EXA2CT

Intel's European Research and Innovation Conference

ENES HPC workshop, Hamburg,

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SEVENTH FRAMEWORK PROGRAMME

e-infrastructure

EXA2CT

CREATING BREAKTHROUGH *INNOVATIVE ALGORITHMS* AND NEW *PROGRAMMING MODELS*, PAVING THE WAY TO EXASCALE FOR *LEADERSHIP CLASS CODES*.

The EXA2CT project brings together experts at the cutting edge of the development of solvers, related algorithmic techniques, and HPC software architects for programming models and communication.

It will take a revolutionary approach to exascale solvers and programming models, rather than the incremental approach of other projects.

We will produce modular open source proto-applications that demonstrate the algorithms and programming techniques developed in the project, to help boot-strap the creation of genuine exascale codes.

Strategy

Start from existing, leadership class applications running on Tier-0 systems today and extract knowledge about them to create the appropriate Proto-Applications.

Enhanced Numerical Algorithms

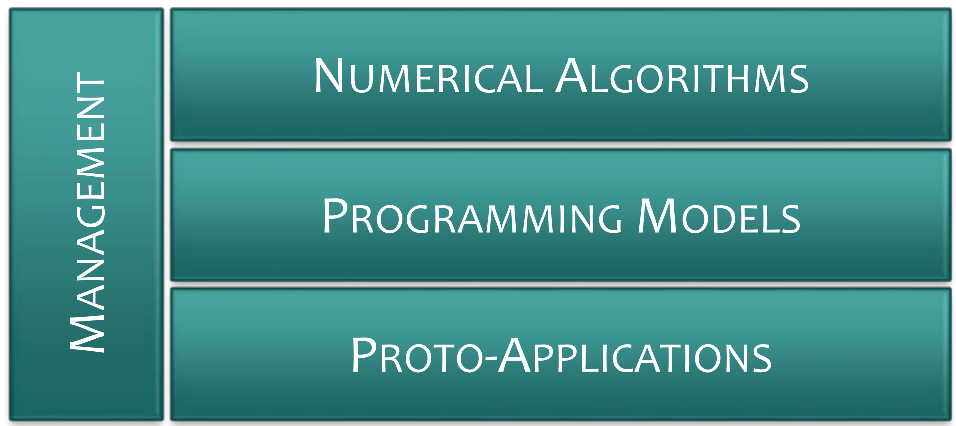
Scalable, Pipelined, Robust Numerical Solvers

