DE LA RECHERCHE À L'INDUSTRIE

SIMULATION FOR FAST TRANSIENT DYNAMICS WITH FLUID STRUCTURE INTERACTION

SOFTWARE ARCHITECTURE FOR NEXT GENERATION SUPERCOMPUTERS

EUROPLEXUS Software

ARISTOTE Seminar
Vincent FAUCHER
CEA/DEN/DANS/DM2S/SEMT/DYN

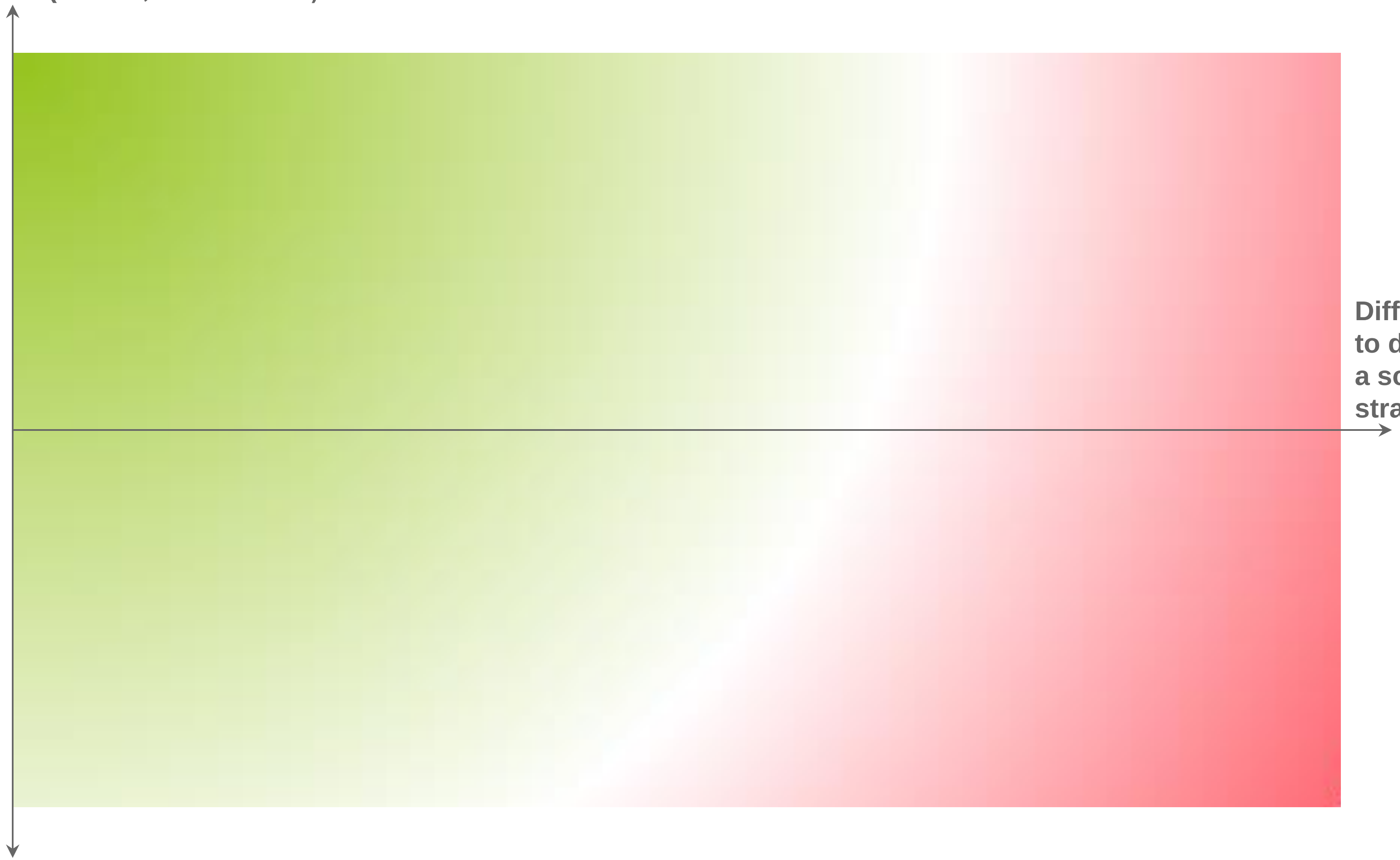
FEBRUARY, 5, 2015

www.cea.fr

OUTLINE

STRATEGIES FOR HPC DEPEND ON THE NATURE OF THE ALGORITHMS…

Access to high performance libraries (PETSc, TRILINOS…)



Difficulty to design a scalable strategy

Straightforward solution

STRATEGIES FOR HPC DEPEND ON THE NATURE OF THE ALGORITHMS…

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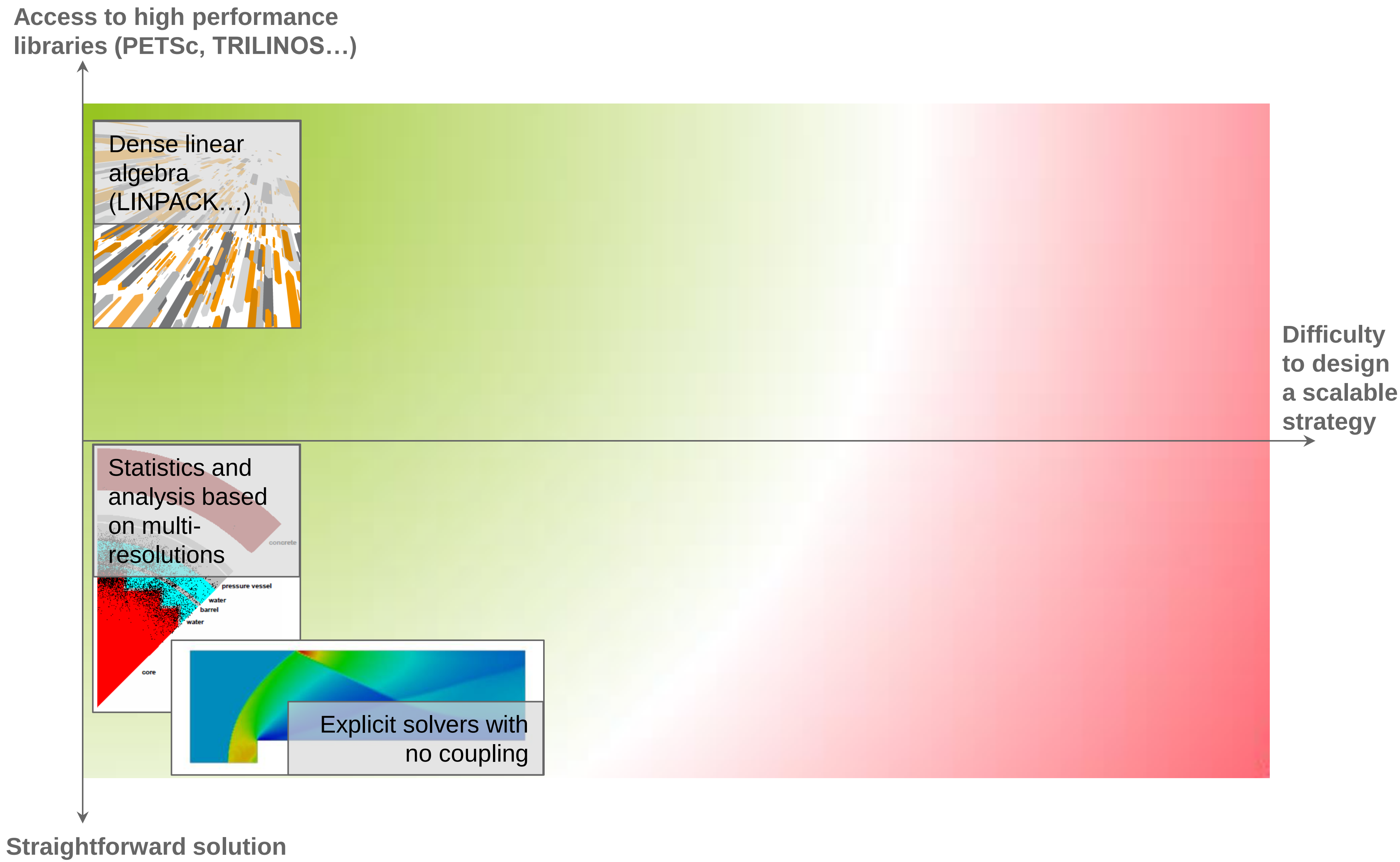

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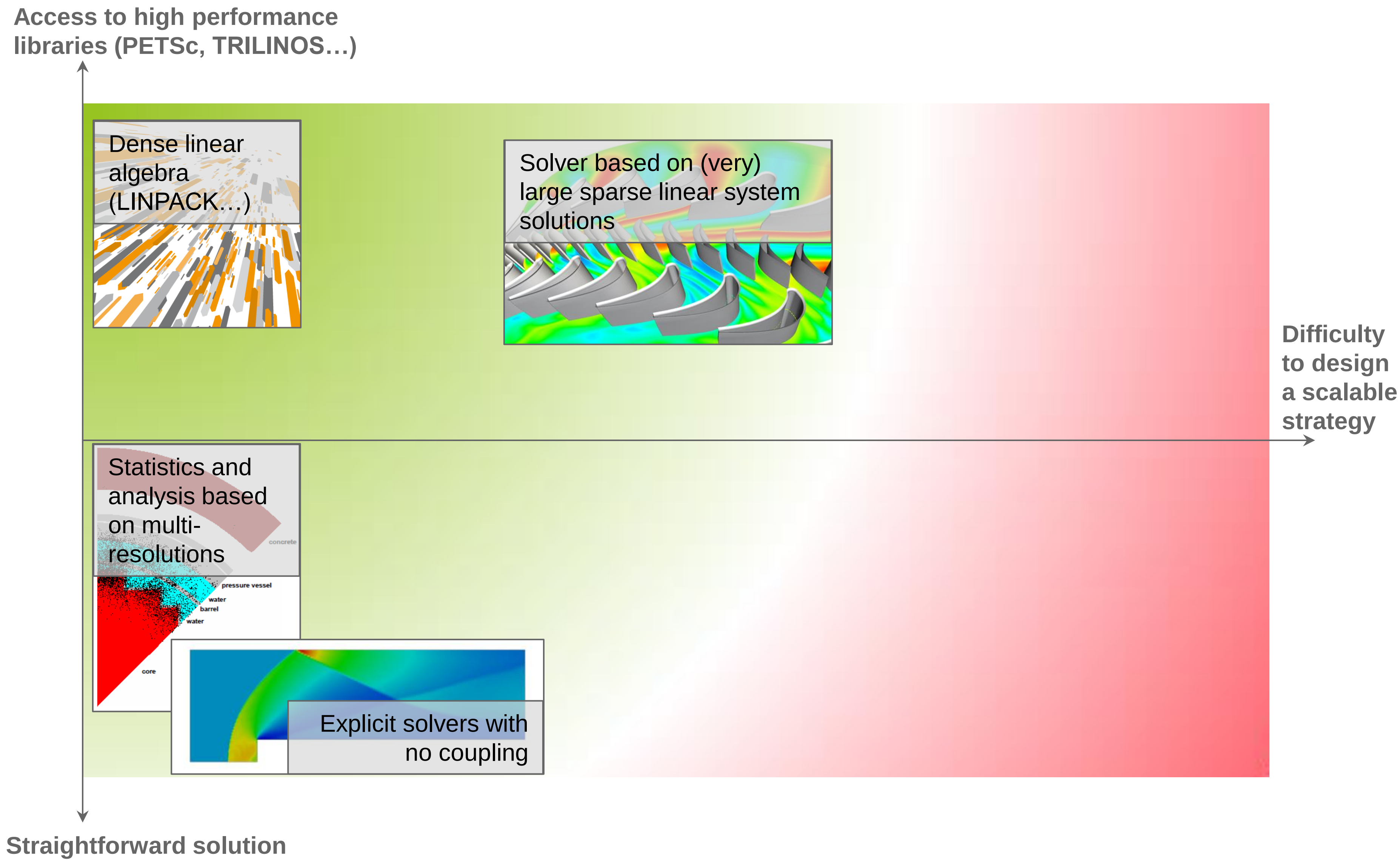

