Le Laboratoire Commun INRIA – CERFACS sur le Calcul Haute Performance

Jean ROMAN

INRIA Bordeaux – Sud-Ouest

IPB et LaBRI UMR 5800

21/09/2010

Objectifs du Laboratoire Commun

- Rassembler le potentiel sur la problématique du calcul intensif et spécifiquement ici du passage à l'échelle pour le calcul péta/exaflops
- Meilleure visibilité et impact vers la communauté académique et vers la communauté industrielle
- Mise en commun de moyens de calcul
- Mise en place d'Actions de Recherche communes
- Premier Comité de Pilotage le 28/09

Le CERFACS aujourd'hui

Métier: le calcul intensif

- Amélioration des méthodes de simulation numériques pour le calcul à hautes performances
- Approche pluridisciplinaire des maths applis aux grands domaines d'application
- Equipes ouvertes au-delà du CERFACS

Participation à "Equi@meso"

Projet dans le cadre des "Equipements d'Excellence"

- coordination GENCI
- augmentation de la capacité HPC d'un certain nombre de meso-centres

Avec volet "Formation"

- Maison de la Simulation + Groupe calcul + CERFACS

CERFACS (+HiePACS)

- Sessions de formation au calcul intensif, aux méthodologies HPC (couplages, assimilation de données, codes de calcul, …)
- Ouvertes aux communautés académiques et industrielles