- that scale up to exascale performance
- that survive hardware failures

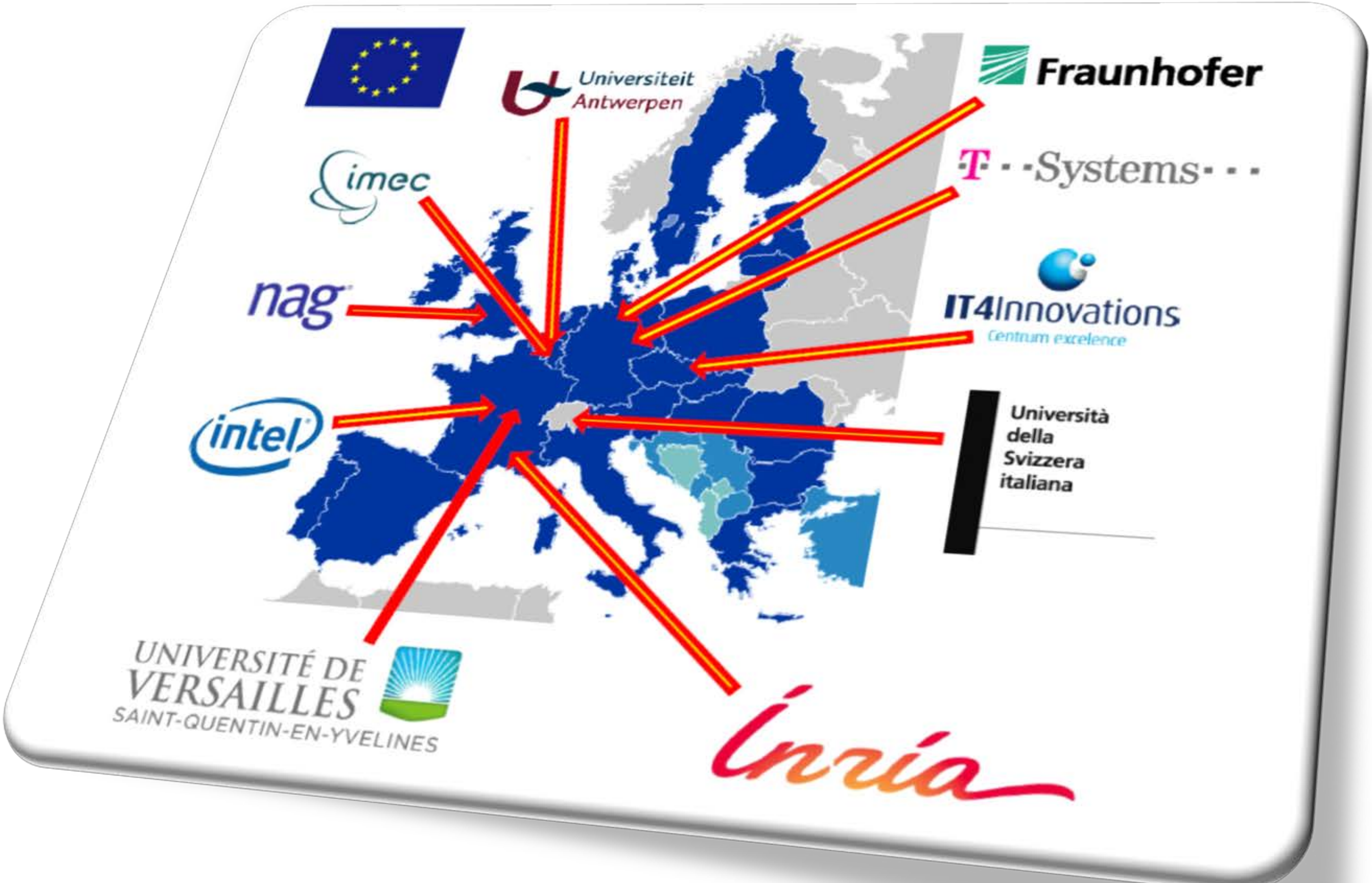
Enhanced Programming Models

GPI/GASPI, Shark,
Irregular Stencil Code, PATUS

- communication model
- to deal with platform heterogeneity
- to deal with resilience



Partners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Numerical Algorithms

Current linear solvers will not scale well to exascale, because of

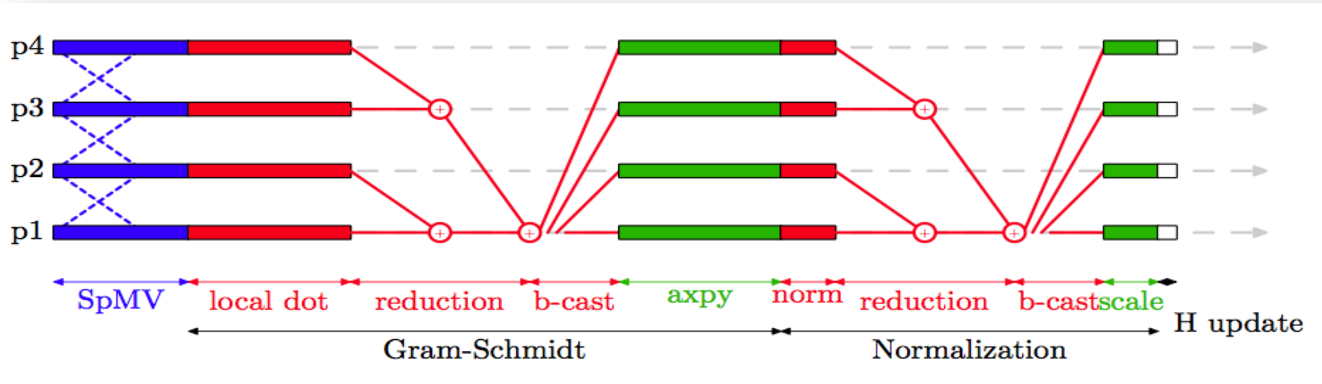
- Global communication
- Bandwidth : Insufficient arithmetic intensity
- Lack of Resilience