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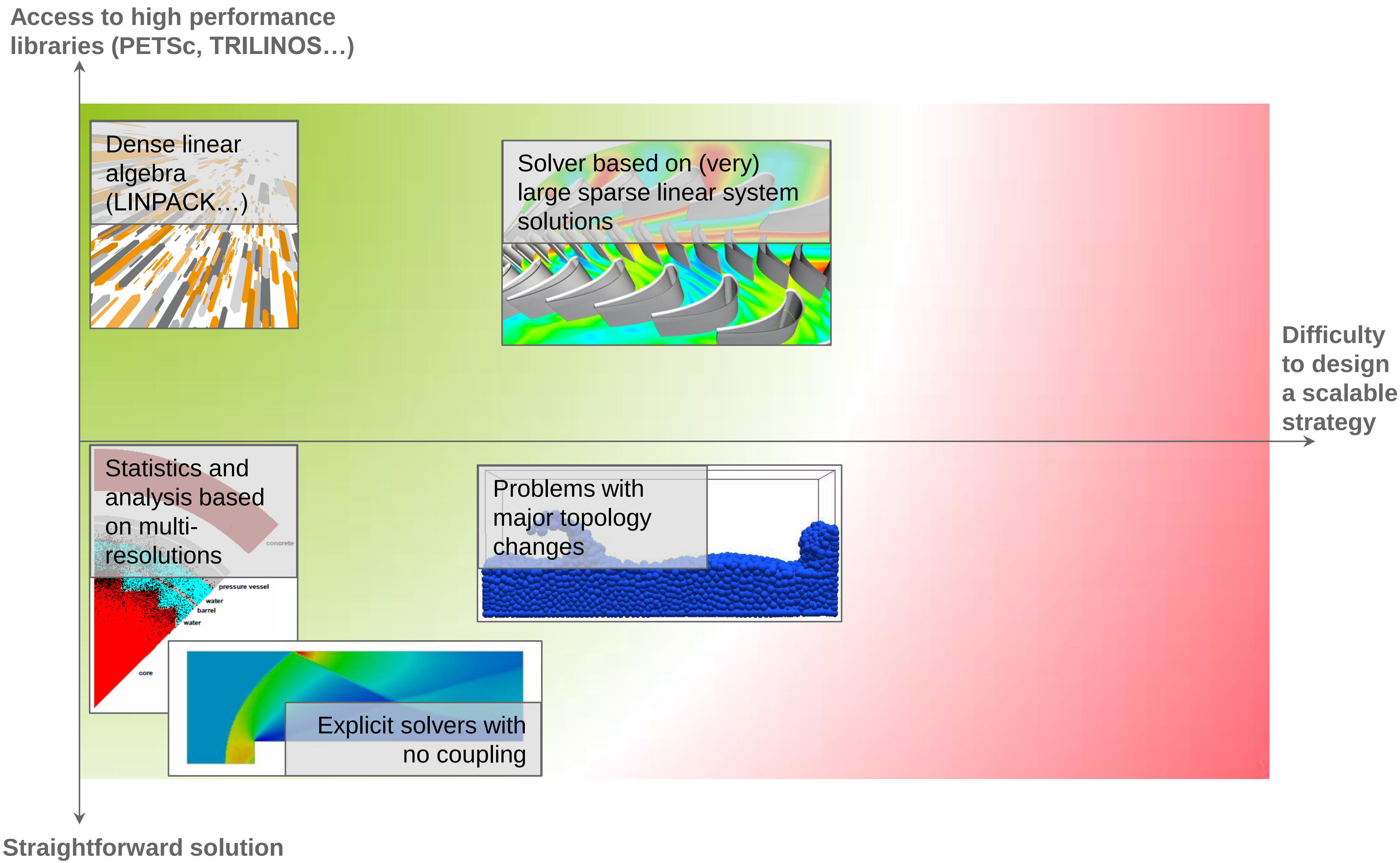

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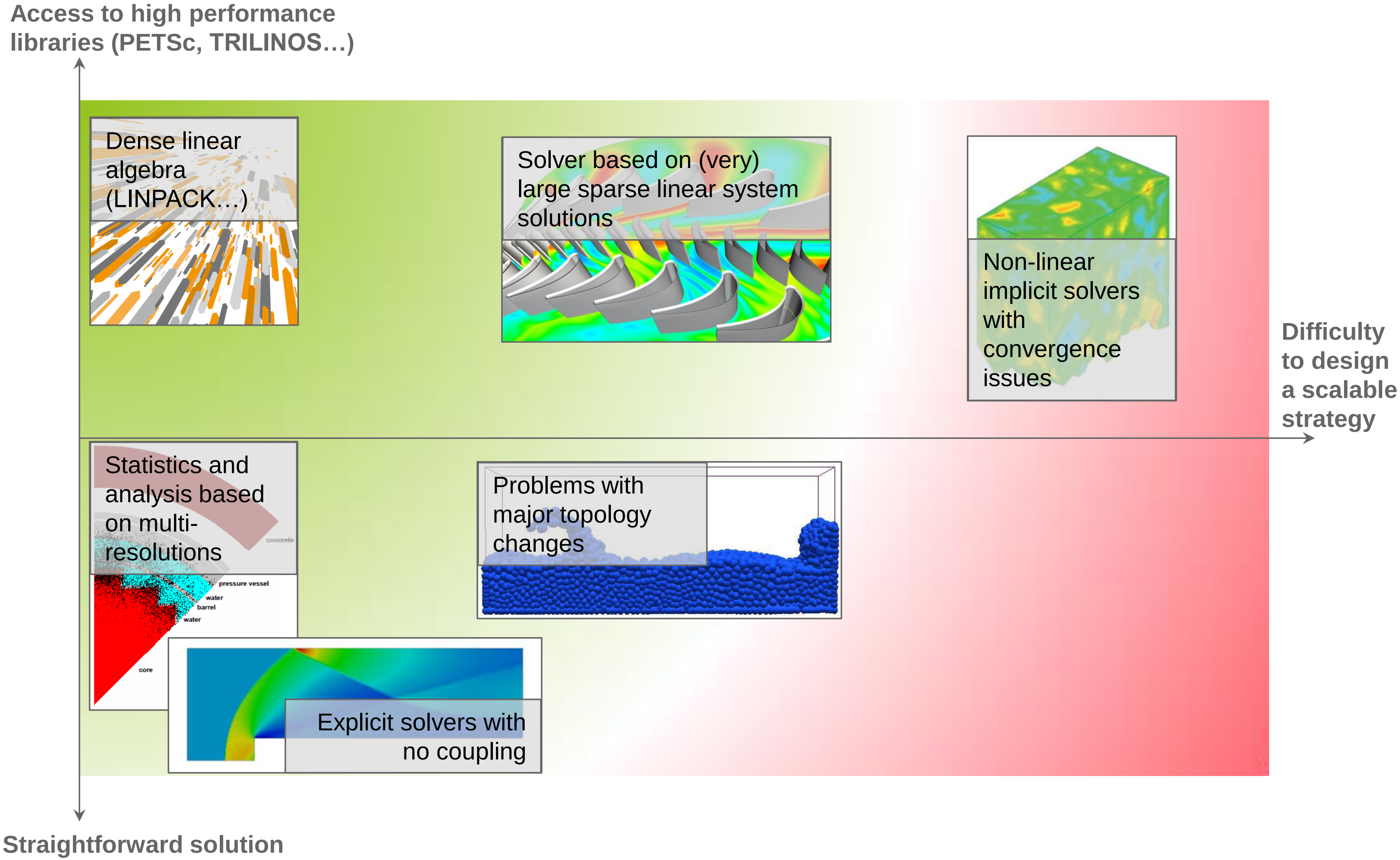

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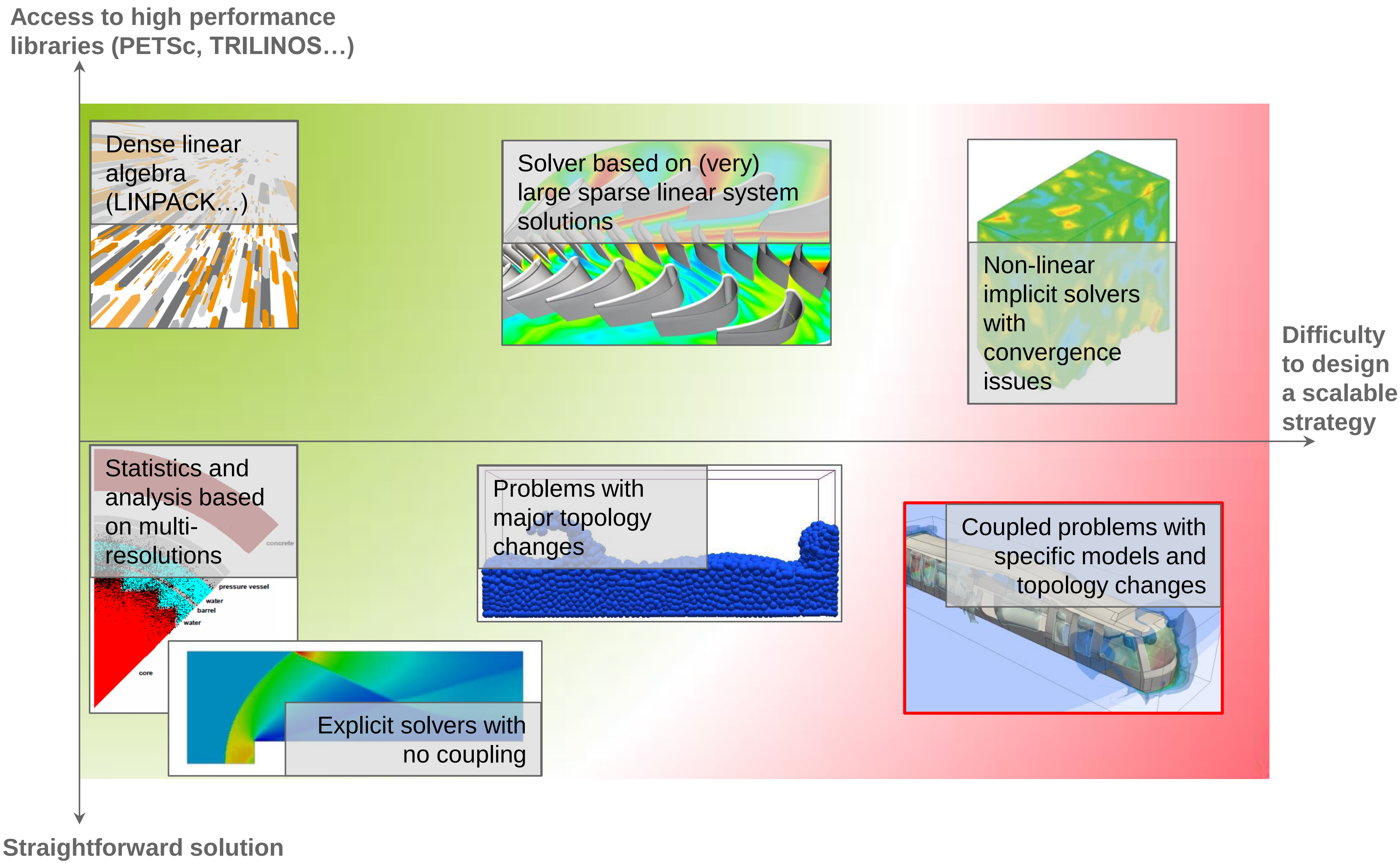

IT IS NOT ALWAYS POSSIBLE TO RESTART FROM SCRATCH…

Why long life applications

- **Repositories of experience and knowledge for research teams**
  - Rise of computational methods since late 70’s
  - Continuous improvement with both new models and methods, guaranty of the sustainability and the implementation of the scientific skills of the teams
  - Integration into external industrial processes

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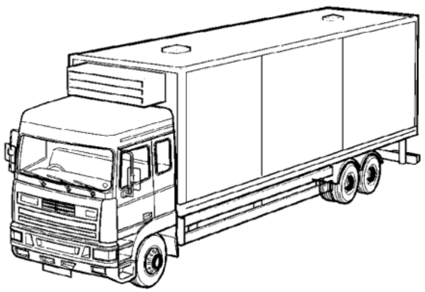
- **Inertia**
  - Complete rewriting process rapidly tedious and out of reach (> 100 000 lines)
  - Development support based on the usage of the application
  - No initial thinking about the life time of applications (otherwise, no Year 2000 bug…)



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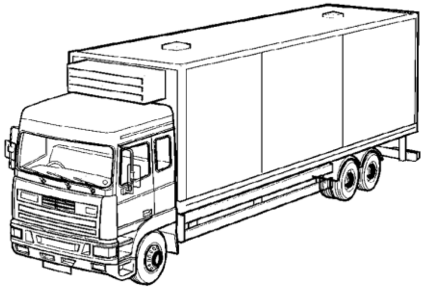

Software identity

- **Main data structure depending on the progamming standards at the beginning of the development**
  - FORTRAN = Formula Translation
  - Convergence on methods emulating dynamic allocation in the early 80’s

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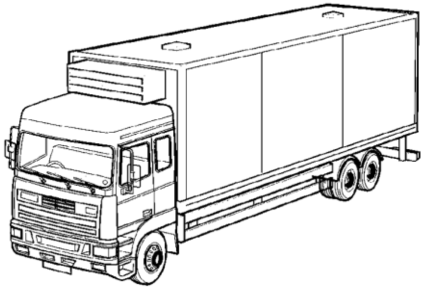

Software identity

- **Main data structure depending on the progamming standards at the beginning of the development**
  - FORTRAN = Formula Translation
  - Convergence on methods emulating dynamic allocation in the early 80's
- **Hardware influence on programming techniques for scientific applications**
  - Vectorial programming for CRAY (80)
  - Share memory OpenMP (90)
  - Distributed memory MPI (fin 90, mi-2000)
  - Everything alltogether, vectorial is back (SIMD), asynchronicity…
  - Hard conversion between programming models
    - Large rewriting and debugging
    - Risk for long immobilization of the application