Le CERFACS aujourd'hui

Société Civile de Recherche

Capital social : 927.200 k€

7 Associés:	CNES	21,3 %
	EADS	9 %
	EDF	21,3 %
	Météo-France	21,3 %
	SAFRAN	9 %
	ONERA	9 %
	TOTAL	9 %

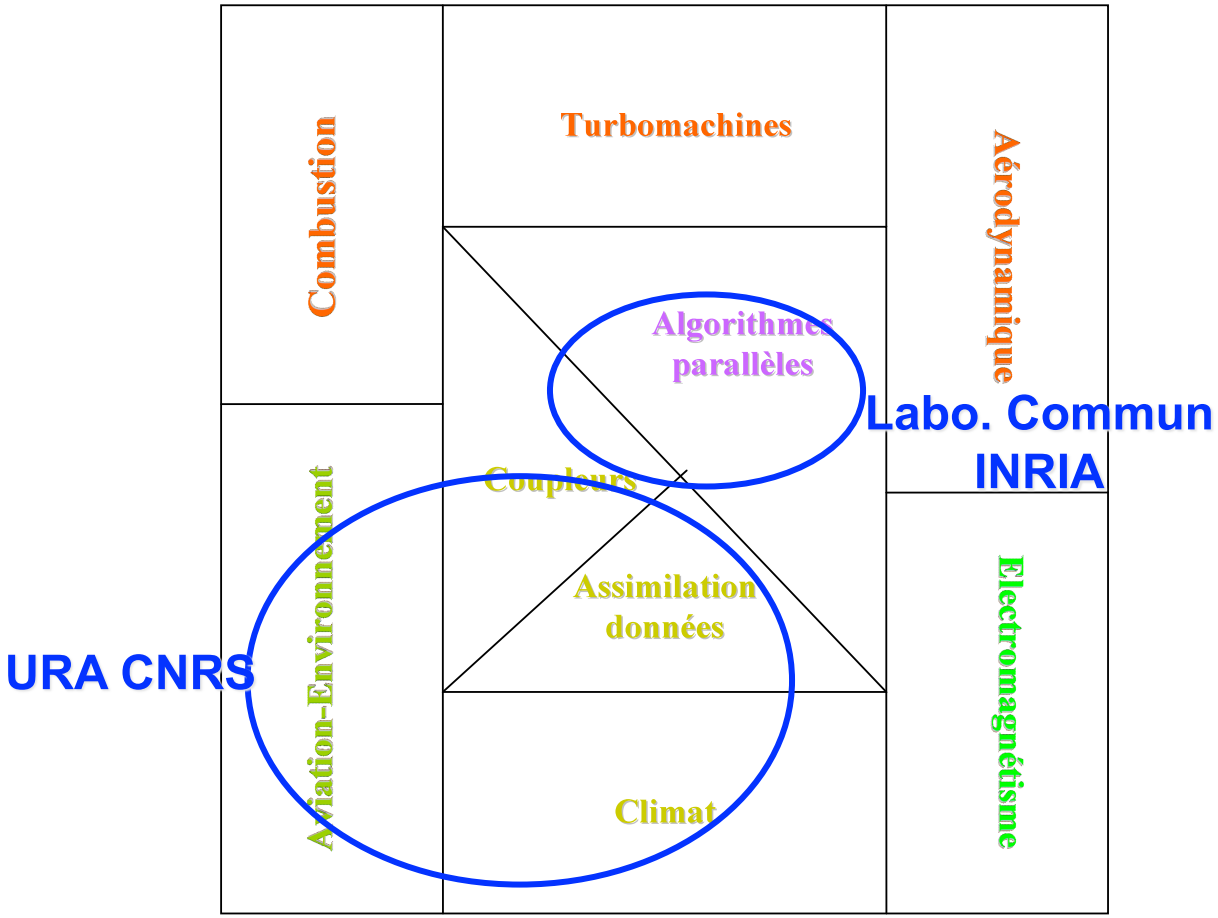
Accords pluriannuels de collaboration

CNRS (Laboratoire Associé, URA 1875)

INRIA (Laboratoire Commun) 

CEA (CCRT)

Le CERFACS aujourd'hui



Algorithmique parallèle, base commune

Etude préconditionnements et solveurs

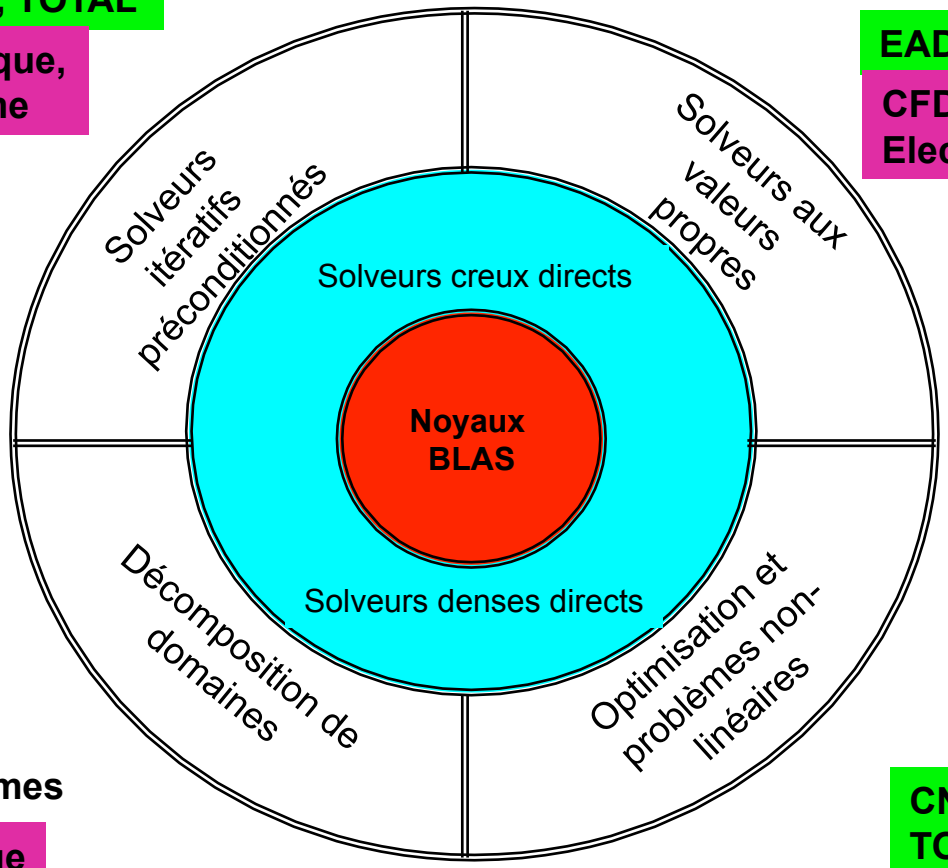
CNES, EADS, EDF, TOTAL

Climat, Géophysique, Electromagnétisme

Intégration dans codes

EADS, EDF, SNECMA

CFD, Climat, Electromagnétisme



Aide et Expertise HPC

CNES, EDF, Météo-F.

