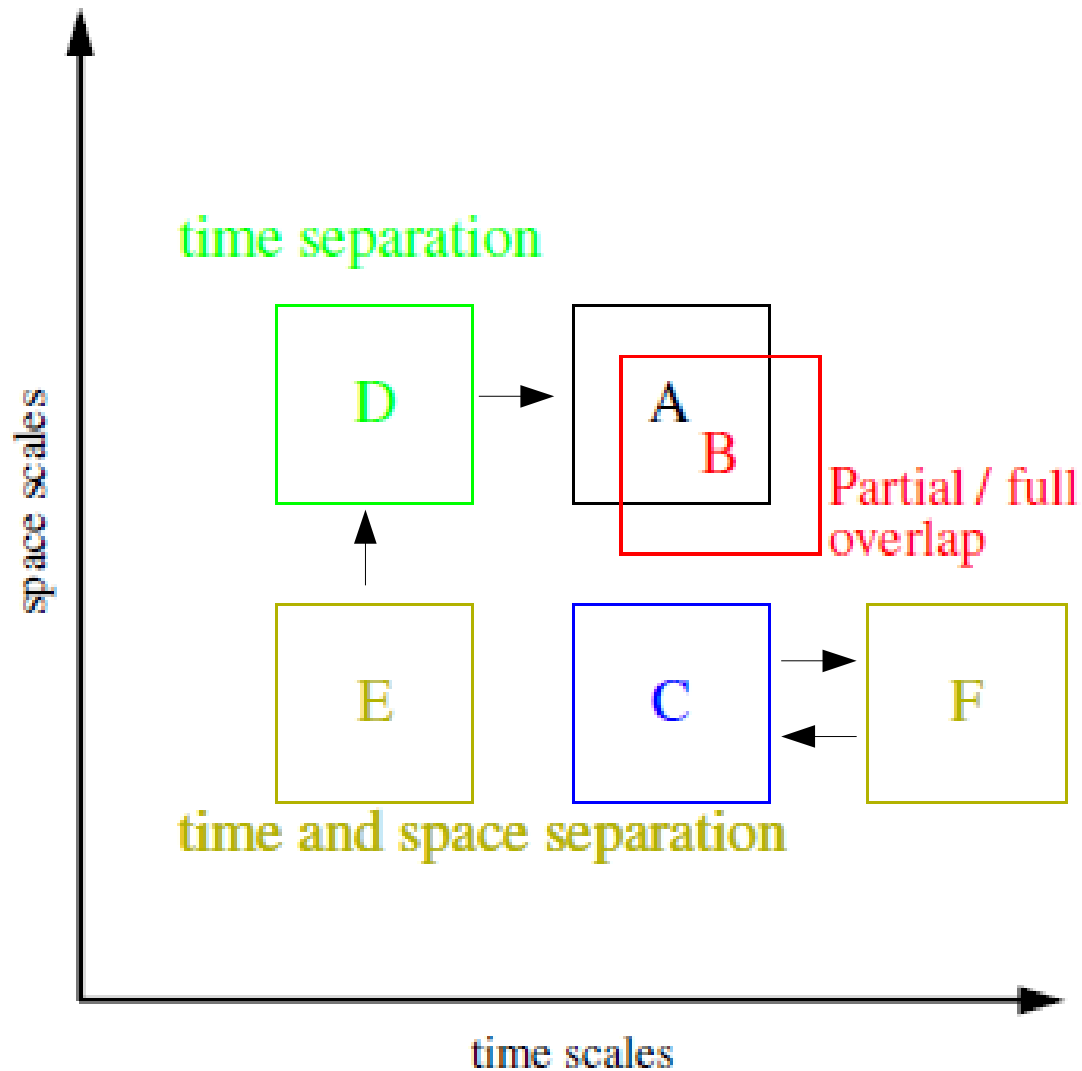
E-Science DMC workshop 2011, Dec 5th 2011, Stockholm

What is multiscale computing?