Beyond state of the art

- Extend communication avoiding/hiding
  - Preconditioning, aug'd/blocked/deflated
- Exploit arithmetic intensity using *tasking models* as backend
- Resilience through interpolation/ABFT
- Application to FETI methods

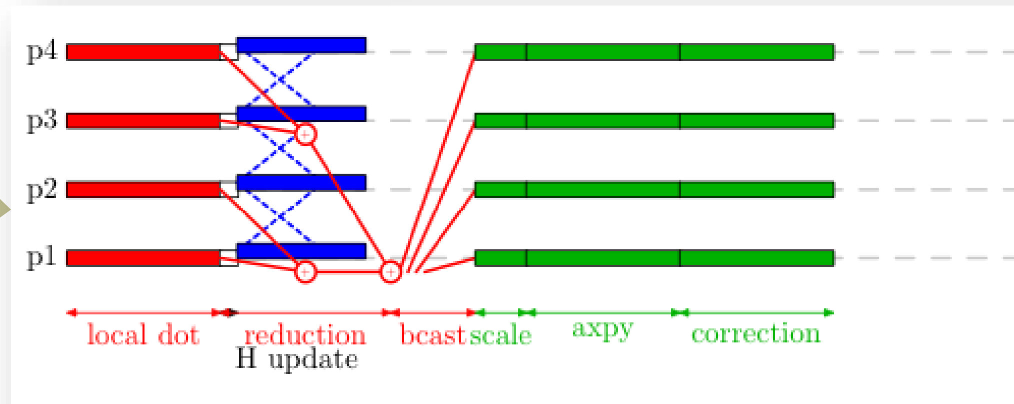
Numerical Algorithms, an example

P. GHYSELS, T.J. ASHBY, K. MEERBERGEN AND W. VANROOSE



Pipelined GMRES overlaps dot-product global communication latency with SpMV

Next generation solvers can hide these latencies and boost performance of a wide range applications in complex systems.



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Numerical Algorithms, an example

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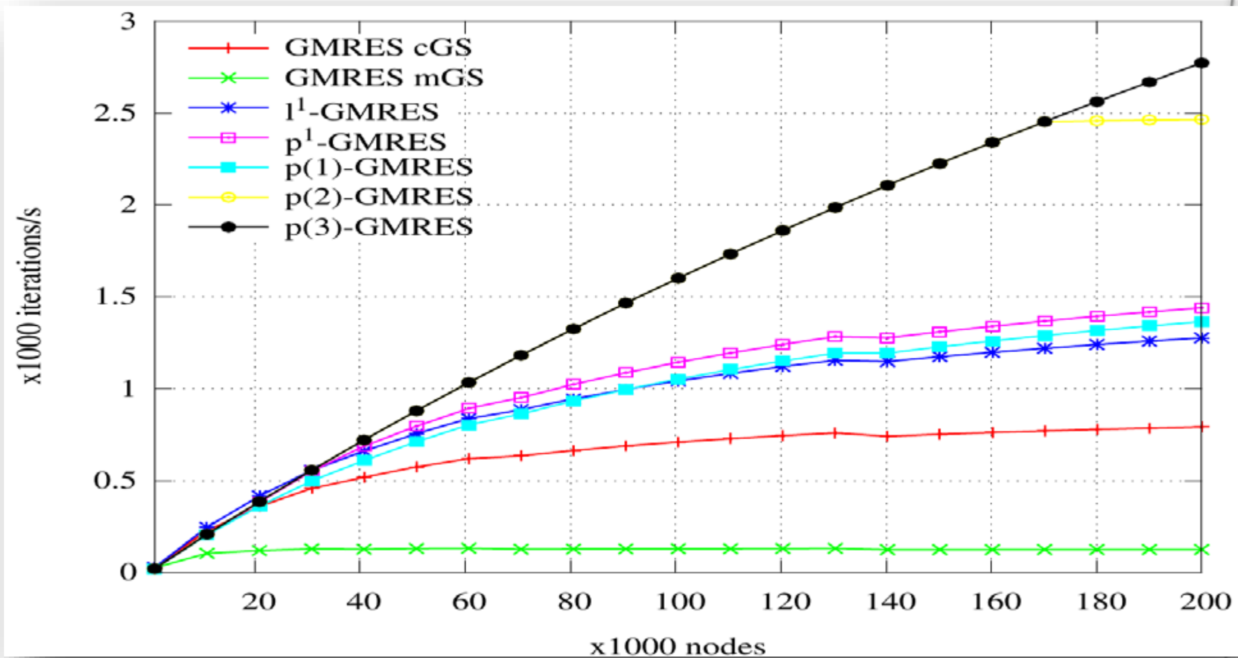
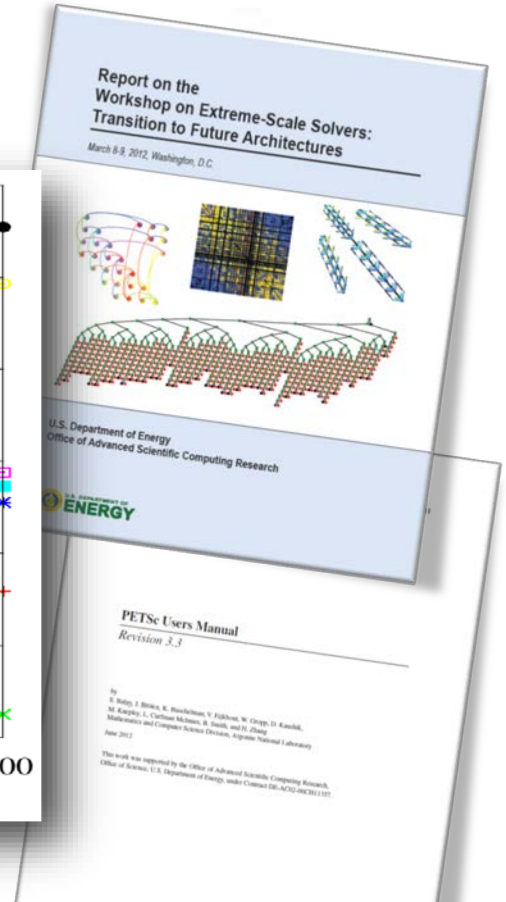
Pipelined GMRES shows significant speedups compared to standard GMRES for strong scaling experiments