EPX: PARALLEL ALGORITHMS FOR FAST TRANSIENT FLUID STRUCTURE DYNAMICS

EUROPLEXUS SOFTWARE

EURDYN (1973-1988)
Fluid-structure fast transient dynamics

PLEXUS (1977-1999)
Fast transient dynamics for accidental situations in the field of civil nuclear energy

PLEXIS-3C (1985-1999)
Data structure derived from PLEXUS
Integration of functionalities from EURDYN (fluid-structure interaction in particular)

H. Bung, P. Galon, F. Bliard, D. Guilbaud, O. Jamond, A. Beccantini

M. Larcher, F. Casadei, G. Valsamos

Co-ownership by CEA/JRC
Development open to a **limited number of Major Partners** (EDF, ONERA)
Distribution by CEA since 2013 : **Production Version** under licence, **Education & Research Version** free for academics

EPX – A QUICK DESCRIPTION (1/2)

- **Local equations**

$$\rho\ddot{\mathbf{q}} + \nabla\cdot\left\{\sigma\left[\varepsilon\left(\mathbf{q}\right)\right]\right\} = \mathbf{f}_{vol}^{str}$$

$$\rho\dot{\mathbf{u}} + \nabla P + \mathbf{f}_{trans}\left(\mathbf{u}\right) = \mathbf{f}_{vol}^{flu}$$

$$\dot{\rho} + \nabla\cdot\left(\rho\mathbf{u}\right) = 0$$

$$\dot{E} + \nabla\cdot\left[\mathbf{u}\left(E+P\right)\right] = 0$$

- **Kinematics constraints**

$$\mathbf{C}\left(\mathbf{q},\dot{\mathbf{q}},\ddot{\mathbf{q}},\mathbf{u},\dot{\mathbf{u}}\right) = \mathbf{S}$$

- **Explicit time integration scheme**

$$\dot{\mathbf{q}}^{n+1/2} = \dot{\mathbf{q}}^{n} + \frac{\Delta t}{2}\ddot{\mathbf{q}}^{n}$$

$$\mathbf{q}^{n+1} = \mathbf{q}^{n} + \Delta t\,\dot{\mathbf{q}}^{n+1/2}$$

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- **Main characteristics**

Geometrically non-linear

$$\varepsilon\left(\mathbf{q}\right) = \frac{1}{2}\left(\nabla\mathbf{q} + {}^{t}\nabla\mathbf{q} - \nabla\mathbf{q}^{t}\nabla\mathbf{q}\right)$$

Conditional stability

$$\Delta t \le \frac{2}{\omega_{max}} \Leftarrow \Delta t \le \frac{l_c}{c}$$

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Link force computation

- Penalty approach:

$$\mathbf{F}_{link}^{n+1} = \mathbf{K}\left(\mathbf{C}^{n+1}\begin{bmatrix} \dot{\mathbf{Q}}^{n+1/2} \\ \mathbf{U}^{n+1} \end{bmatrix} - \mathbf{S}^{n+1}\right)$$

☑ *Explicit link forces*
☒ *Choice of penalty coefficients*
☒ *Impact on time integration stability*

- Dual approach:

$$\mathbf{F}_{link}^{n+1} = {}^t\tilde{\mathbf{C}}^{n+1}\mathbf{\Lambda}$$

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☑ *Exact link verification*
☑ *No impact on time integration stability*
☒ *Matrix system to build and solve*

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- **Discrete system**

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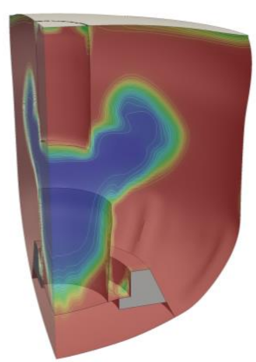
- *Candidates selection*
- *Writing the kinemtic relations*
- *Spatial sorts, inclusion and intersection computations*

Crash with self-contact



Explosion in vessels with immersed structures

EPX – A QUICK DESCRIPTION (2/2)

Discrete system

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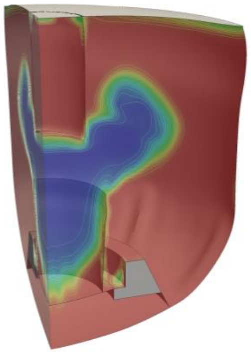

Explosion in vessels with immersed structures

Main task 3 = Link force computation

- *Condensation onto the Lagrange Multipliers*

$$\tilde{\mathbf{C}}^{n+1} \begin{bmatrix} \mathbf{M}_S & \\ & \mathbf{M}_F^{n+1} \end{bmatrix}^{-1} {}^t\tilde{\mathbf{C}}^{n+1} \mathbf{\Lambda} = \tilde{\mathbf{C}}^{n+1} \begin{bmatrix} \mathbf{M}_S & \\ & \mathbf{M}_F^{n+1} \end{bmatrix}^{-1} \mathbf{F}^{n+1} - \tilde{\mathbf{S}}^{n+1}$$

$$\Leftrightarrow \mathbf{H}^{n+1} \mathbf{\Lambda} = \mathbf{B}^{n+1}$$

- *Linear solution and scatter of the forces*

EPX – A QUICK DESCRIPTION (2/2)

Discrete system

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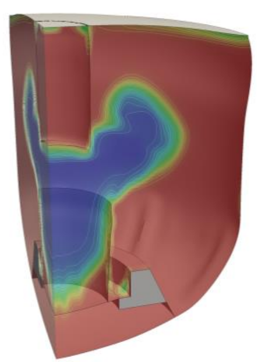


Explosion in vessels with immersed structures

Main task 3 = Link force computation

- *Condensation onto the Lagrange Multipliers*

$$\tilde{C}^{n+1}\begin{bmatrix} M_S & \\ & M_F^{n+1}\end{bmatrix}^{-1} {}^t\tilde{C}^{n+1}\Lambda = \tilde{C}^{n+1}\begin{bmatrix} M_S & \\ & M_F^{n+1}\end{bmatrix}^{-1} F^{n+1} - \tilde{S}^{n+1}$$

$$\Leftrightarrow \boxed{H^{n+1}\Lambda = B^{n+1}}$$

- *Linear solution and scatter of the forces*

EPX – A QUICK DESCRIPTION (2/2)

Discrete system

$$\begin{bmatrix} M_S & \\ & M_F^{n+1} \end{bmatrix} \begin{bmatrix} \ddot{Q}^{n+1} \\ \dot{U}^{n+1} \end{bmatrix} + {}^t\tilde{C}^{n+1}\Lambda = \underbrace{\begin{bmatrix} F_{vol}^{str} \\ F_{vol}^{flu} \end{bmatrix}^{n+1} - \begin{bmatrix} F_{int}\left(Q^{n+1}\right) \\ F_\rho\left(U^{n+1}\right) + F_{trans}\left(U^{n+1}\right) \end{bmatrix}}_{F^{n+1}}$$

$$\tilde{C}^{n+1} \begin{bmatrix} \ddot{Q}^{n+1} \\ \dot{U}^{n+1} \end{bmatrix} = \tilde{S}^{n+1}$$

$$[\rho]^{n+1} = [\rho]^n + F_\rho(U)$$

$$[E]^{n+1} = [E]^n + F_E(U)$$

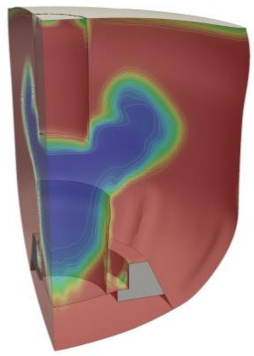
Main task 1 = Elementary loop

- *Stress computation* (constitutive laws, equations of state)
- *Fluxes computation*
- *Heterogeneous individual costs*

Main task 2 = Writing kinematic constraints

- *Candidates selection*
- *Writing the kinemtic relations*
- *Spatial sorts, inclusion and intersection computations*

Crash with self-contact



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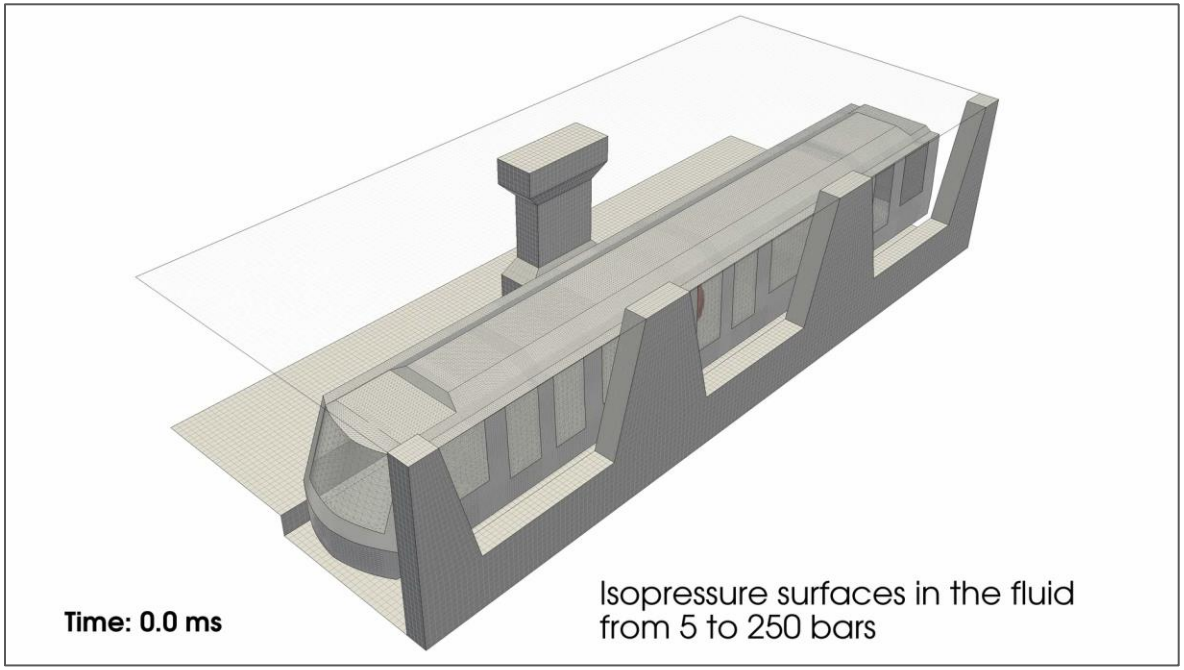
Principal characteristics

- Many specific algorithms (formulations and links)
- Various relative weights of the main tasks
- Very specific parallel strategy

EPX: SOME ILLUSTRATIONS



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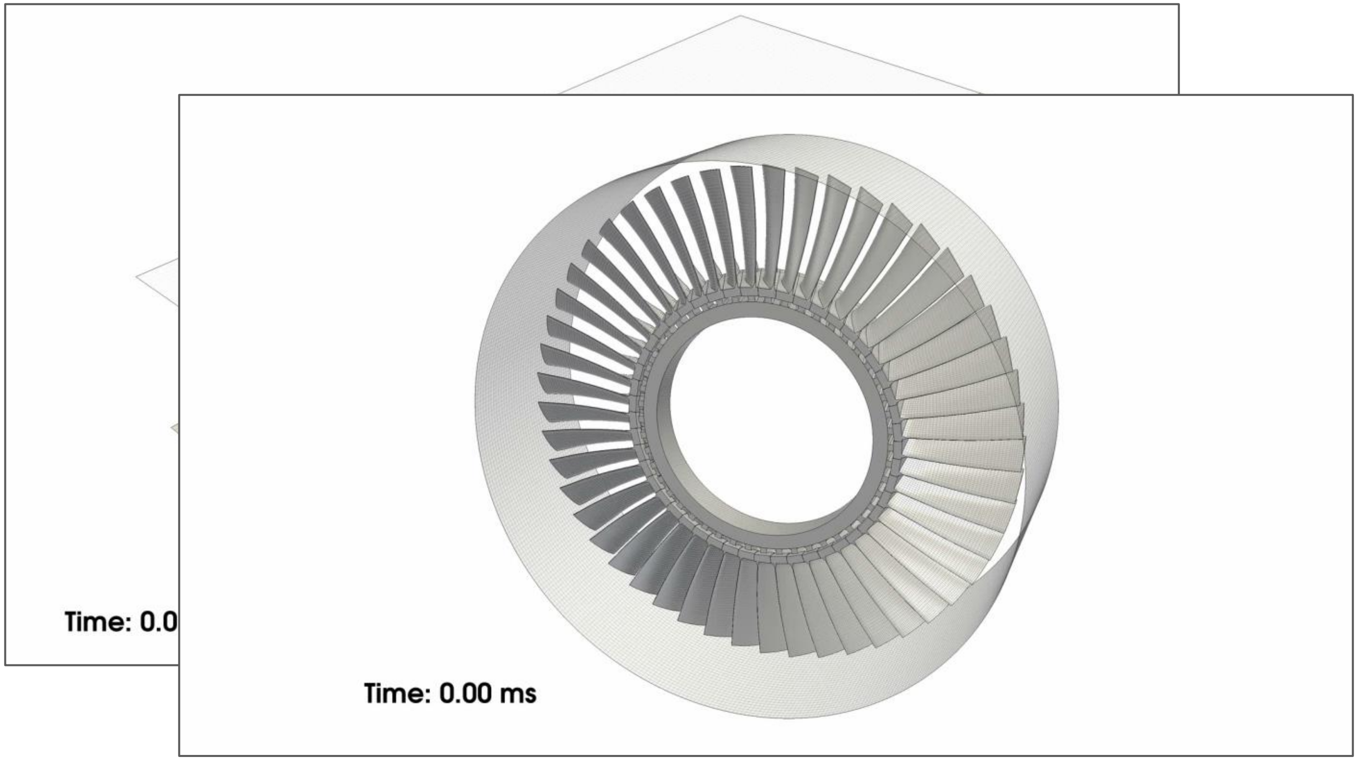

