A PERSPECTIVE ON HIGHPERFORMANCE COLLABORATIVE
PLATFORMS FOR
MULTIDISCIPLINE SIMULATION &
OPTIMIZATION

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Outline

INRIA Example Scenario Multidiscipline challenges **HPC Contributions Workflows** Conclusions





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INRIA Key figures

Jan. 2008



A workforce of 3,800

including 2,000 paid by INRIA

2,800 scientists 950 PhD candidates (400 from abroad) 500 post-docs and engineers

1050 staff 468 research scientists 560 ETA 300 interns

120 projects in FP6 and 30+ in FP7

Budget: 180 M€ (tax not incl.) 20% from contracts, licenses, 8% from Europe





INRIA organization

Research projects

• The key organization: 180 project-teams (10-20 persons, 4 years, 10-90% funding)

Research centers

 Decentralized, self-supporting structure with strong connections with the regional environment, no intermediate administrative level

Scientific and functional departments

Coordination and organization role

Discussion structures

 Center Committee in the research centers and discussion committee at the national level

Evaluation bodies

 Research Projects Committee in the research centers, Evaluation Committee at the national level

Steering bodies

• Research centers management teams, national management committees





KEY-WORDS

• What: COLLABORATIVE INTEGRATION PLATFORMS

• How: DISTRIBUTED HIGH-PERFORMANCE ENVIRONMENTS

Programming & Communication

Where: INNOVATIVE MULTIDISCIPLINE APPLICATIONS

Modeling & Simulation







• PROVIDE SEAMLESS & CONFIGURABLE PLATFORMS

• SUPPORTED BY:

- **1 HIGH-PERFORMANCE DISTRIBUTED SYSTEMS**
- 2 CONFIGURABLE & RESILIENT SYSTEMS

3 - PROGRAMMING MODELS & TOOLS for DISTRIBUTED COMPUTING

Technology Push

APPLIED TO LARGE-SCALE INNOVATIVE MULTIDISCIPLINE APPLICATIONS

Application Pull





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Aeroelastic Simulation: M=0.8, Nz=1, Z=11277 m









Fluid Structure Interaction: Process Overview

Aero-structural Design Process



Process definition







Innovative multidiscipline Applications

Combine algorithms and methodologies







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Multiphysics challenges

- Reduce time to market, design better & faster
- Use efficient, robust & validated methodologies & tools
- Set-up collaborative teams, procedures & workplans
- Deploy & take-up HPC resources
- Design large-scale multiphysics simulation & optimization •
- Contribute to knowledge for safer, cleaner, quieter designs
- Contribute to virtual flight tests, virtual certification by 2020

Transport & Aeronautics Vision 2020





Multiphysics Design, simultation & optimization

nesting complex multidiscipline processes



HPC Contributions: ongoing efforts

- High-Performance Computing era: multi-core, GPU,...
- Heterogeneous, parallel, grid and distributed computing
- Sustainable, affordable, mature, HPC & wide-area computing
- Collaborative environments: //viz+HPC, VR workbenches, ...
- Disseminate in many domains: genomic, seismic, aerospace, medical, chemical, automotive, astrophysics, energy...

The e-science era





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HPC: from Mega-Flops to Exa-Flops...

CDC6600	Cray2	ASCI Red	Blue Gene /L Roadrunner		
1MFlops	1GFlops	1TFlops	.5PFlops	1PFlops	1EFlops
1964	1985	1997	2007	2008	2018
10**6 flops	10**9	10**12	#10**15	10**15	10**18





HPC: the road to Exascale computing...

- Exascale 2018 plan at Intel: computing power >> Moore's law
- Blue Waters (NCSA), INCITE (US): free petascale for industry
- RIKEN KEISOKU (Japan), DEISA, PRACE (EU) INITIATIVES
- MOSART, CRESCENDO, NURESIM (CEA nuclear plant sim)
- ITER Tokamak fusion facility, Argonne, Oak Ridge, MIT Labs Blue Gene /L (.5 Pflops), /P (3 Pflops), /Q (10 Pflops), ...





ISSUES

- COMPUTING POWER IS NOT: WHAT ARE THE ISSUES ?
- TECHNOLOGY BARRIER PLAGUES HPC DISSEMINATION
- HETEROGENEITIES PLAGUE MULTIPHYSICS SIMULATION
- CULTURE & IPR PLAGUE COLLABORATIVE WORK...
- NEED TO DEVELOP COMMON APPROACHES
- •••• PETASCALE DATA MANAGEMENT ISSUE



FOCUS

- NEED TO SOFTEN ACCESS TO HPC TECHNOLOGY
- METHODS & TOOLS TO SUPPORT HETEROGENEITIES
- EXPLORE, DESIGN, COMBINE NEW APPROACHES
- EXPERIMENT ON LARGE-SCALE TESTCASES
- NEED TO DEVELOP COMMON COLLABORATIVE TOOLS
- •••• AUTOMATE SCENARIO DEPLOYMENT & EXECUTION





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OPEN ISSUES

- USERS NOT AWARE OF UNDERLYING HW, OS, GRIDS...
- DISTRIBUTION, FAILURE, SECURITY TRANSPARENT
- COMPOSE & REUSE LEGACY TOOLS, CODES, APPs
- NO USE OF EXOTIC LANGUAGES & COMMANDS : GUI++
- COMPLIANT WITH CURRENT & UPCOMING STANDARDS CORBA, SOA, WSDL, WSRF, OGSA, Globus GT3 & GT4, UNICORE...