Report on the Workshop on Extreme-Scale Solvers: Transition to Future Architectures

March 8-9, 2012, Washington, D.C.

U.S. Department of Energy
Office of Advanced Scientific Computing Research

ENERGY

PETSc Users Manual
Revision 3.3

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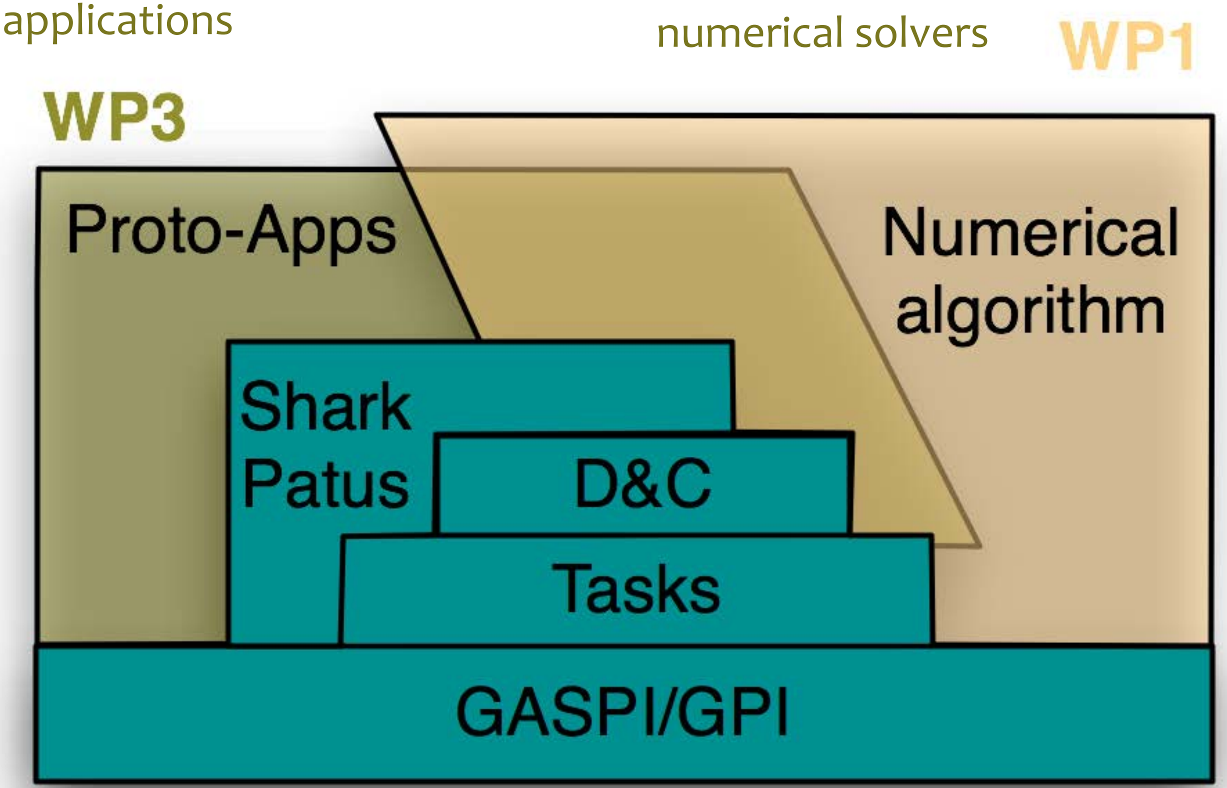
WP1 in a nutshell