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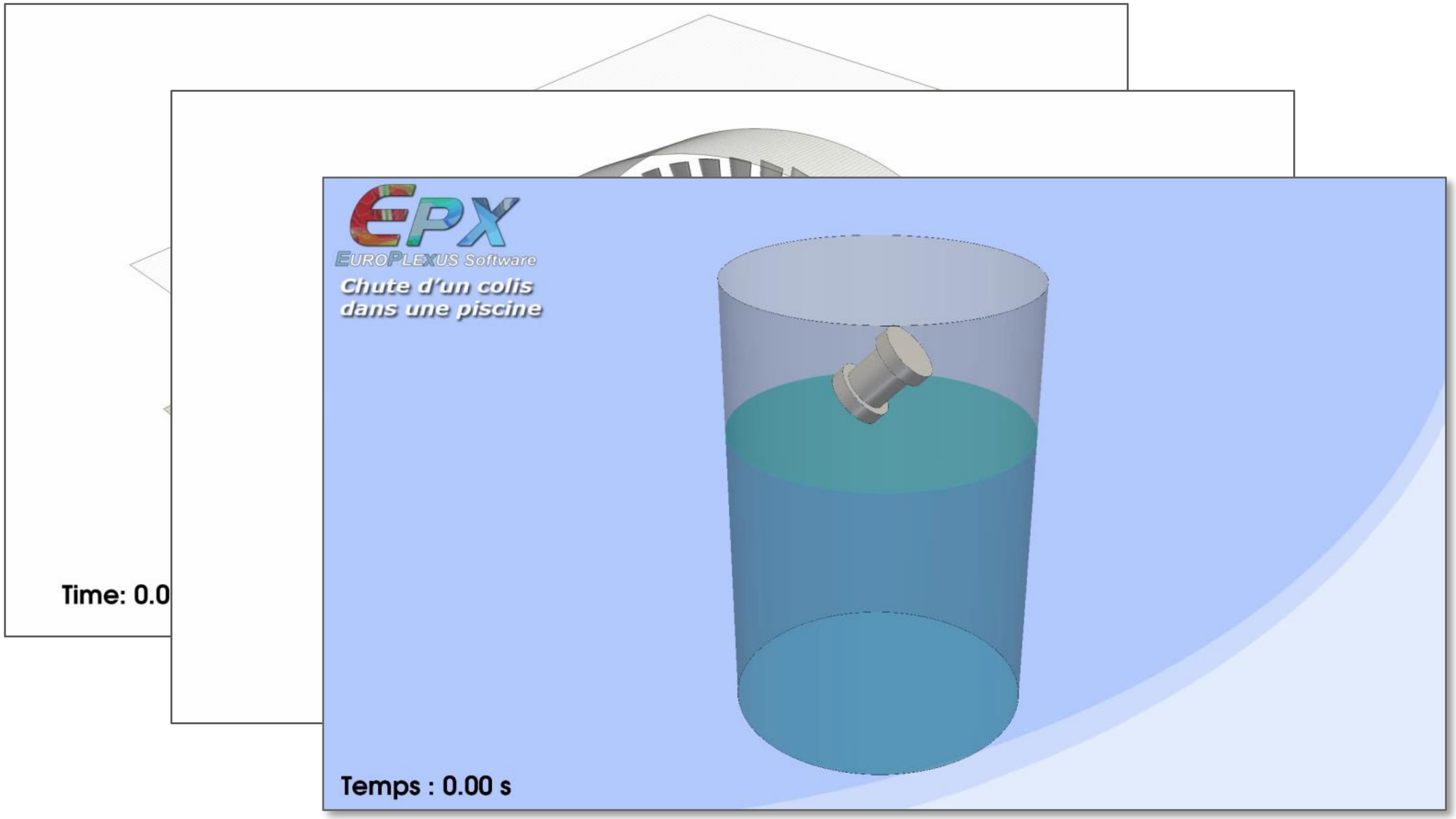

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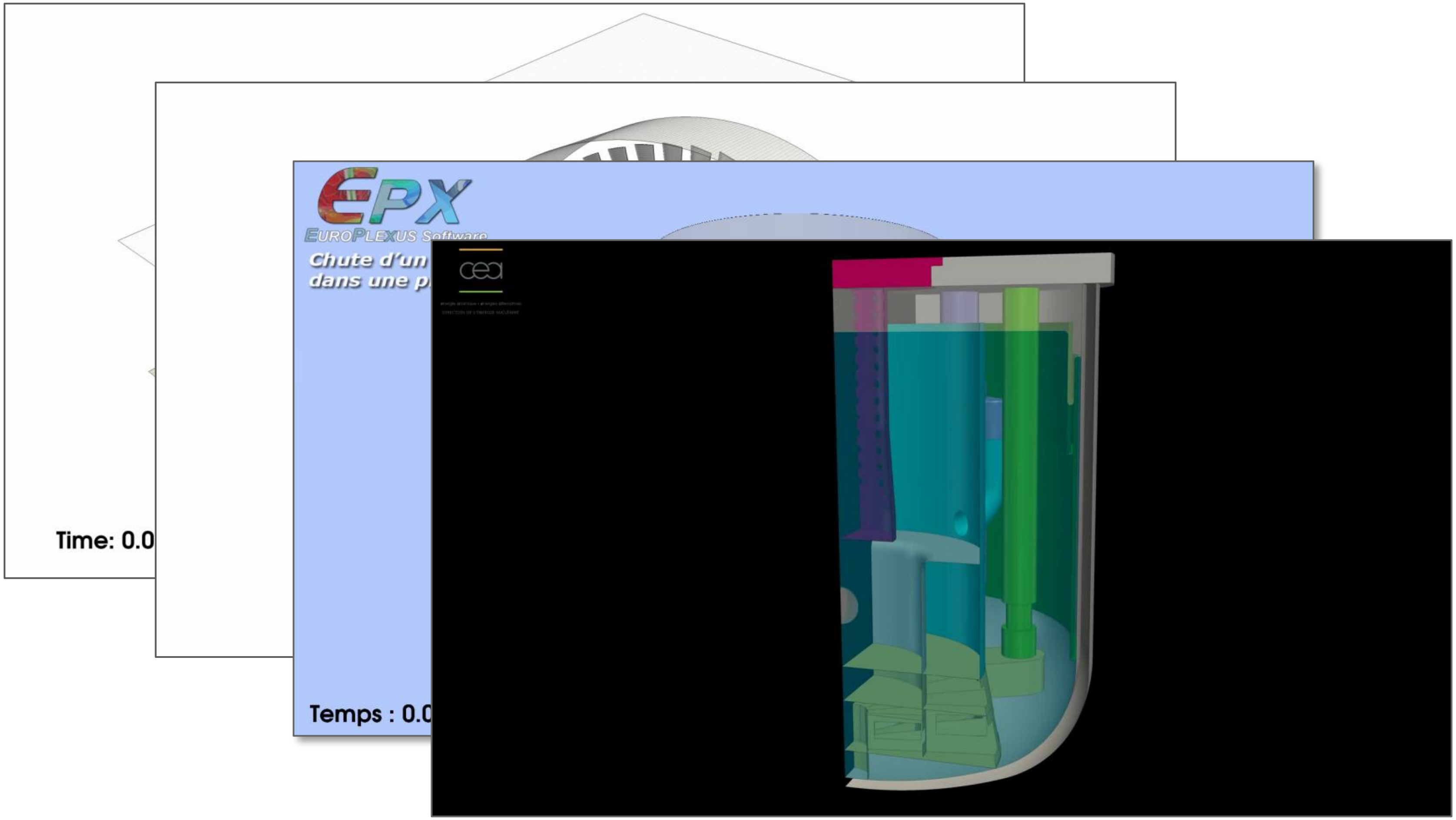

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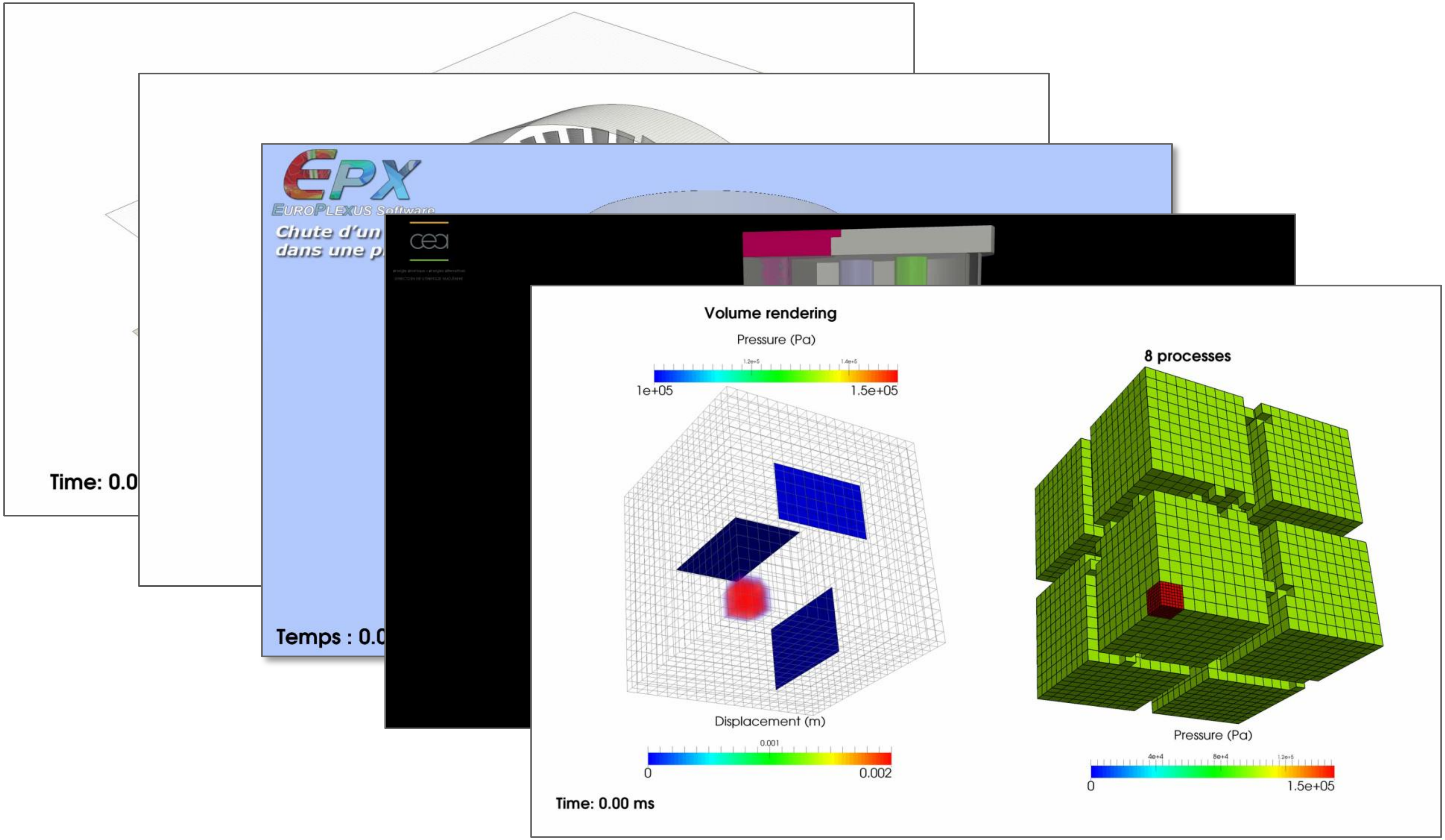

EPX: GLOBAL PARALLEL STRATEGY

- **Distributed memory on cluster nodes**
  - Domain Decomposition through *Recursive Orthogonal Bisection*
  - Generic approach for any kind of kinematic constraints
    - Inter-domain detection of connected entities
    - Specific solver preserving scalability for the computation of link forces
  - Dynamic Domain Decomposition
    - Mandatory to handle large topological changes in the system

Initial situation on a given subdomain

Same subdomain after half a turn of the rotor

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(Advanced) shared memory inside subdomains

- Use and development of the KAAPI library (INRIA, http://kaapi.gforge.inria.fr)
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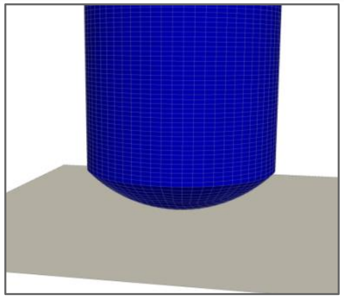