Aérodynamique, Combustion, Assim. Données

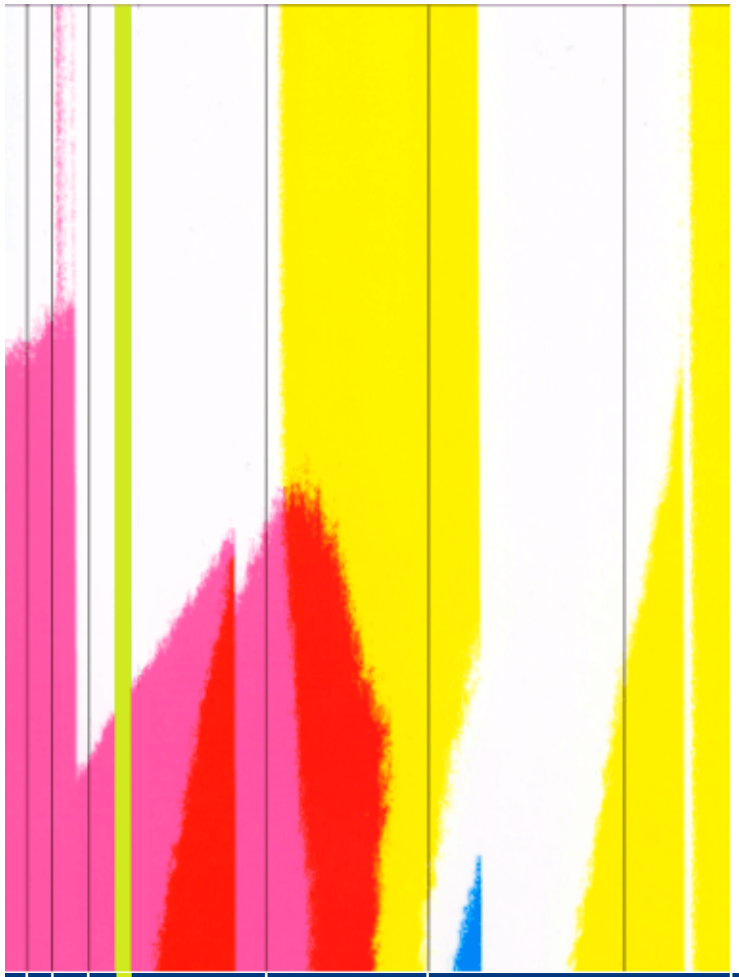
Nouveaux algorithmes

Aérodynamique

Solveurs optimisés/

CNES, EADS, Météo-F., TOTAL

Electromagnétisme, Géophysique



HiePACS
High-End Parallel Algorithms for Challenging Numerical Simulations

INRIA Bordeaux - Sud-Ouest
PRES de Bordeaux
CNRS (LaBRI UMR 5800)