- Communication hiding, pipelining global reduction
  - Wim Van Rose, University of Antwerpen
- Communication avoiding, increasing arithmetic intensity using matrix power kernel based on stencil compiler (PATUS)
  - Olaf Schenk, USI
- Resilience by interpolating missing data
  - Luc Giraud and Laura Grigori, INRIA
- FETI benchmarks with coarse operators
  - Tomas Kozubek, IT4Innovations
- Communication avoiding at the level of the preconditioner

WP2 Organization

Proto-Applications
Extract representative proto-applications from HPC applications

Enhance Numerical Algorithms
Scalable and robust numerical solvers



Enhance Programming Models
Improve efficiency, robustness and scalability of GPI/GASPI , Shark , PATUS and leverage task parallelism

WP2-Programming Models

Current HPC programming models don't scale very well

- *MPI*, *OpenMP*, Vectorization

  ... too complex
- *PGAS* Languages

  ... are a partial solution

Beyond State of the Art

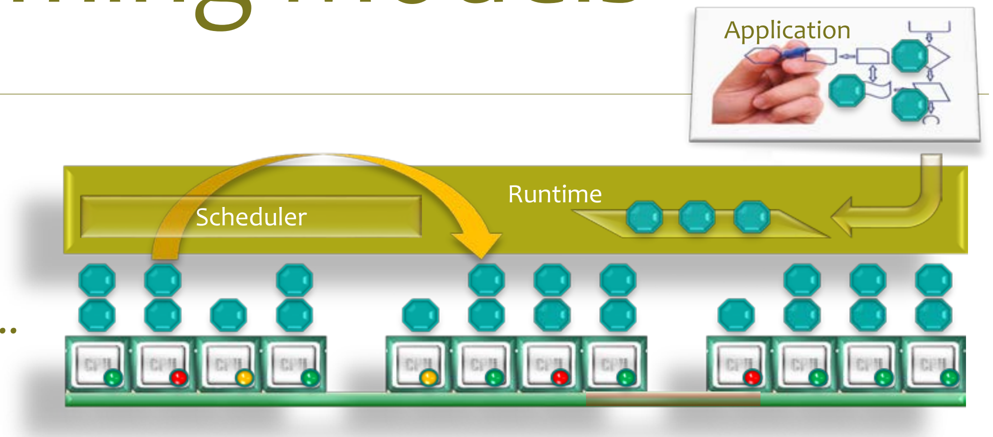
- Extend PGAS with Tasking Models

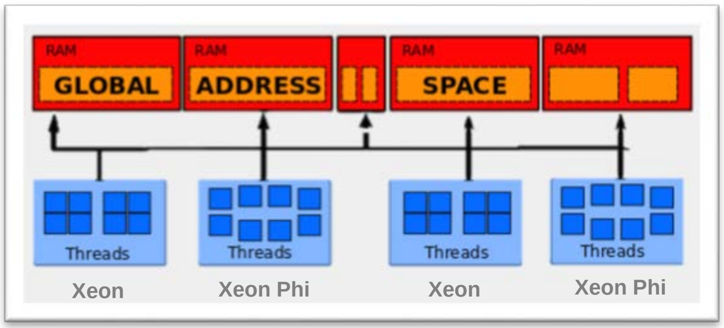
  ... starting from *GASPI*
- High Level Libs : *Patus*, *Shark*
- Resilience : Software that survives failures

WP2-Programming Models

Tasks

Formulate your program in terms of logical tasks, instead of threads
Threading Building Blocks , Cilk™ Plus, ...