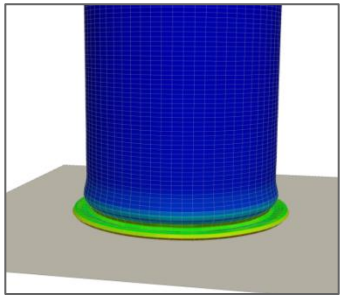

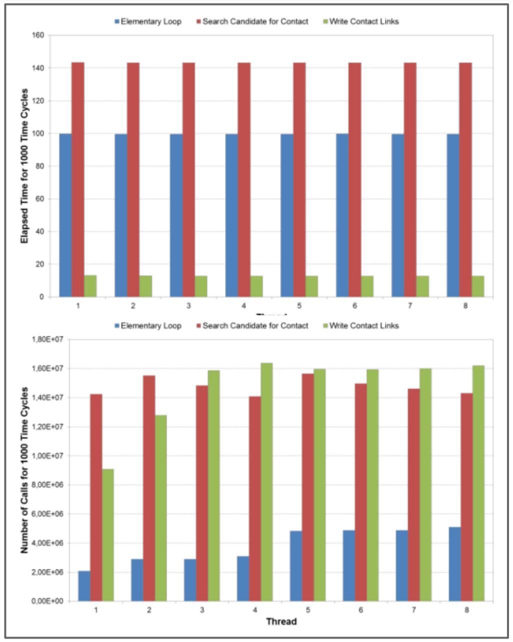

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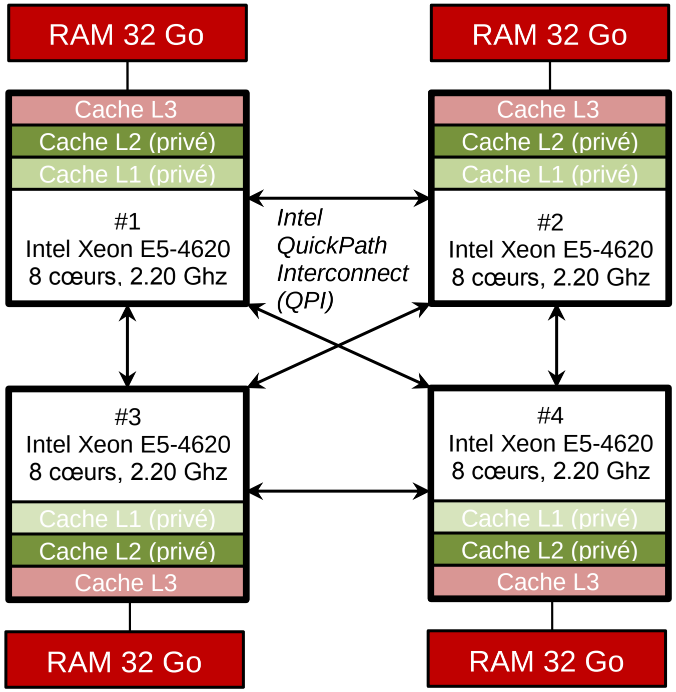
- **Tests on PRACE/Curie supercomputer**
  - Preparatory Access in 2012
  - Scalability achieved for >= 1 024 cores

EPX: SHARED MEMORY OPTIMIZATION FOR MULTI-PROCESSOR NODES (1/2)

- **Target architecture**



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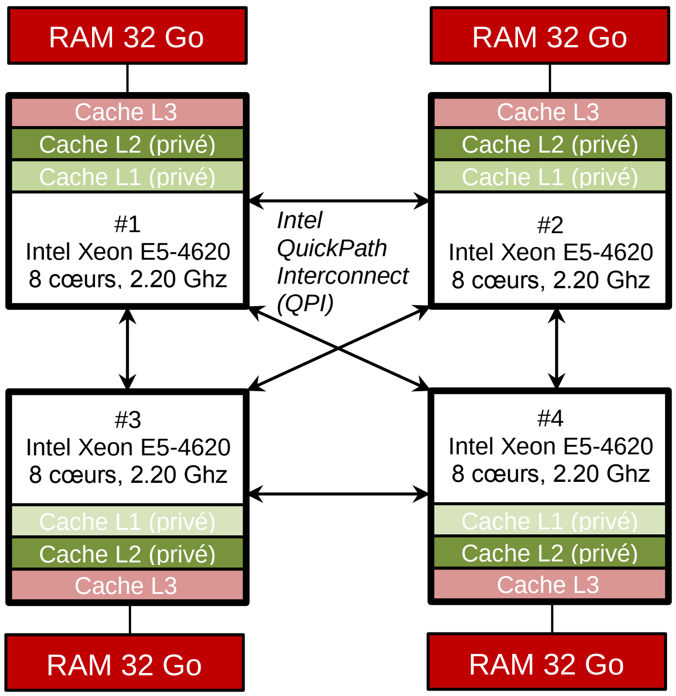

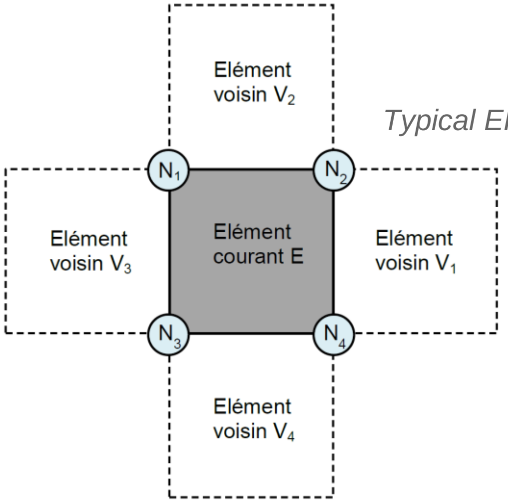

Typical EPX cell

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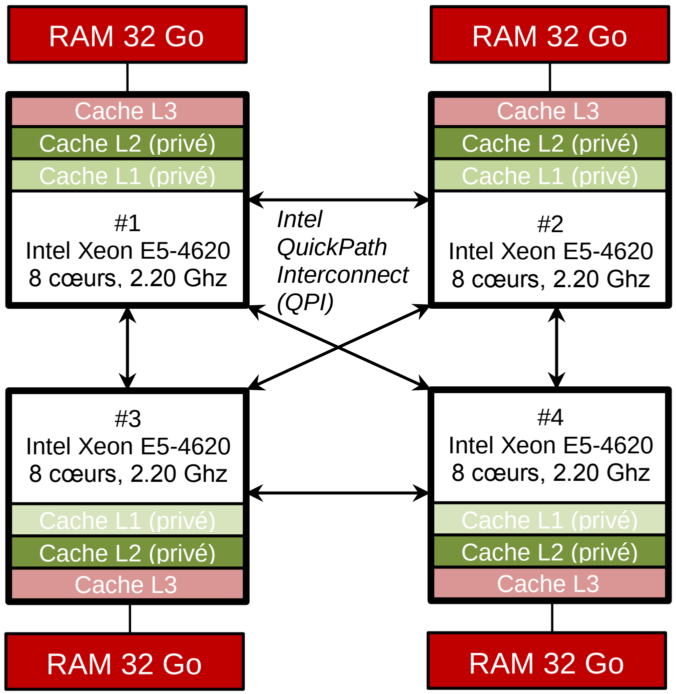

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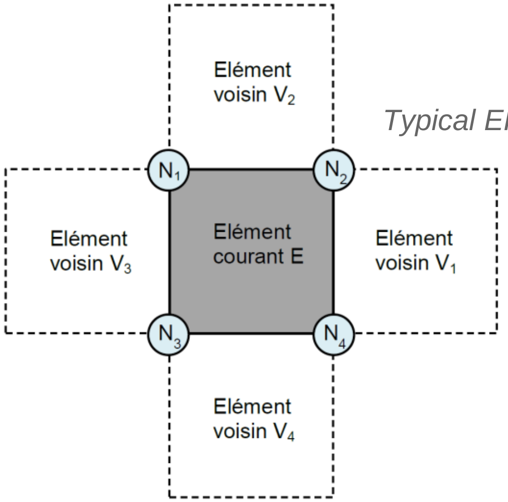
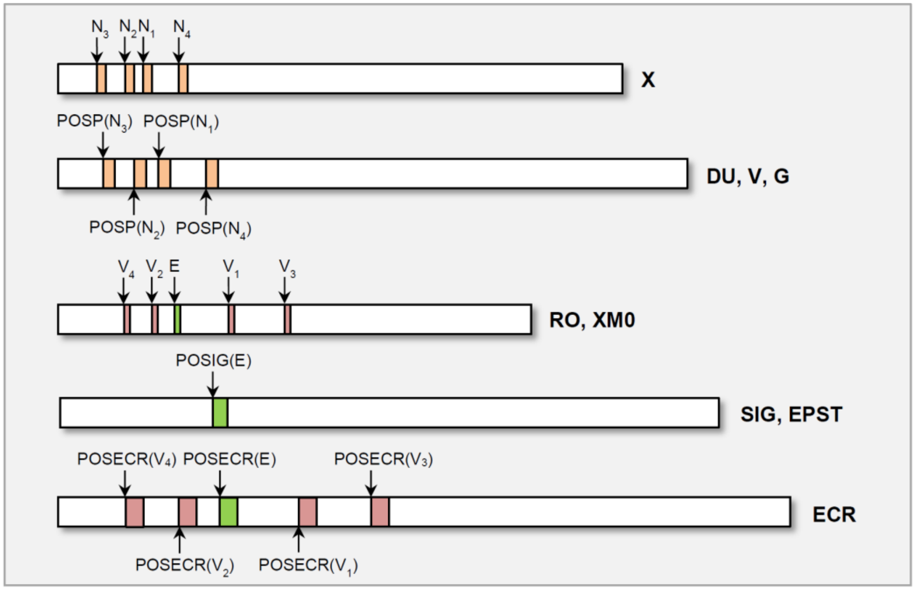


Data placement in memory



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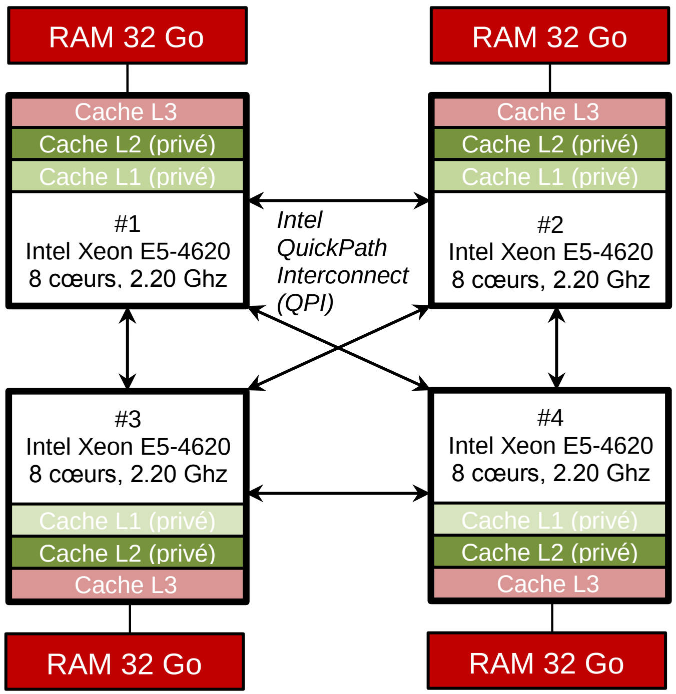
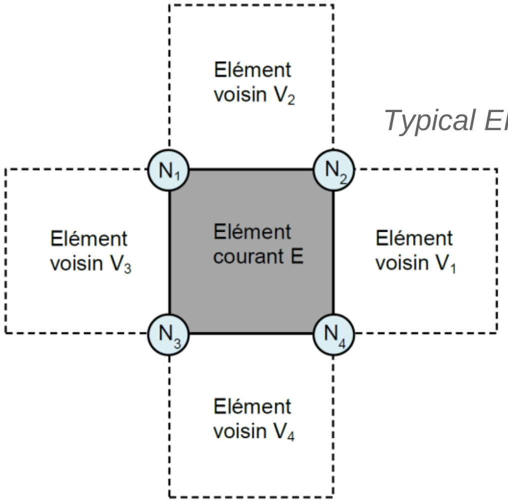


Problematics

- Global data structure inherited from past choices
- Lack of scalability for the elementary loop using threads on several sockets



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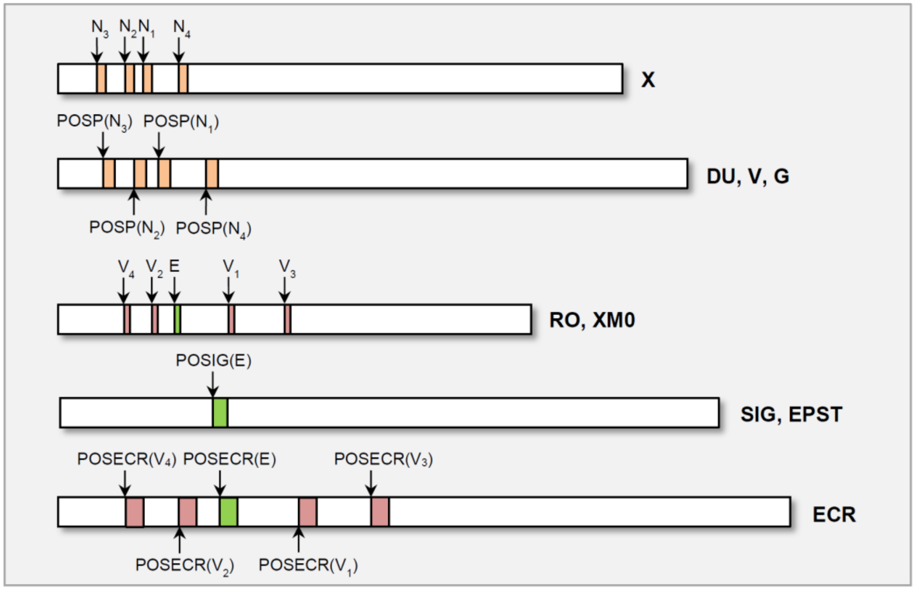