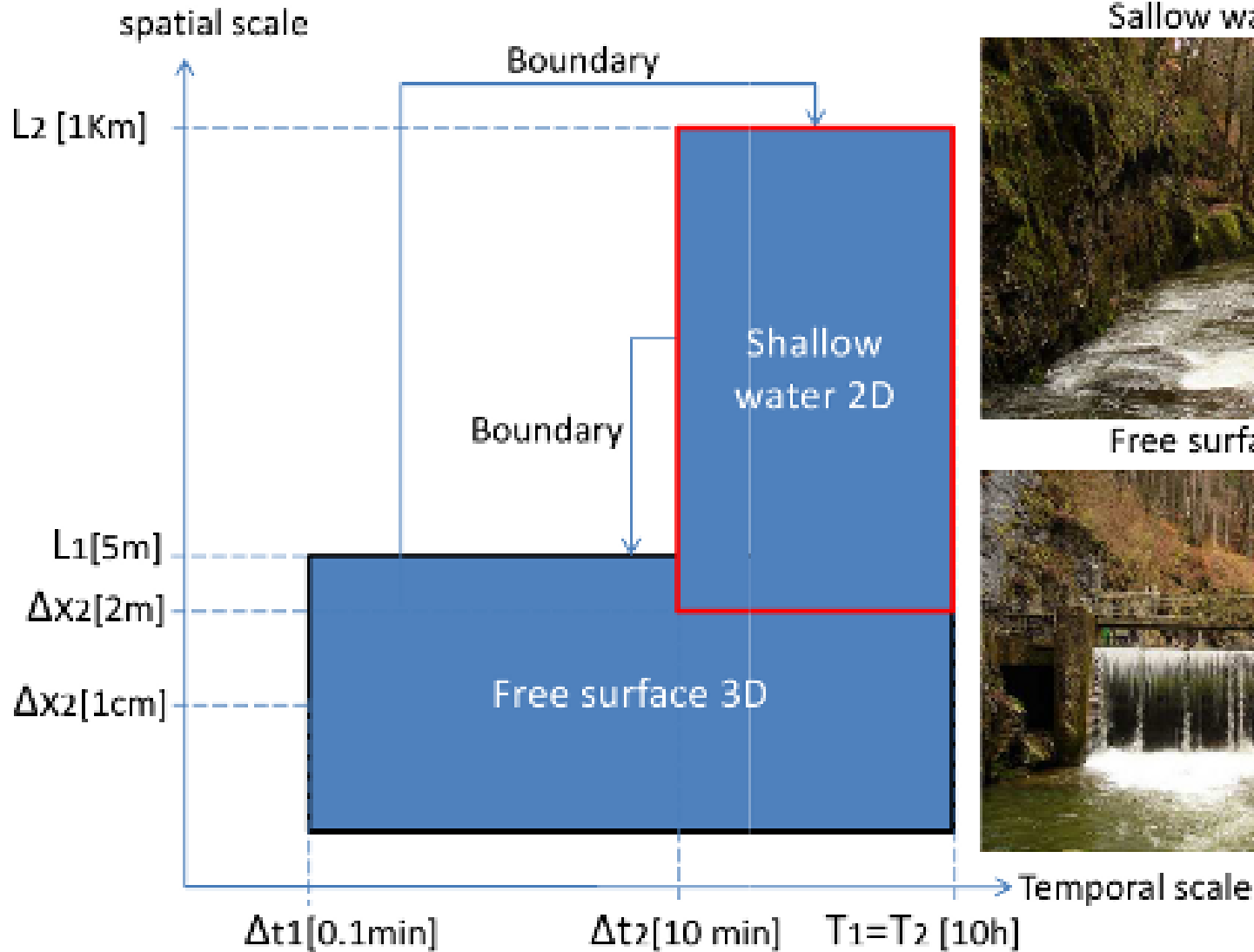
- Goal: Accurately resolve phenomena on a range of scales (e.g. spatial or temporal scales), using a hybridized method.
- Applications consist of multiple 'subcodes':
 - each of which tackles an aspect of the problem for a single (spatial or temporal) scale.
- Coupling between subcodes can be loose (one-directional dependencies) or tight (with cyclic dependencies).