GASPI – a *PGAS API*

- is not a new language or a language extension, but complements existing languages *(library approach ~ MPI)*
- Support for resilience

  e.g. time-out mechanisms for all non-local procedures

GASPI + Tasks ➔ extreme scalability

Opportunities : Heterogeneous execution platforms for tasks, task/data migration, task/data resilience, ...

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EXA2CT-WP2 Contact

GASPI/GPI

- Christian Simindinger [1]
- Valeria Bartsch [2]
- Mirko Rahn [2]

D&C and Task programming

- Eric Petit [3] (WP leader)
- Christian Simmendinger [1]

Resilience

- Valeria Bartsch [2]
- Mirko Rahn [2]

Shark and Patus

- Roel Wuyts [4]
- Olaf Shenk [5]

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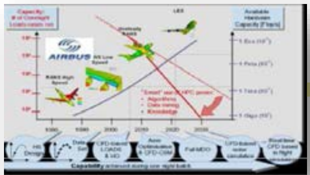
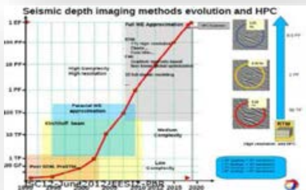
[2] @itwm.fraunhofer.de
[3] @prism.uvsq.fr
[4] @imec.be

Proto-Apps

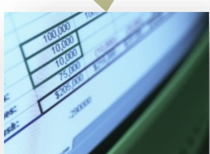


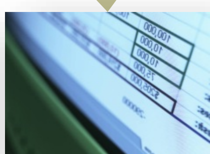


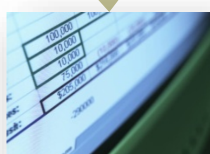
Sometimes considered identical to
Mini-apps, *Proxy-Apps*, *Skeleton Apps*

However proto-apps are not reduced version of real-world applications, they are specifically designed to be :

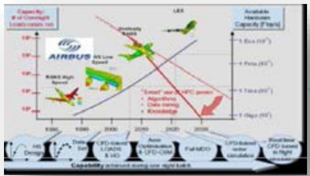
- demonstrating high scalability for re-factored applications
- encapsulating essential characteristics:
  - New exascale algorithms
  - Advanced parallel implementations

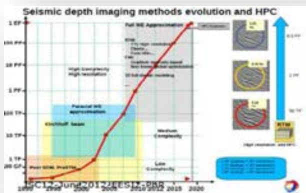






Proto-Apps



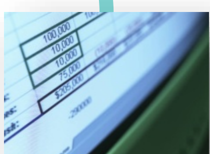


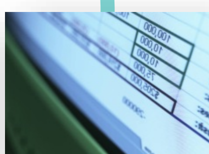
Scientific & Industrial Board

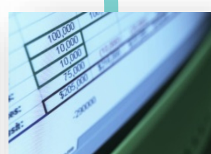
- Define the selection of the proto-apps
  - Have a say in the definition of the targets
    - Are preferred partners in the take-up of the results
      - Will get help in translating the proto-app (back) into the reference applications

Reference Application Areas

- Computational Fluid Dynamics for Aerospace, combustion
  - Structural Mechanics Analysis
    - Geophysics
      - Material sciences
        - And others …