Research Action of the joint
Lab. INRIA - CERFACS on HPC

INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

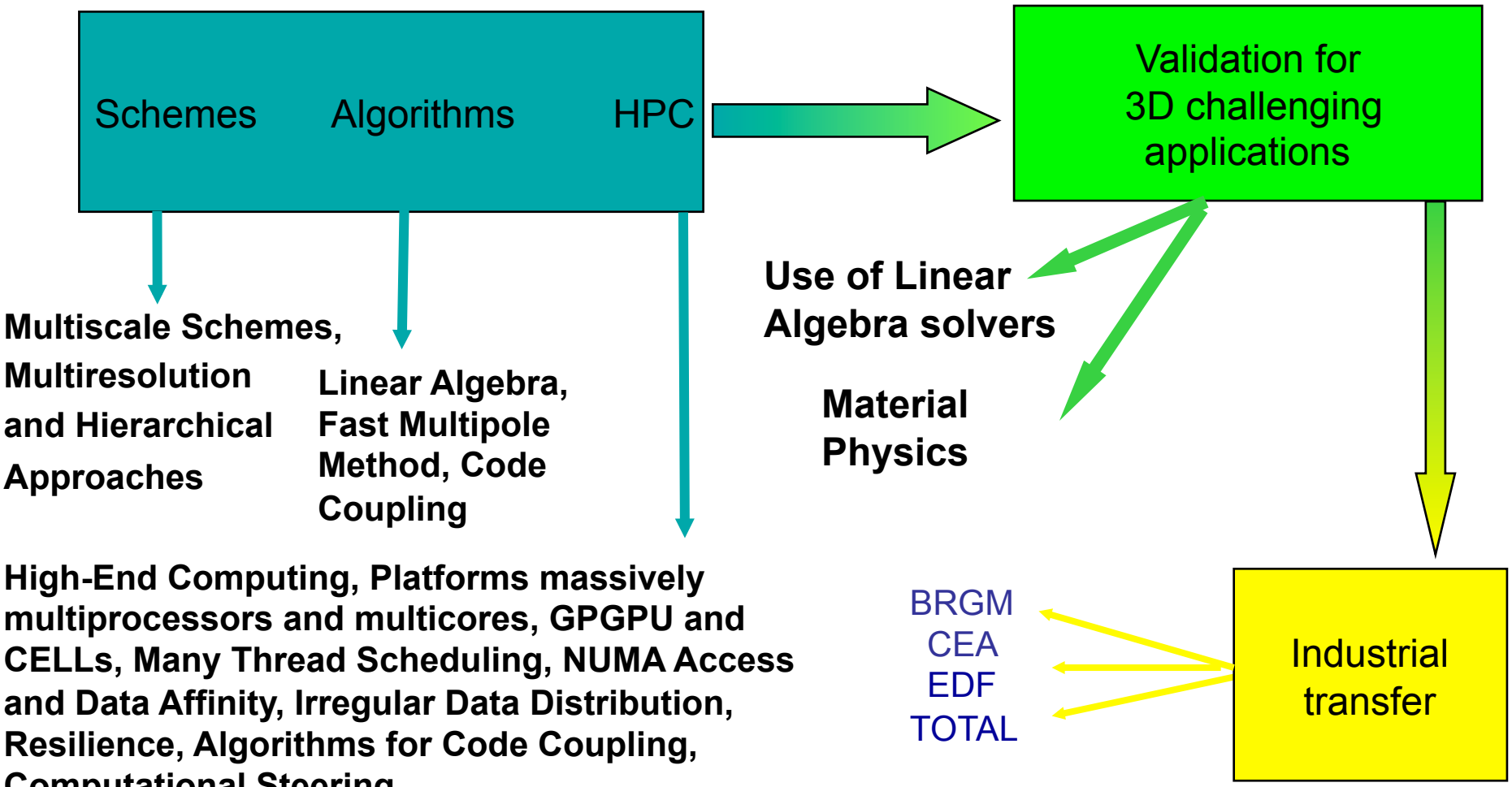
INRIA

centre de recherche BORDEAUX - SUD-OUEST

CERFACS

HiePACS : a multidisciplinary approach

Scientific Objectives



Frontier Simulations, Towards Peta/Exascale Computing (Urbana Champaing, NCSA)

Project-Team Composition

- **Scientific leader**

  Jean Roman [On INRIA secondment, Professor at IPB]

- **Scientific Advisor**

  Iain Duff [Senior Scientist, Leader of the ALGO project, CERFACS]

- **INRIA members**

  Olivier Coulaud [Research director]

  Luc Giraud [Research director since 1st September 209]

  Emmanuel Agullo [Junior research scientist since 1st January 2010]