- Multiscale methods allow researchers to simulate systems by taking the best of both worlds.
 - Microscopic detail in the most critical subsections of the problem.
 - Efficiency and problem size advantages of macroscopic simulations.
- Multiscale simulations are highly modular.
 - No large monolithic codes.
 - Easy to flexibly compose new scenarios.

Scale Separation Map



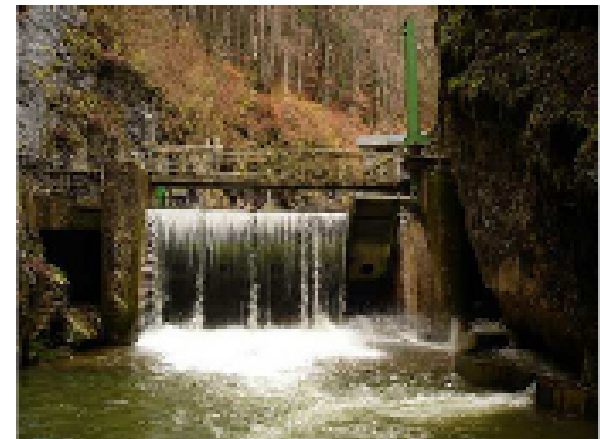
Example: Canals



Sallow water 2D



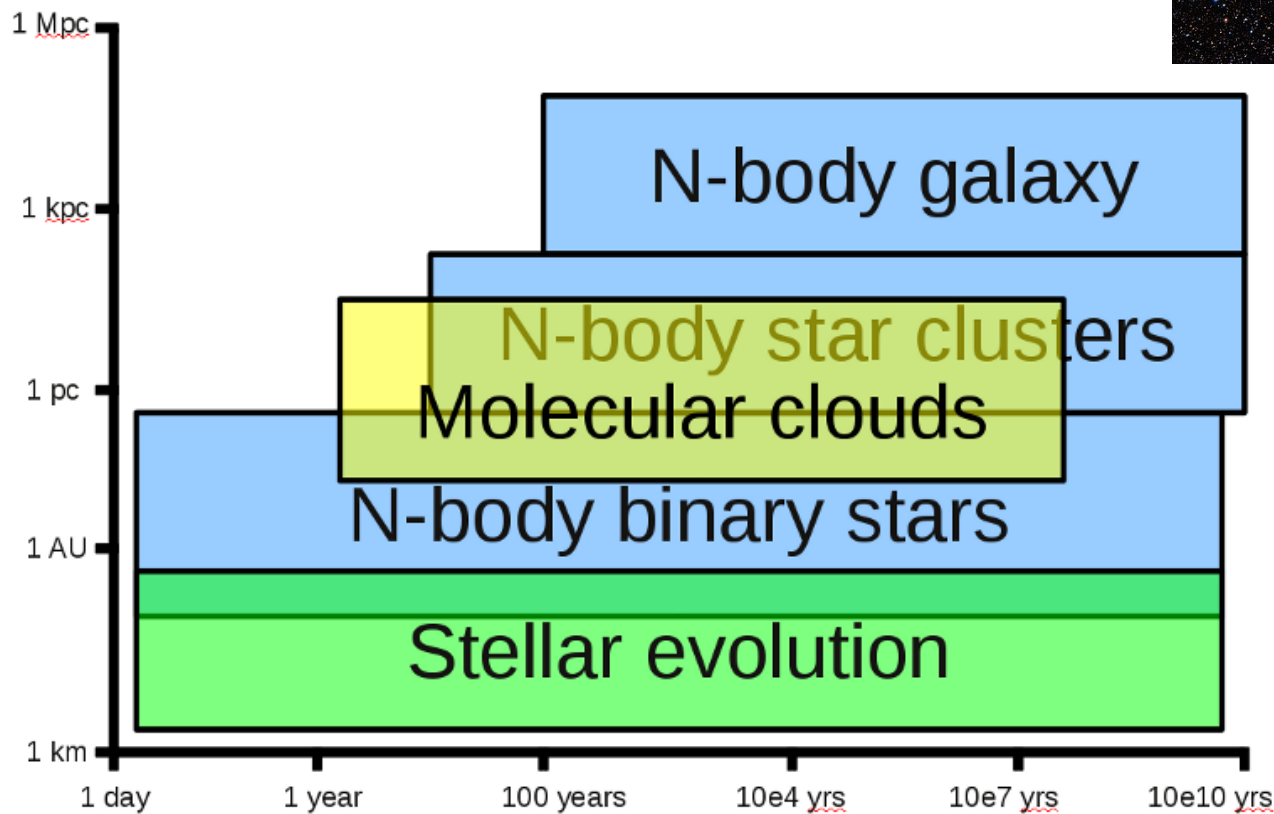
Free surface 3D



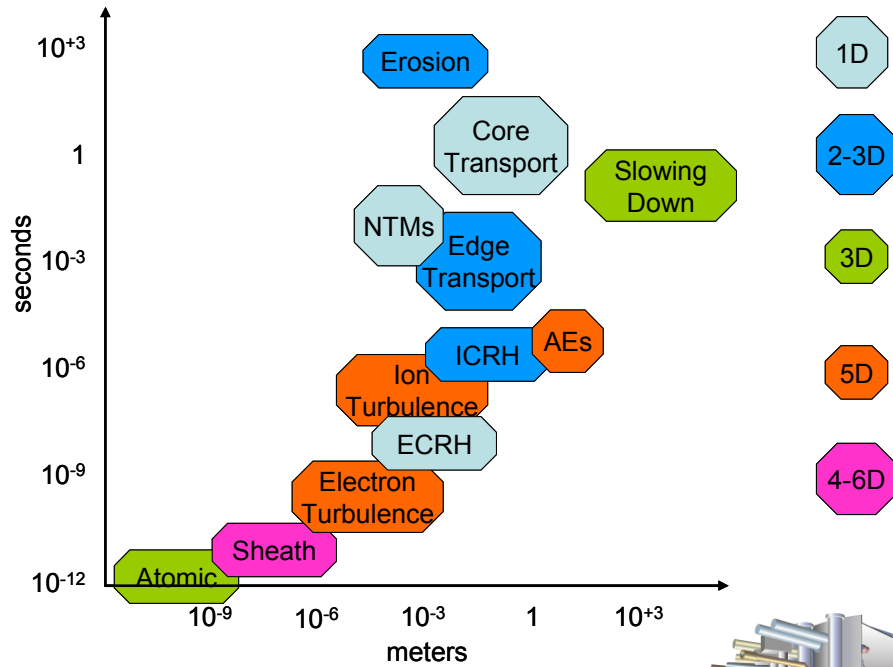
Example: Astrophysics



M31, or Andromeda



Example: Fusion

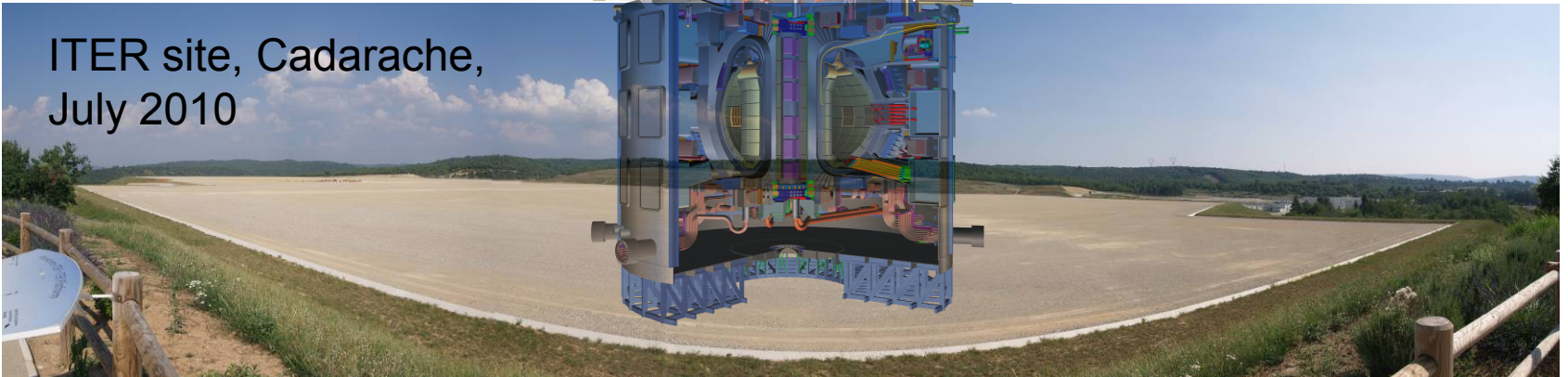


Task Force on Integrated Tokamak Modelling

Goal : run these coupled simulation codes to explore physics for existing tokamaks and for future devices (ITER, DEMO, power reactors)