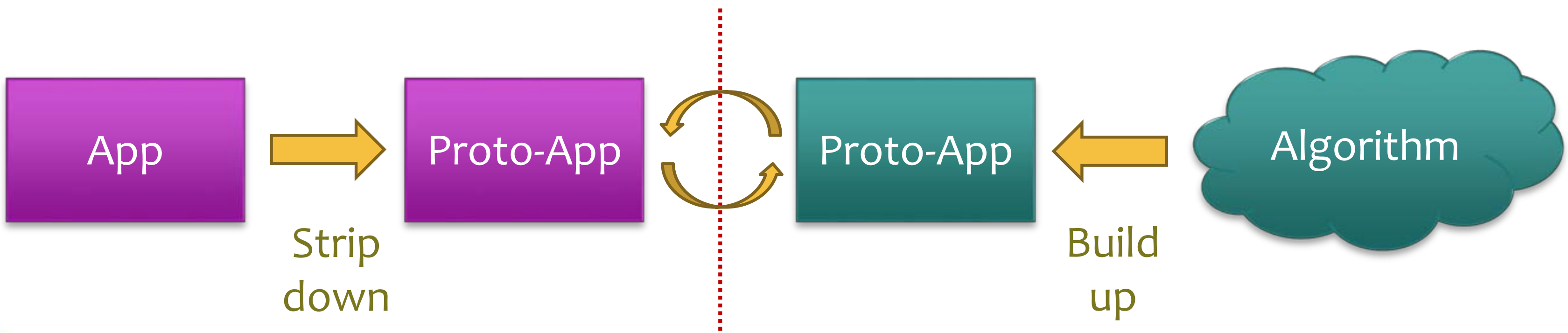


Proto-app development questions

- Discussion with WP1 & WP2: what proto-app description?
  - Numerics-oriented: actually functional (computes)
  - Dataflow-like description (tasks + dependencies)
  - Communication-oriented (profiling-parameterized « sleeps »)

Abstraction

Coupling to implementation



Presently 8 reference applications

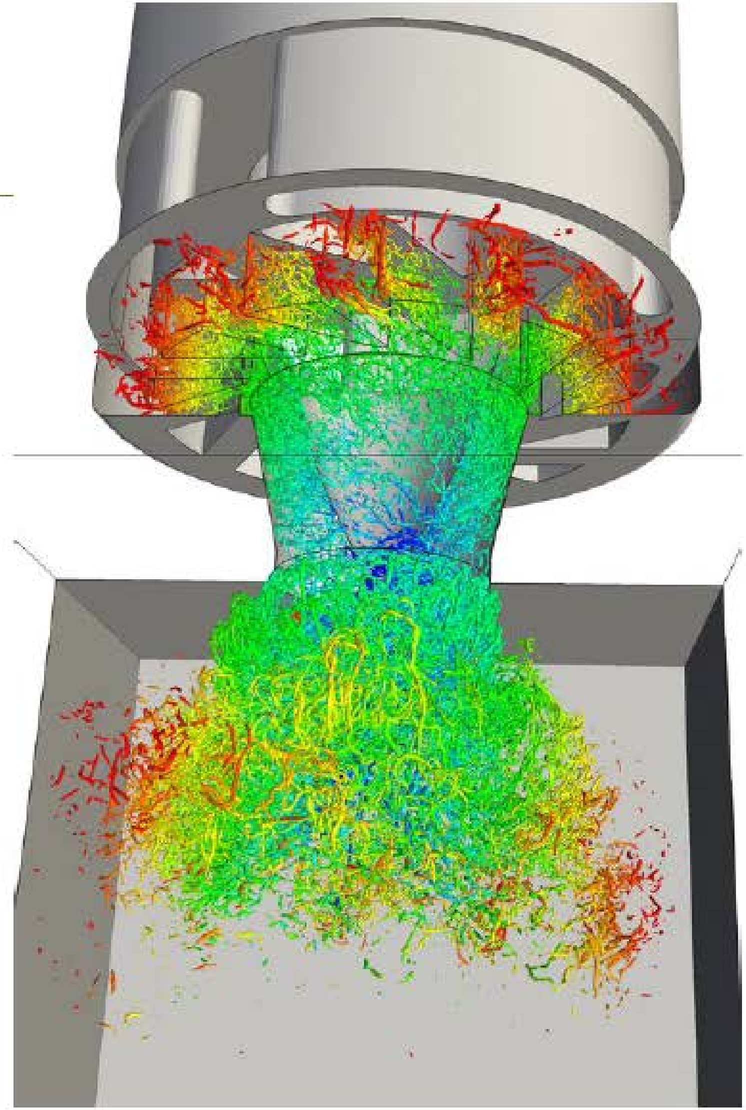
Code	Domain
YALES2	**CFD combustion**
TAU	**CFD**
SPECFEM3D	**Seismology**
elsA	**CFD**
MUPHY	**Fields/particles multiphysics**
Aeronautics code	**CFD**
GYSELA	Fusion
Quantum Espresso	Quantum chemistry
Climate	**Climate science**