- **CERFACS members**

  Xavier Vasseur [Senior Scientist, Member of the ALGO project, CERFACS]

  X [Senior Scientist, Member of the ALGO project, CERFACS, *to be recruited*]

- **PRES de Bordeaux members**

  Aurélien Esnard [Assistant professor at Bordeaux 1 University]

  Abdou Guermouche [Assistant professor at Bordeaux 1 University]

- **Post-doctoral fellows**

  Pavel Jiranek [Funding from CERFACS, Member of the ALGO project]

  Y and Z [Fundings from CERFACS, Members of the ALGO project, *to be recruited*]

- **Ph. D. students**

  Rached Abdelkhalek [Funding from TOTAL since 22 January 2008]

  Mathieu Chanaud [Funding from INRIA and CEA since 1st December 2007]

  Fabrice Dupros [Funding from BRGM and ANR CIGC NUMASIS (2005) since 1st January 2007]

  Jérôme Soumagne [Funding from Europe FP7/ICT/FET NextMuSE STREP since 1st April 2009]

- **Technical staff**

  Damien Genet [Funding from ANR CIS NOSSI (2007) since 1st September 2008]

  Yohan Lee-Tin-Yien [Funding from INRIA, ADT ParScaLi, since 7th December 2009]

- **Research scientist (partners)**

  Pierre Fortin [Assistant professor at Paris 6]

  Guillaume Latu [Assistant professor at ULPS and CEA Cadarache]

Scientific Foundations

- High performance computing on next generation architectures
- High performance solvers for linear algebra problems
  - Hybrid direct/iterative solvers based on algebraic domain decomposition
  - Hybrid solvers based on a combination of multigrid methods and direct solvers
  - Linear Krylov solvers
  - Eigensolvers
- High performance Fast Multipole Method for N-body problems
- Algorithms for code coupling in complex simulations

Application domains

- Material Physics and multiscale simulations *(CEA Saclay and DPTA CEA Ile-de-France)*
- Application customers of high performance linear algebra solvers : *BRGM and TOTAL (GPU, seismic imaging), CEA-CESTA (electromagnetism), EDF (structural mechanics)*

General High-Performance framework

- Modern (future) platforms:
  - Massively multiprocessor and multicore
  - Hierarchical structure
  - Huge number of computational resources
  - Heterogeneous resources (a node may contain multicores, GPUs, ...)

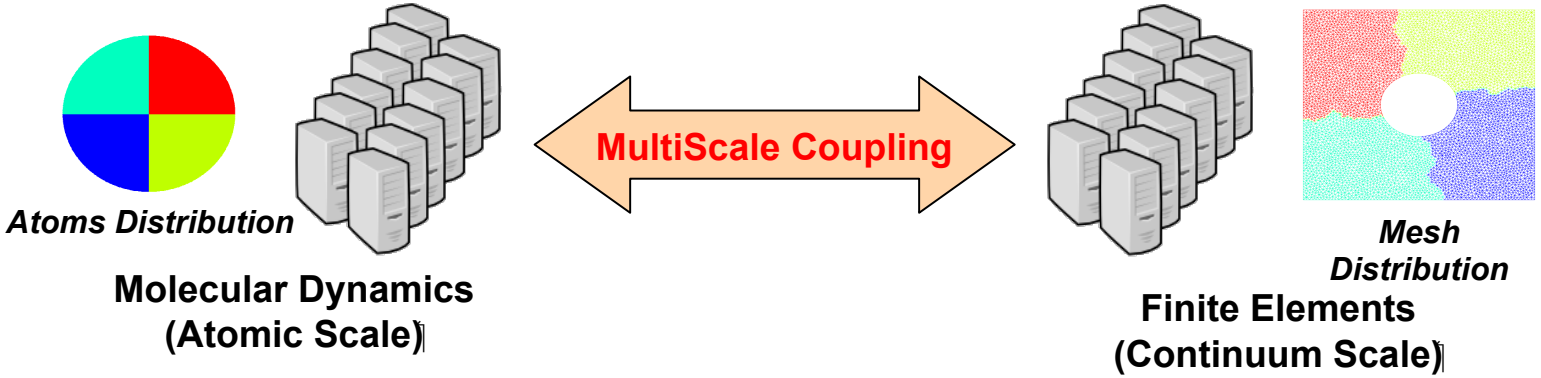
→ Necessity to adapt/design (new) algorithms to efficiently exploit these platforms