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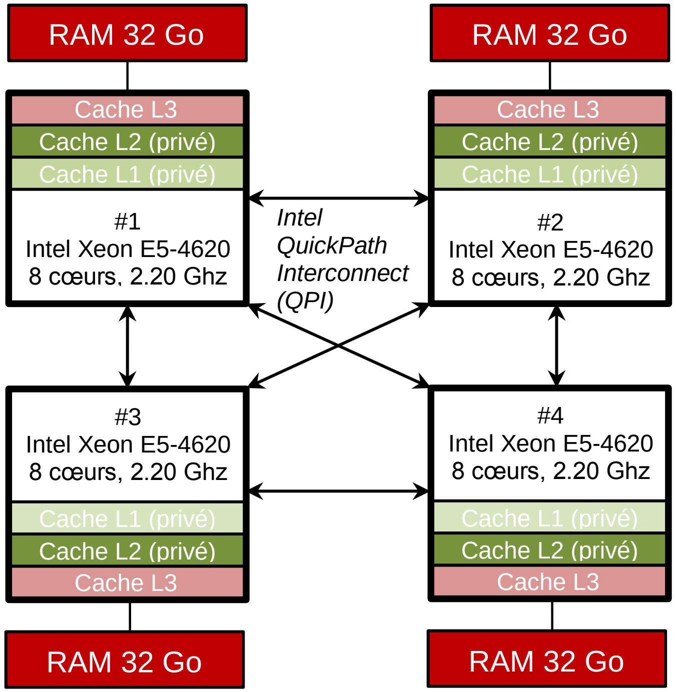

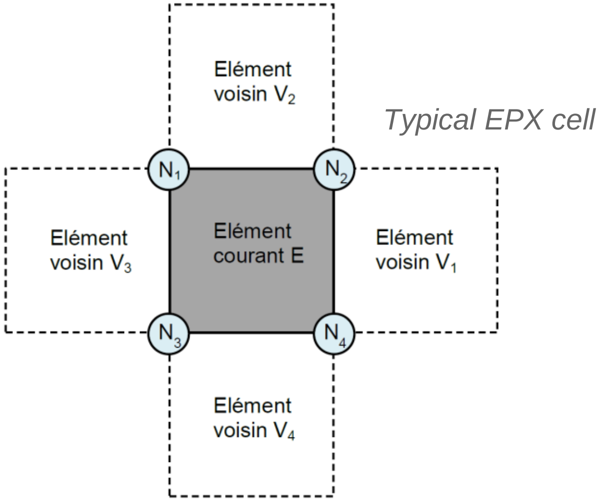

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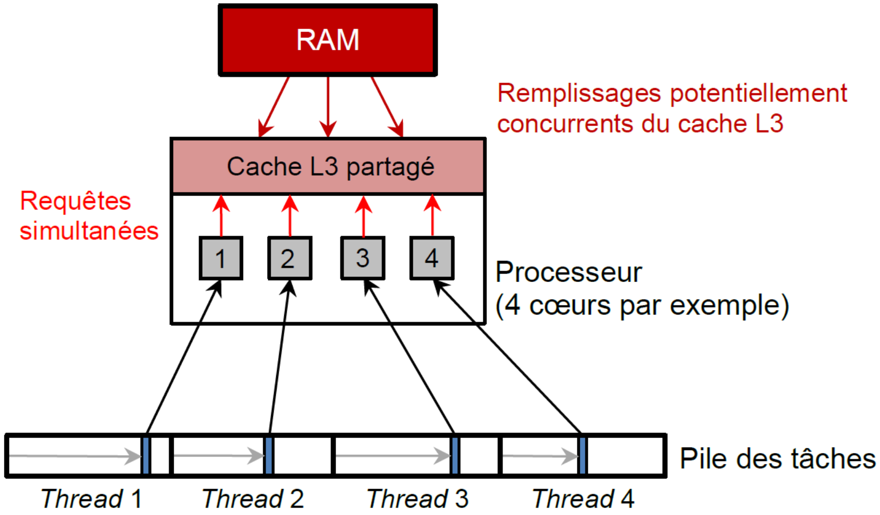

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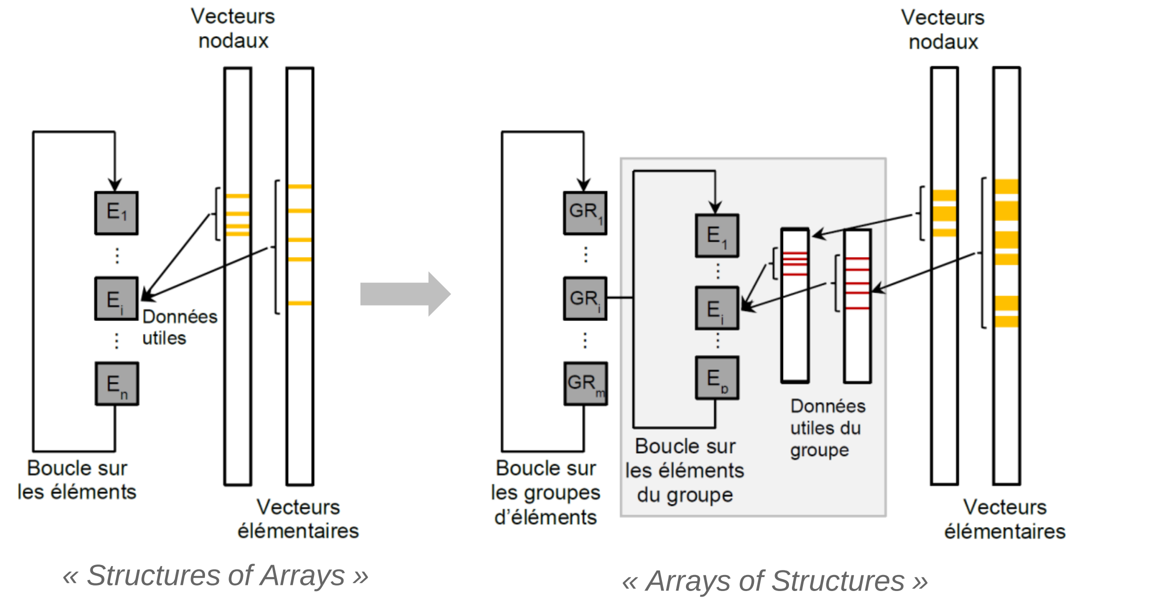
- On-going optimization (PhD M. Sridi, CEA, INRIA, 2013-2016)



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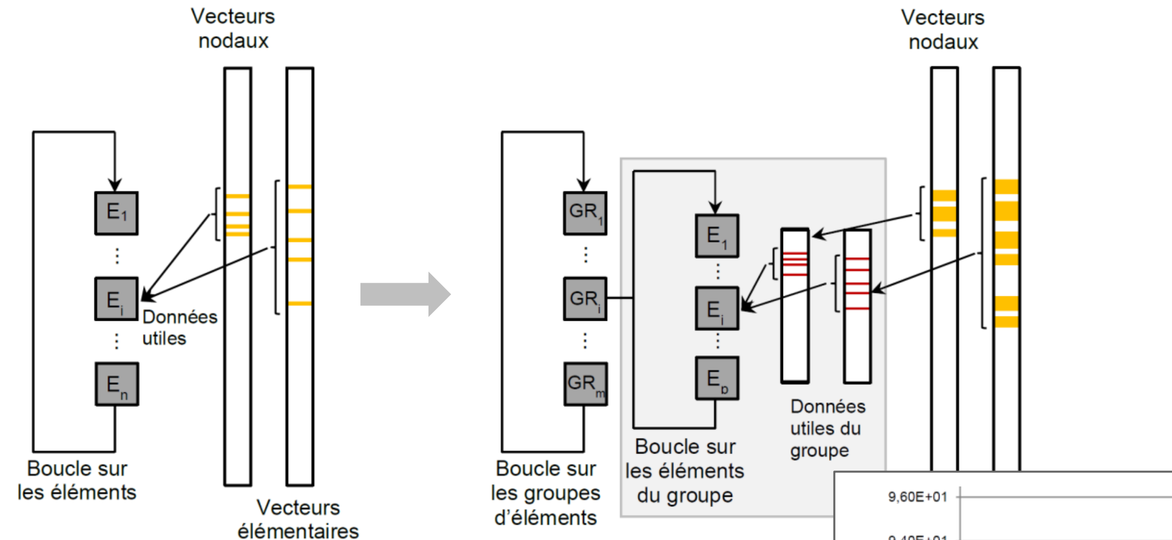
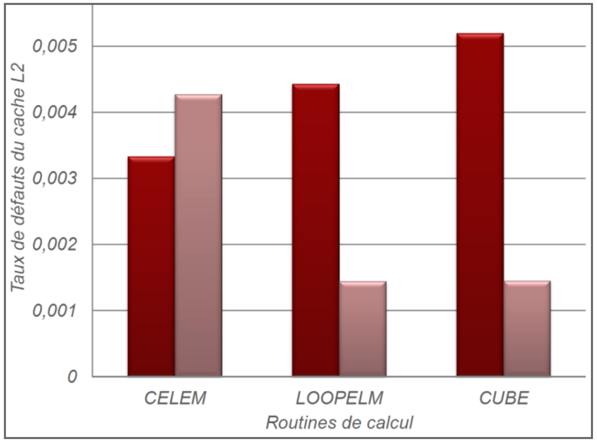
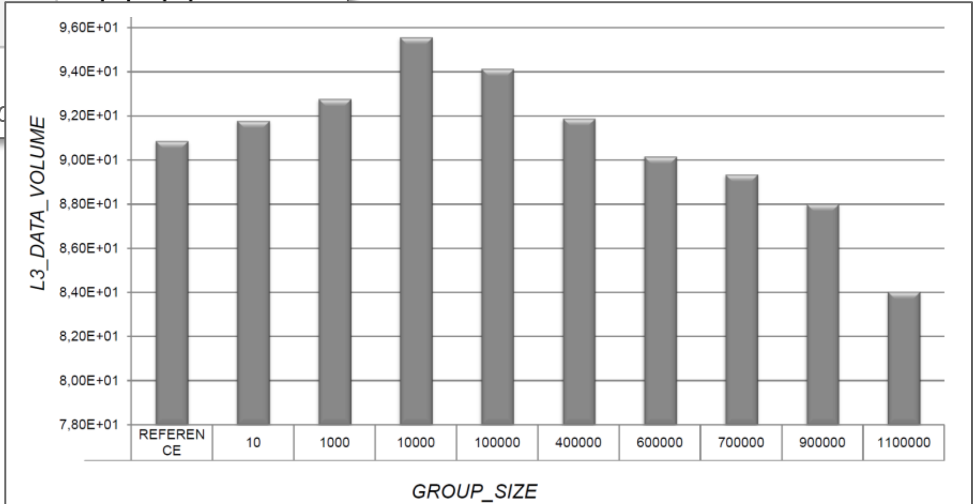


« Structures of Arrays »