Reference applications features

- Strong scaling is a popular scalability model
  - Time to solution drives most industrial codes
- Some use cases for weak scaling
  - Multi-scale physics (YALES2)
  - Higher resolution (Climate, muphy)
  - More complex physics (elsA)
- Some very precise answers about target problem sizes
  - YALES2
  - TAU
- Most science is done on 1k-10k cores
- I/O is a recurring problem
- Fault tolerance: not a lot of feedback beyond checkpoint/restart

Test Cases

- Getting suitable test cases is crucially important to us
  - Should show good scalability, up to a point
  - Should also show performance issues
  - Should be representative of genuine application usage



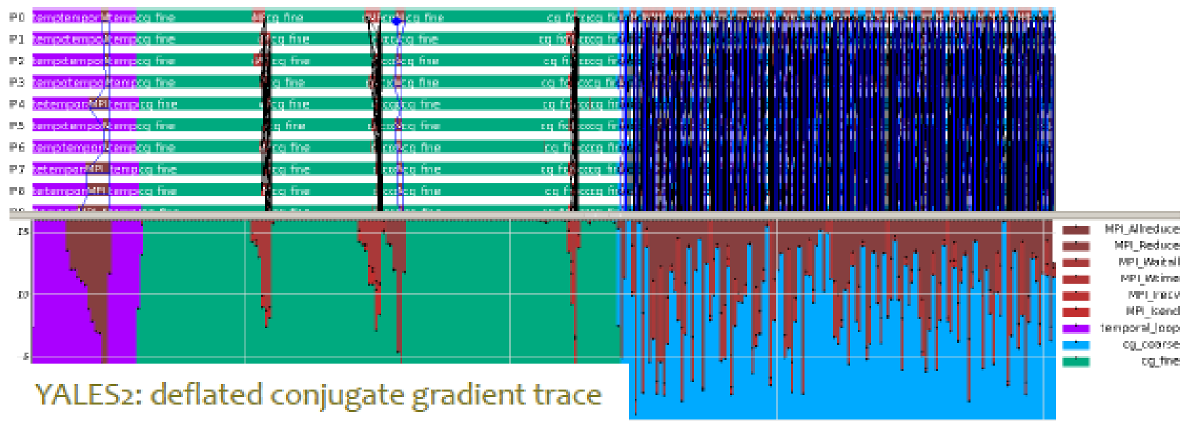
YALES2, PRECCINSTA 2.6B test case (V. Moureau)

YALES2 status update

- Questionnaire feedback received
- Two main development cases identified:
  - CFD linear solvers
    - Good scaling up to 16k cores
    - Want to reduce cell count/core, from 100k to 10k: strong scaling
    - Main identified issue: deflated preconditioned CG
  - Reactive code (combustion)
    - Large computational imbalance across MPI domains
    - MPI task scheduler (dynamic load balancing) scaling up to 1k cores
    - Performance issues beyond that

Application Profiling

- Understanding both node-level performance and parallel scalability
  - In-depth, **quantitative** knowledge of application runtime behaviour is vital for building proto-apps
- Detailed analysis greatly facilitated by access to relevant source code
  - Allows targeted instrumentation
  - When not possible, extensive work on code owner's part is to be expected



YALES2: deflated conjugate gradient trace

YALES2: deflated CG

- Conjugate gradient on 2 levels
  - Main grid
  - « Deflated » level (typically 200x coarser than main grid)
- Scalability issues
  - Extremely fine-grained MPI comms, esp. at deflated level
  - Global comms. (sychronizing) for norm and dot product computations

WP3 Roadmap

- NAG
  - Mike Dewar and Chris Goodyer
- Intel Exascale Lab, France
  - Omar Awile, Thomas Guillet, Marie-Christine Sawley
- Prepare the list of reference applications
- Profile and help refactoring reference applications
- Prepare the library of protoapplications for Opensource release

Dissemination

- EPCC workshop with all 6 Exascale EU projects
  - GASPI tutorial
- ISC booth and BOF
- TERATEC, July 1 and 2nd

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