Distributed Workflows: customization

FOCUS ON APPLICATION & USERS





40 ans



30

Workflow contributions to Multiphysics Design

- DECLARATIVE REPRESENTATION OF HETEROGENEOUS DISTRIBUTED INTERDEPENDENT COMPUTATIONS
- AUTOMATE & MANAGE COMPLEX DISTRIBUTED COMP.
- USED AS COMPLEX APPLICATION FACTORIES
- RUNTIME BINDING
- IN PLACE REFERENCING
- EXHIBIT MULTI-DISCIPLINE INTERACTION PROTOCOLS
- DATA STREAMING FOR ASYNCHRONOUS // COMPUTAT.





Workflow contribution to Multiphysics Design

- MANY WORKFLOW candidates: Taverna, YAWL, Pegasus...
- WORKFLOW BUS
- SHARE & COMPOSE WORKFLOWS
- SERVICE ORIENTED ARCHITECTURES
- REUSABLE TRACEABLE COMPOSITE WORKFLOWS
 <u>REPRODUCIBILITY</u>, <u>PROVENANCE OF DATA</u>



Workflows for Multiphysics Design

- PLUG-IN COMPONENTS, DATABASES AND SOFTWARE
- INTERACTIVE MULTI-USER PLATFORMS
- MULTI-DISCIPLINE TRIAL/ERROR ENVIRONMENTS
- EXHIBIT APPLICATION DEPENDENCIES

• COMPUTATIONAL STEERING = ON-LINE MONITORING + INTERACTIVE STEERING





OPEN ISSUES

• FLEXIBILITY (i.e. dynamic (re)-configuration), USER EXCEPTION HANDLING (i.e. parameter updates)... DISTRIBUTED PAUSE, ROLL-BACK, RESTART... RESILIENCY, PETA-SCALE VOLUMES DATA...

COLLABORATION on WORKFLOWS

• China, Finland, ...

- VIRTUAL FLIGHT-TESTS IN AERONAUTICS Vision 2020
 - FP7 Transport (Aeronautics) Call 2009...
- FLUID-STRUCTURE APPLICATIONS IN AUTOMOBILE

• OMD2 (ANR) : RENAULT, TAO, OASIS, ECN, EMSE, ENS Cachan, UTC, SIREHNA, ACTIVEON...





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To summarize

- Workflows are formal specifications of scientific processes: data collection, analysis, computation & publication
- Support sharing scientific processes descriptions across organizational and discipline bounderies
- Ability to evolve processes, compare, identify differences
- Solve heterogeneity in large-scale multiphysics apps
 - implementations: application orchestration & choreography
 - computing environments: supercomputers, large clusters, ...

The snowball effect...





CONCLUSION

GH-PERFORMANCE COMPUTING PLATFORMS

LARGE SCALE MULTIDISCIPLINE APPLICATIONS ON COLLABORATIVE ENVIRONMENTS

LARGE-SCALE MULTI-DISCIPLINE OPTIMIZATION FLEXIBLE, RESILIENT, EFFECTIVE

DISTRIBUTED PLATFORMS

RE-CONFIGURABLE, FAULT-TOLERANT





CONCLUSION

TOWARDS VIRTUAL FLIGHT-TESTS



HIGH-PERFORMANCE COLLABORATIVE PLATFORMS

« THE DIGITAL DYNAMIC AIRCRAFT »





REFERENCES







Links

- IEEE Computer, December 2007, Examining the Challenges of Scientific Workflows
- NSF Workshop, Arlington (Va), 1-2 May 2006 <u>http://vtcpc.isi.edu/wiki/index.php/Main_Page</u>
- Ter@Tec Initiative (France) High-Performance Numeric Simulation http://www.teratec.fr/
- LARGE-SCALE DISTRIBUTED INFRASTRUCTURES
 Open Science Grid, TeraGrid, NMI, NAREGI, PRACE...
- IEEE Technical Committee on Scalable Computing Workflow Management in Scalable Computing Env. http://www.swinflow.org/tcsc/wmsce.htm





Links

• vl-e

University of Amsterdam, http://www.vl-e.nl

- PRACE Partnership for Advanced Computing in Europe Persistent HPC service & infrastructure http://www.prace-project.eu
- CCGRID'09 Cluster Computing & Grid Conf. Lyon (F) May 2008, Shanghai May 2009, Melbourne 2010 <u>http://www.ens-lyon.fr/LIP/RESO/ccgrid2008/</u> <u>http://grid.sjtu.edu.cn/ccgrid09/</u>
- e-Science 2008 4th IEEE Intl Conf. University of Indiana, Indianapolis, December 2008
- Grid Applications and Middleware Workshop Wrocaw, Poland (GAMW'2009), Sept. 2009