General High-Performance framework

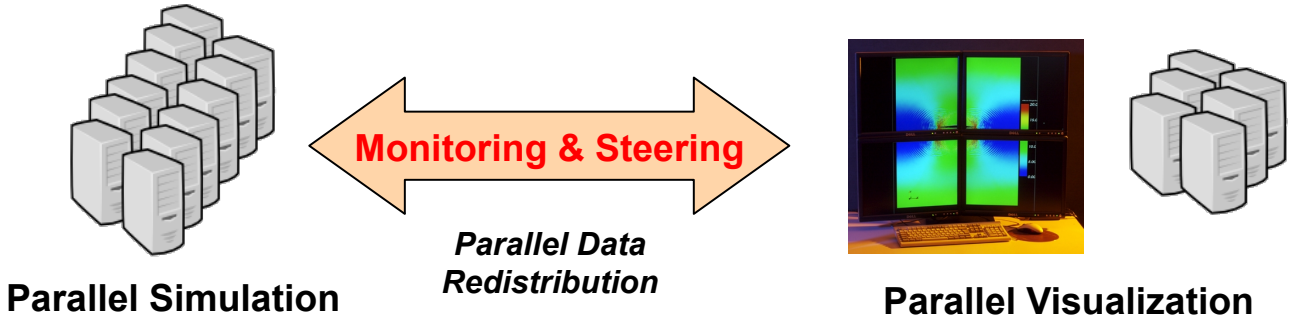
- Scalability issues:
  - Use of hierarchical approaches (i.e, Multi-level parallelism)
  - Need of finer grained algorithms
- Performance & modern architectures:
  - The grain of computation is the key:
    - On regular multicores very fine grain is needed
    - On GPUs (for example) coarse grain tasks are necessary
  - How to mix fine and coarse grained tasks to efficiently exploit all the resources?
  - How about memory hierarchy (NUMA effects are becoming larger and larger, etc ...)?
- Data related issues:
  - How to efficiently store huge amounts of data on disks (I/O related topics like overlapping, perfetching, etc ...)
  - How to be able to deal with the problem of resilience in the context of our target applications ?

Works on Coupling

- Code Coupling in Material Physics with LibMultiScale
  - Coupling schemes in crack propagation, difficult load balancing pb, ...



- MxN Computational Steering with the EPSN framework
  - Parallel online visualization, steering of coupled simulations, ...



New Research Axis on Coupling

Efficient algorithms for code coupling in complex simulations

- Efficient and accurate schemes for multiscale simulations
  - Mixing micro and macro scales is required for accuracy, but scalability is still challenging !
- Coupling of complex simulations based on the graph/hypergraph model
  - Modelling and partitioning the complete coupled application
- Interacting with complex coupled simulations and their data
  - Steering by direct-image manipulation, checkpointing/restart, dynamic load balancing, ...

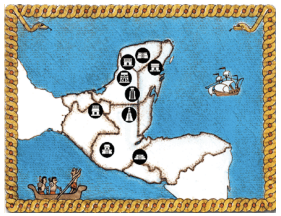
Material Physics

Two main classes of applications

1. Compute « in silico » properties (optical, ...) for new materials

   Hybrid organic-inorganic nanocomposites

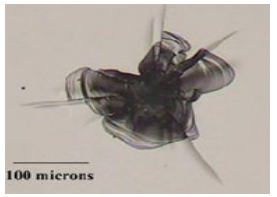
   - Nontoxic coating and robust pigment
   - Optical storage and switch