« Arrays of Struc



L2-Cache misses reduction



L3-Cache filling improvement

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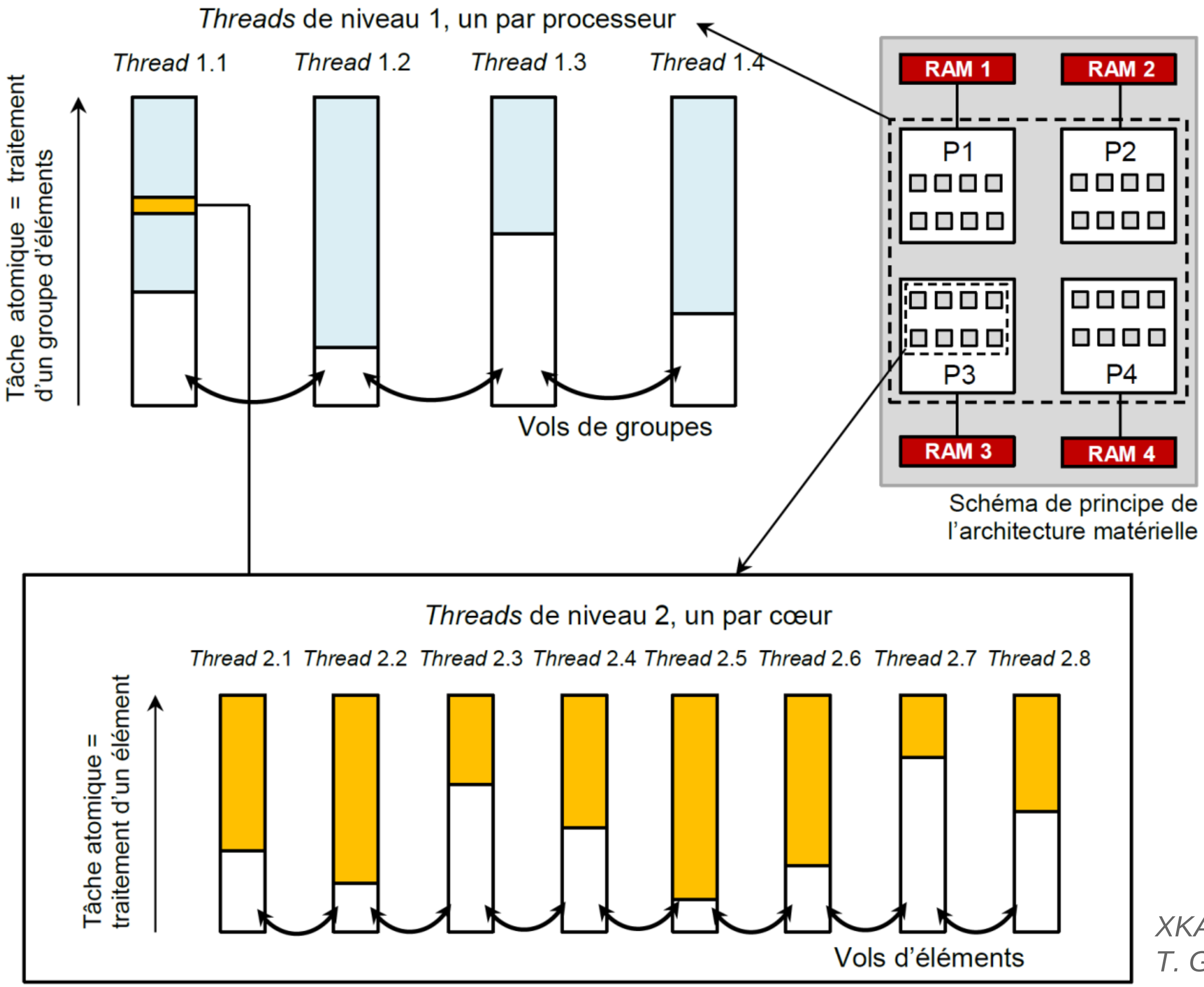

XKAAPI – v3, 2015, January
T. Gautier, INRIA

STRATEGY TOPICS FOR EXASCALE COMPUTING

STRONG OPTIMIZATION VS GENERALITY & FLEXIBILITY

- **Petascale = (big) clusters of PCs + accelerators**

  - Performance obtained from precisely mastering data exchanges and memory accesses
  - Relevant due to relative architectural uniformity
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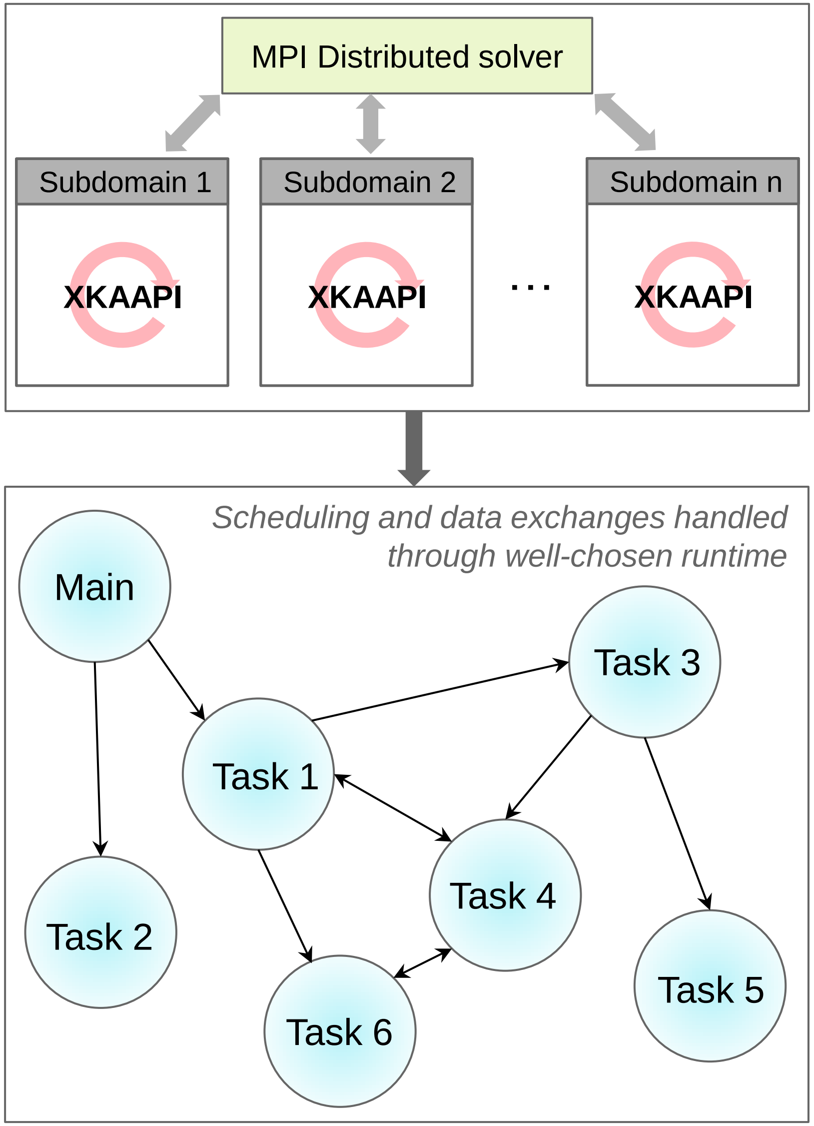

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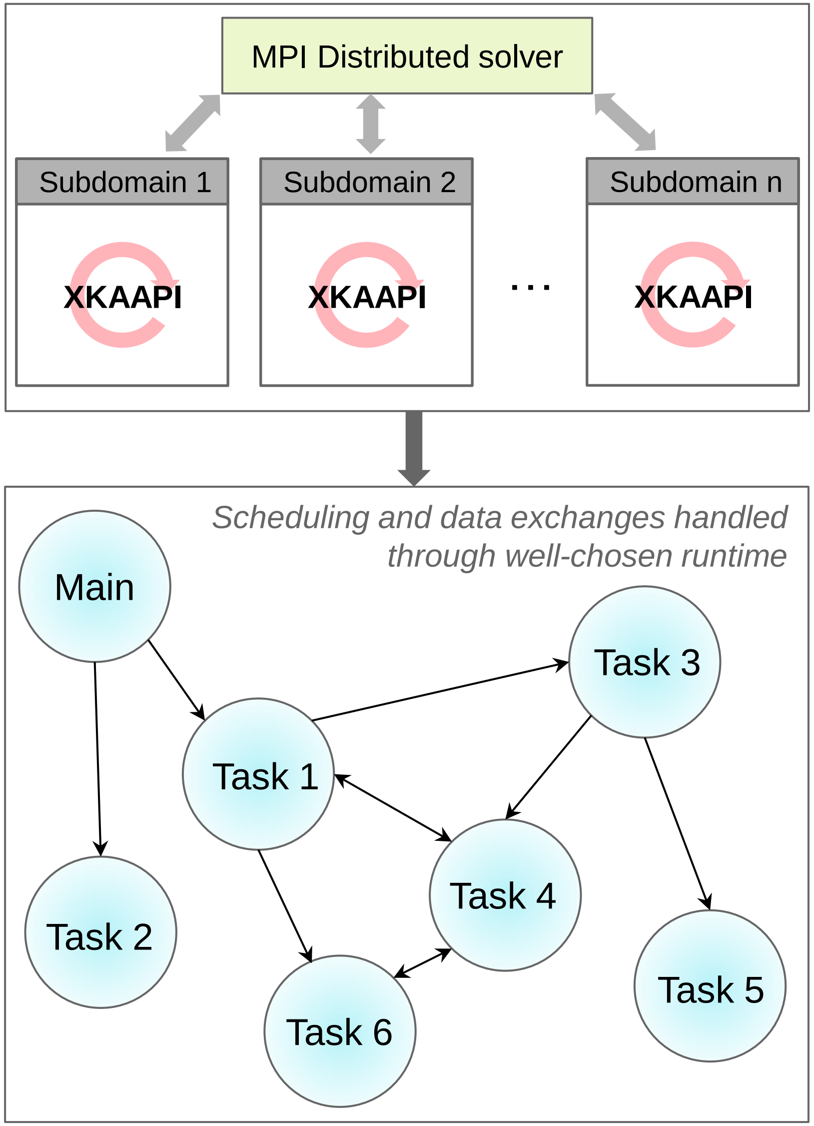

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- **Shortcomings**
  - Runtime must handle efficiently shared and distributed exchanges
  - Deep evolution of the data structure to expect…

NEED FOR ASYNCHRONICITY AND ASSOCIATED ISSUES

- **Need for asynchronicity**
  - Minimum constraints on data flow
  - Fill-in the computing cores at their maximum

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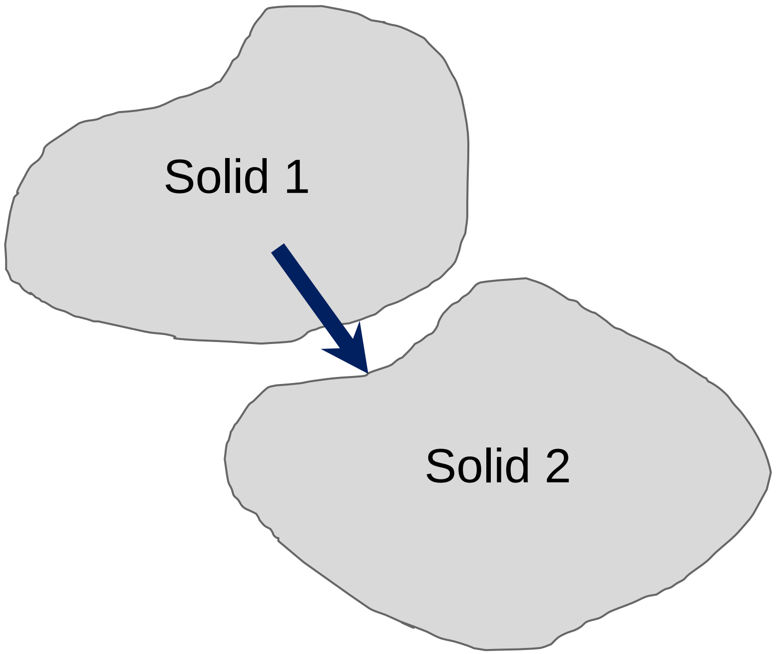

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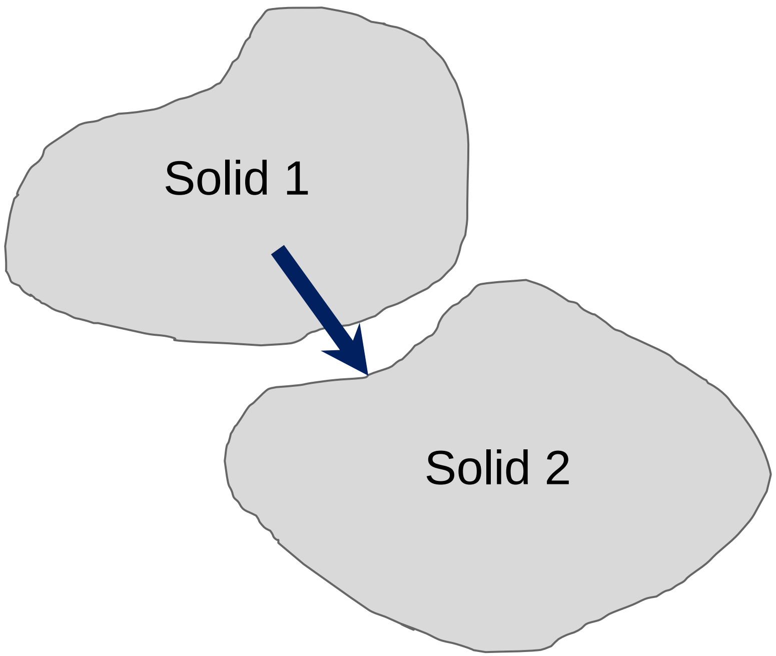

Task 1	Task 2	Task 3
Elementary forces with solids 1 & 2	Contact detection between solids 1 & 2	Link force computation