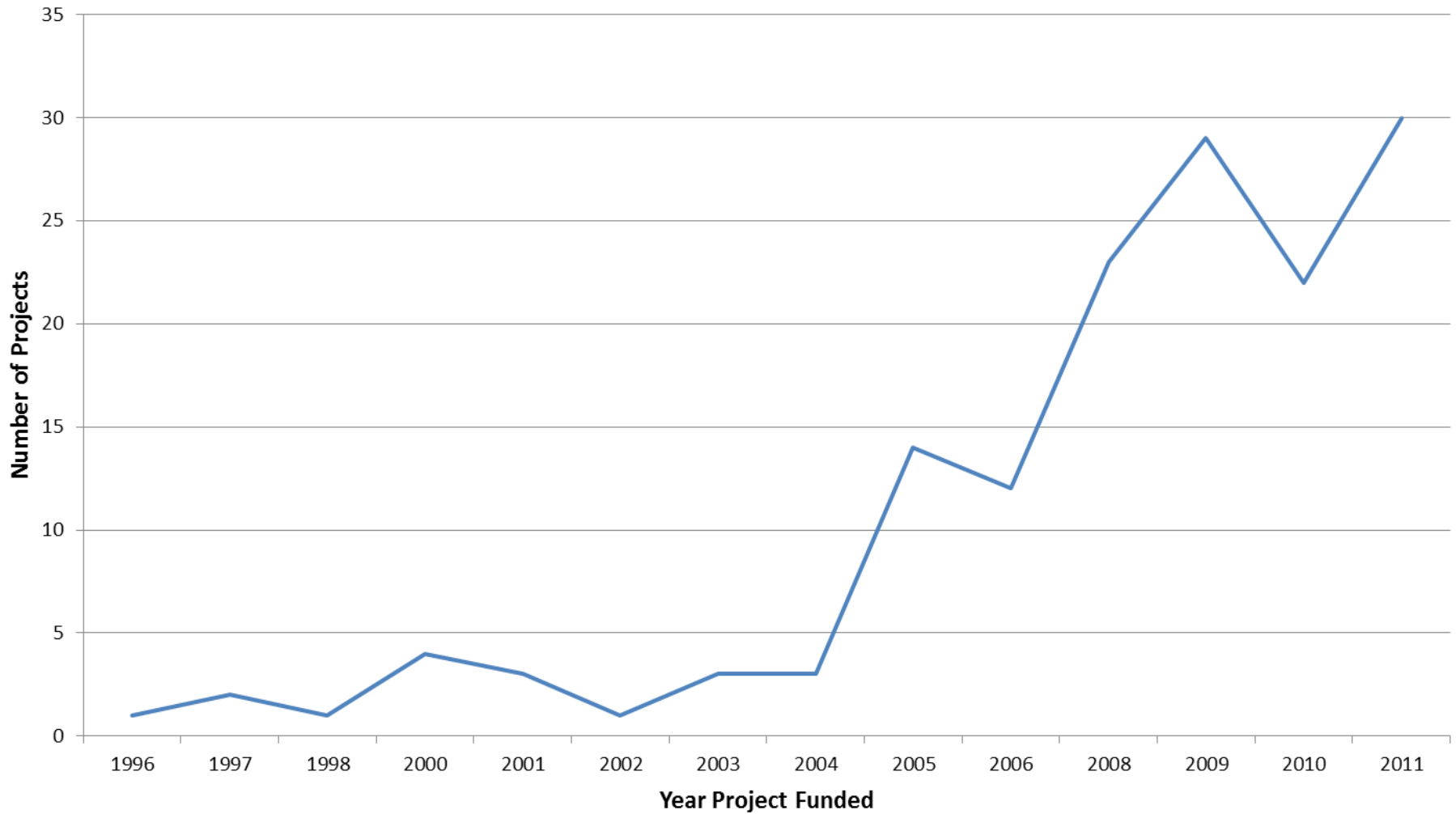


ITER site, Cadarache, July 2010

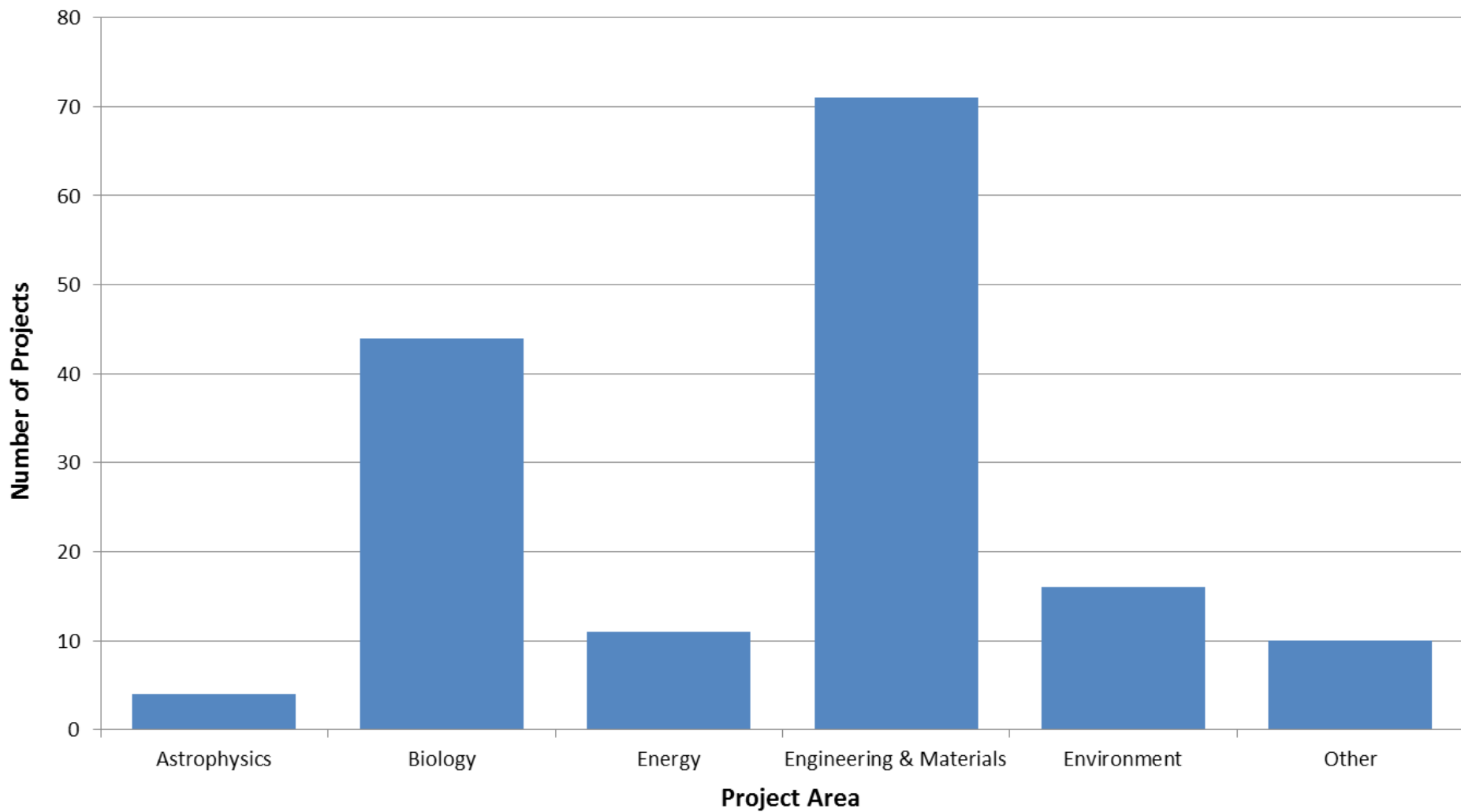


- What the taxonomy contains:
- Reviews of multiscale computing efforts in a range of domains:
 - Astrophysics, Systems Biology, Engineering, Material Sciences, Energy and Environmental Sciences.
- An investigation of multiscale EU projects.
- A characterisation of coupling toolkits originating from various communities.
- This work is not (yet) exhaustive, so all feedback is more than welcome!

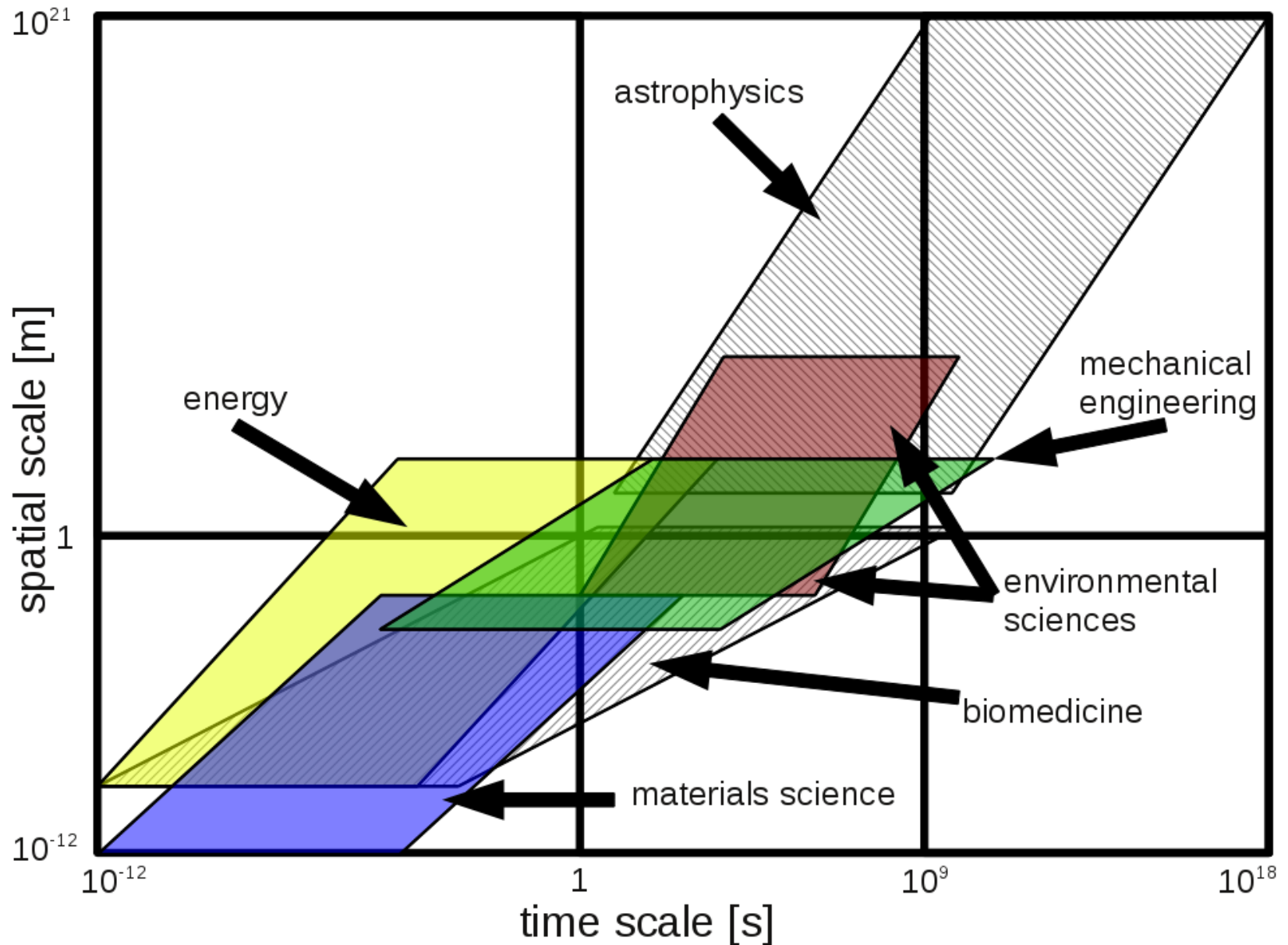
Number of EU Funded Multi-scale Projects by Start Year