Peinture murale, site de Cacaxtla

2. Failures

   - megaJoule laser (crack propagation)
   - Nuclear reactor (dislocation simulation)

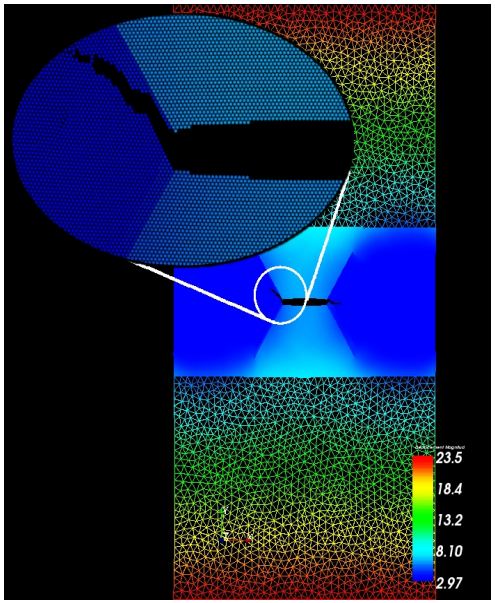


Features

- Multiscale simulation (quantum to continuum)
- Large system, complex algorithms not well studied mathematically

Feed research activities in numerical schemes, FMM and code coupling

Material Failures

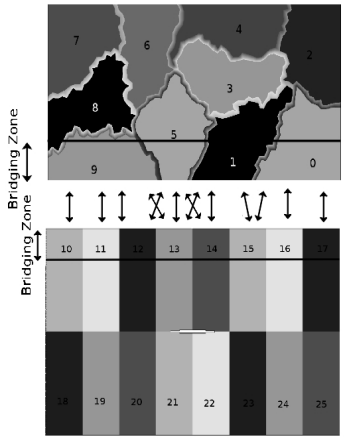


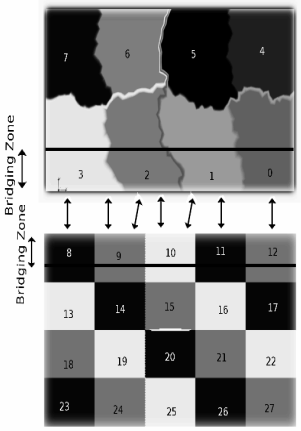
Crack propagation

Multiscale simulation – Atomic-To-Continuum model

Difficulties

- Transmit information between two different scales
  wave reflections, …
- Perform simulation at a given temperature, pressure, …
- Efficient Data distribution for scalable simulation





Software packages

- Environment for computational steering : EPSN
  - Former ScAlApplix EPI
  - ACI-GRID, ARC RedGRID, ANR MASSIM - ANR CIS NOSSI

    http://www.labri.fr/projet/epsn - http://gforge.inria.fr/projects/epsn

- Hybrid parallel linear solver : MaPHYS (Massively Parallel Hybrid solver)
  - Algorithmic study: A. Haidar PhD at CERFACS
  - Software prototype: ANR Solstice and Associated INRIA team PhyLeas with Univ. Minnesota
  - INRIA ADT to consolidate the prototype software (2 year engineer)

Projects

- Ongoing
  - ANR NOSSI (Material Physics), SOLSTICE (Linear sparse solvers for frontier simulations)
  - ITN FP7 MyPlanet (Eigensolvers)
  - G8 proposals : Exascale computing and EXATOM

- Accepted in 2010
  - ANR BLANC : RESCUE (Resilience for numerical algorithms)
  - ANR COSINUS : OPTIDIS (Dislocation dynamics)
  - France-Berkeley Fund (Hybrid solvers : MPI+Thread implementation, Unsymmetric and indefinite systems)

- TOTAL : 2 new Ph. D. (Mesh refinement for elastodynamics problems – P. Thore (*) ; Highly scalable hybrid solvers for wave propagation in frequency regime in heterogeneous media - H. Calendra)

- Collaborations with others CERFACS teams : EMA (*), CFD (MyPlanet), meeting planed at the beginning of October (5^{th})