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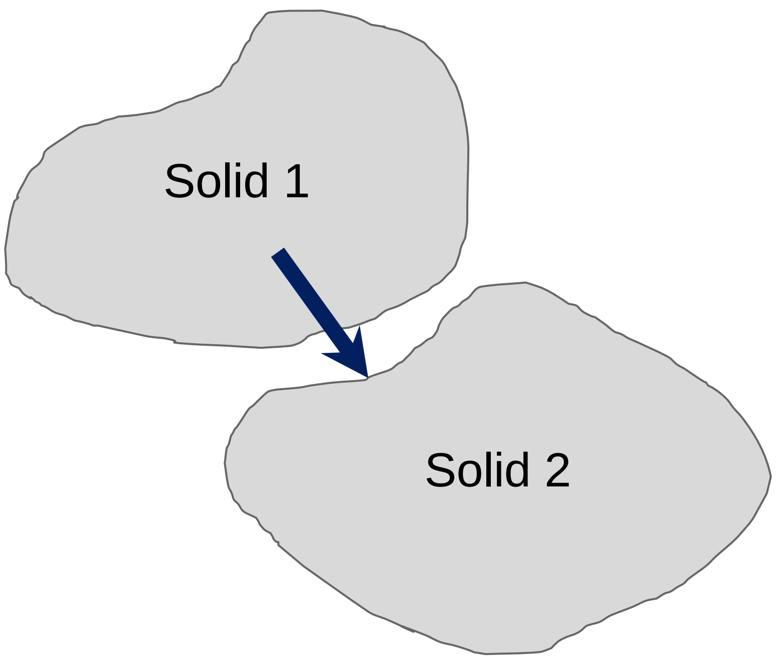

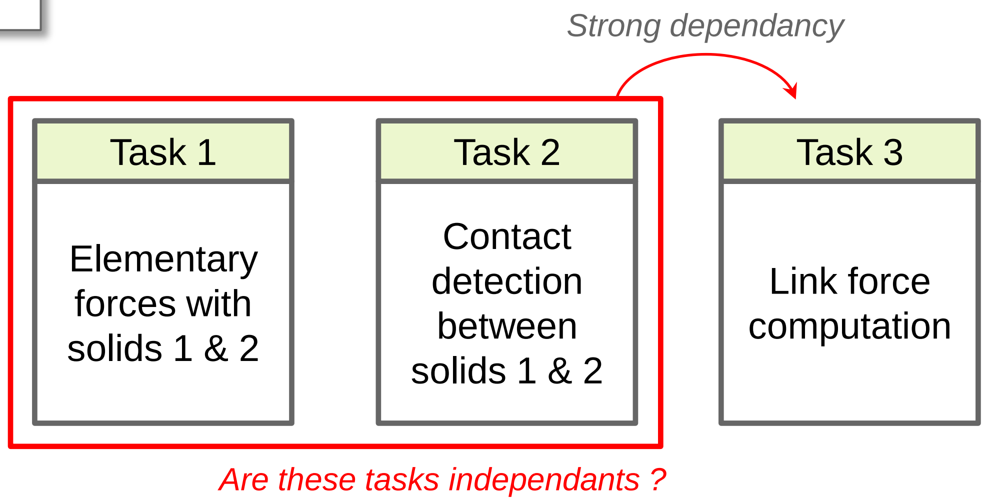

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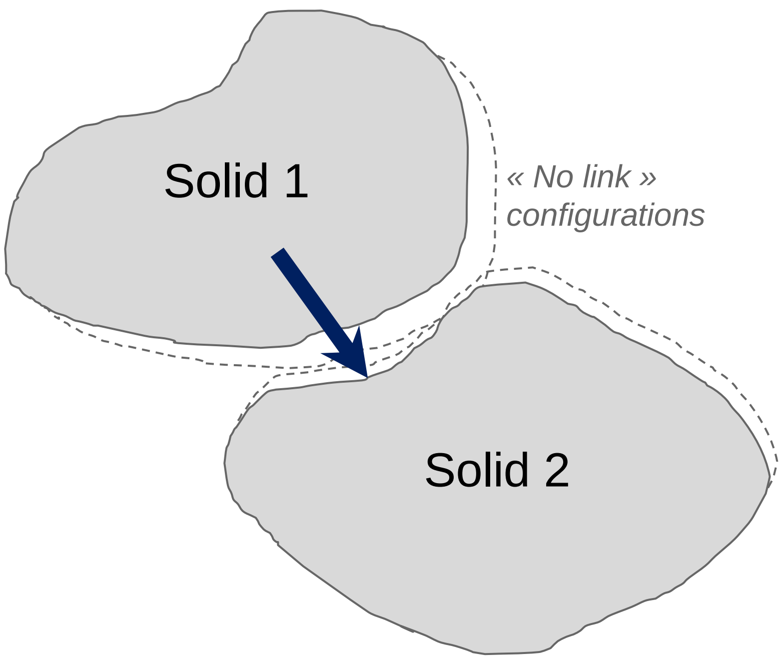

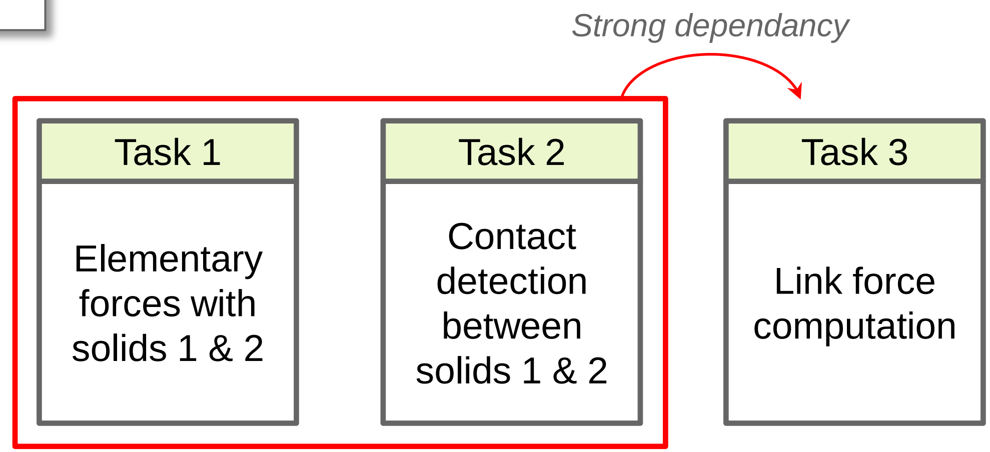

Are these tasks independants ?

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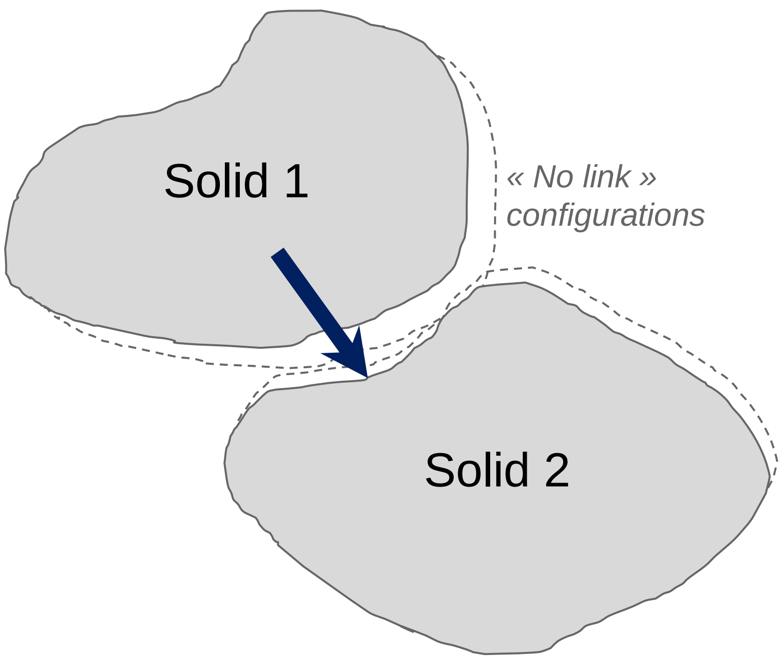

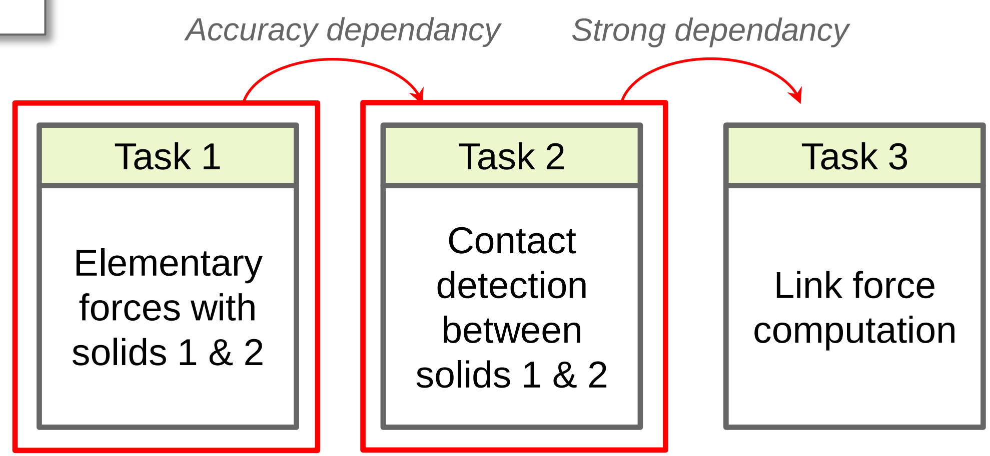

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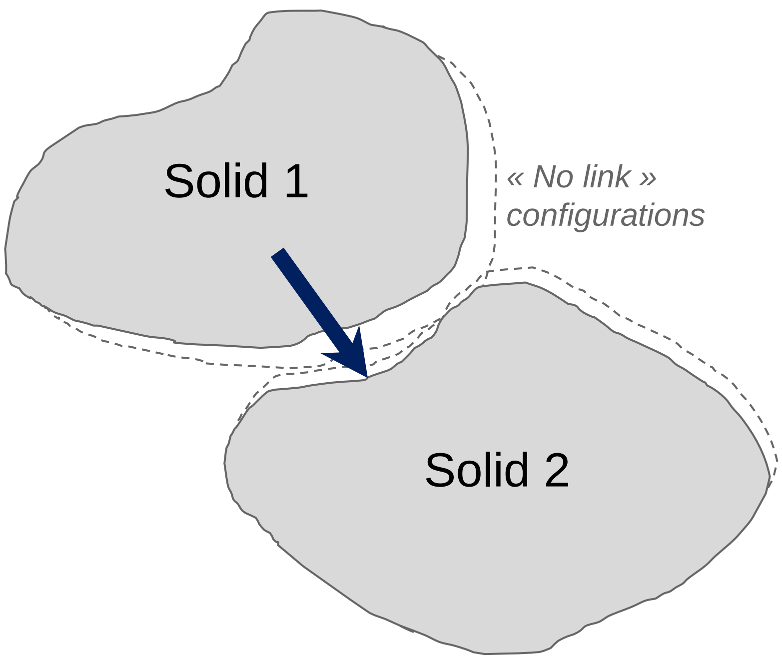

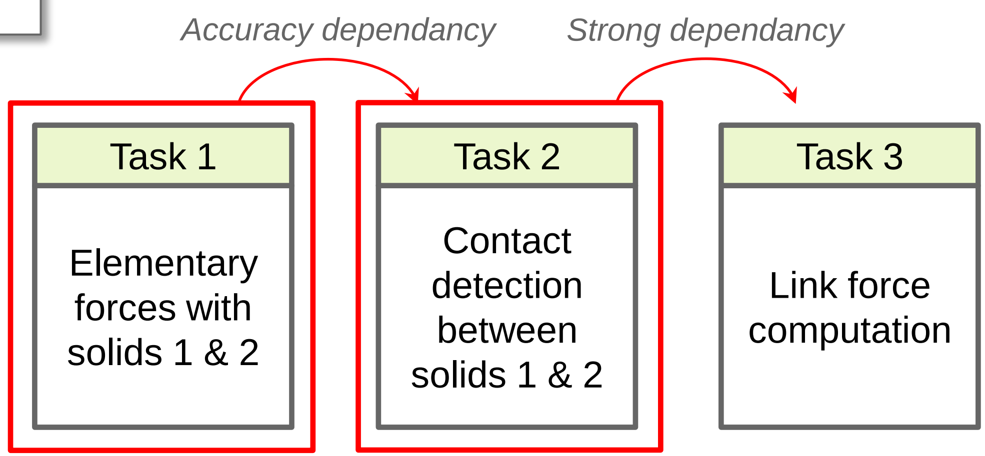

- **Beware the priorities**
  - Final cut in the hands of physics and applied mathematics
  - Asynchronicity implies strong algorithmic innovation

SOME CONCLUSIONS AND PROSPECTS

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- **Main conclusions for explicit fluid-structure dynamics**
  - Petascale
    - Efficiency for Petascale obtained through combining distributed and shared memory
    - Optimization sticking closely to the hardware main characteristics
    - Use of middleware runtime for dynamic scheduling anytime possible
  - Extension to exascale
    - Need for asynchronous algorithms preserving the accuracy of the physical solution
    - Potential restructuration of the data flow to transfer the adaptation to hardware to a generic runtime

- **Prospects**
  - Autotuning for the application to correct itself seeking optimal parallel performance
  - Need for robust on-the-fly diagnostics (internal or external)
  - Continuous algorithmic innovation for load-balancing (growing interest for AMR…)

EUROPLEXUS Software

http://www-epx.cea.fr

THANK YOU FOR YOUR ATTENTION

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Direction de l'Energie Nucléaire
Département de Modélisation des Systèmes et Structures
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