EU Funded Multi-scale Projects by Area



SSM of various domains



Coupling Frameworks



| name | domain of origin | generic? | parallel? | distributed? | loose coupling? | tight coupling? | coupling abstractions | built-in unit conversion? | year of last public release |
|---------------------|------------------|----------|-----------|--------------|-----------------|-----------------|-----------------------|---------------------------|-----------------------------|
| AMUSE [12] | astrophysics | no | yes | yes | yes | yes | none | yes | 2011 |
| FLASH [14] | astrophysics | no | yes | no | yes | yes | none | yes | 2011 |
| GridSpace [64] | sys. biology | yes | yes | yes | yes | no | MML [65] | no | 2011* |
| MCT [53] | environment | yes | yes | yes | yes | yes | none | yes | 2009 |
| MUSCLE [66] | sys. biology | yes | yes | yes | no | yes | MML [65] | no | 2010* |
| OASIS | environment | no | yes | no | no | yes | none | no | 2011 |
| OpenMI | environment | no | yes | yes | yes | yes | yes | yes | 2011 |
| PALM | environment | yes | yes | no | no | yes | none | no | 2011 |
| Pyre Framework [54] | environment | yes | yes | no | yes | yes | none | no | 2005 |
| SWIFT [45] | energy | yes | yes | yes | yes | no | yes | no | 2011 |
| SWMF [11] | astrophysics | no | yes | no | yes | yes | none | yes | not public |
| UAL | energy | yes | yes | yes | yes | yes | none | no | 2011 |

- Clear organizational differences between multiscale communities in different domains.
 - e.g.: astrophysics aims for domain-specific, while systems biology aims for general-purpose coupling tools.
 - Material sciences rarely use coupling frameworks altogether, opting to use hand-written scripts instead.
 - Also differences in sizes of multiscale projects between different domains.

- We have provided a review of existing multiscale communities.
 - This review is an on-going effort.
- The multiscale modelling and simulation community is rapidly growing:
 - How do we ensure that no efforts are needlessly duplicated and that the existing knowledge is obtained by newcomers to the field?
- The favored approaches to tackle multiscale problems differ heavily between scientific domains.
 - What are the reasons for these differences?
 - Could a lack of cross-disciplinary interaction cause communities to seek suboptimal approaches for multiscale computing?

Acknowledgements

- Thanks go out to:
 - The MAPPER consortium as a whole.
 - Krzysztof Kurowski
 - Ilya Saverchenko
 - Kasia Rycerz
 - Alfons Hoekstra
 - Marian Bubak
 - Werner Dubitzky
 - Bastien Chopard
 - Dave Coster
 - Par Strand
 - James Suter

