Arcane/ArcGeoSim, a software framework for geosciences simulation

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Outline

these are the questions.

- Who are IFPEN ?
- What was our problem… ?
- … and our solution ?
- A solution but another problem ?
- Current activities.
Vocation

- IFPEN is a public research and training player (EPIC – Etablissement Public à caractère Industriel et Commercial -- state-owned industrial and commercial establishment)
- It has an international scope, covering the fields or energy, transport and the environment
- From research to industry, technological innovation is central to all its activities

Mission

- Growth in energy demand
- Climate change
- Long development time of REs
- Requirement for qualified personnel
- Economic competitiveness

As part of the public-interest mission with which it has been tasked by the public authorities, IFPEN focuses on:

- providing solutions to take up the challenges facing society in terms of energy and the climate, promoting the emergence of a sustainable energy mix
- creating wealth and jobs by supporting French and European economic activity and the competitiveness of related industrial sectors
Strategic positioning

- **Sustainable Resources**
- **Eco-efficient Processes**
- **Eco-friendly Production**
- **Innovative Transport**
- **Renewable Energies**

**OIL AND GAS**

= 50% of R&I activities

**NEW ENERGY TECHNOLOGIES**

= 50% of R&I activities

**ENERGY TRANSITION**

- Providing environmentally-friendly technologies and pushing back the current boundaries of oil and gas reserves
- Producing environmentally-friendly fuels and chemical intermediates from fossil resources
- Producing energy while mitigating the environmental footprint
- Developing fuel-efficient, environmentally-friendly transport
- Producing fuels, chemical intermediates and energy from renewable sources
Geosciences Software Development

A suite for geosciences engineering

Complete modeling & simulation workflows

Facing reality

Modeling the past, planning the present

Modeling the present, predicting the future
Motivations

2005, back to the origin

- New parallel hardware architectures
  - Linux cluster, multi-core processors
- Needs for new physical models and advanced numerical methods
- A wide range of applications in geosciences: reservoir, basin, CO$_2$ but few common services
- Increasing cost to
  - maintain old scalar applications
  - parallelize these applications
  - implement advanced numerical methods
  - industrialize current R&D

Move or die : a new generation of simulators
An HPC framework for a new generation of simulators

As a key for competitiveness:
- Thru an hardware abstraction
- And low level optimizations

For an higher productivity in challenging environment:
- With an high level programming

Why and How

Reliability is not “the fifth wheel of the wagon”
- By defining a “standard” coding
- Given by a frame to the developer
- With an automated environment to enforce quality

Performance

Developer Friendliness

Rational Development

Robustness
What framework ?

A. Building a new one from scratch
   - A custom made framework …
   - … which may reinvent the square wheel
   - How to estimate its cost ?
   - What delay before the first commercial product ?

B. Using an existing framework
   - And following legacy choices
   - What continuity ? / what autonomy ?
     - As a customer or as a partner ?
What is Arcane?

An high level design to speed up development

- **Developer-friendly API**
  - Based on an Object Oriented language: C++
    - The highest performance OO language
    - But sometimes too tricky? (template, memory…)
  - With a C# binding for higher level programming
  - For any physical/numerical developer
    - To write code mostly as sequential procedures in service containers
    - With some wrappers for common usages
  - With common code services for computational sciences
    - I/O management (XML, HDF5)
    - Parallel management (data migration/synchronization/partitioning…)
  - With common concepts for mesh oriented simulations
    - 2D/3D unstructured distributed mesh, variables, groups, items
      (node, edge, face, cell, dof, particle, link…) …
What is Arcane?

An high level design for lower level optimizations

- **Hardware Abstraction and Performances**
  - Message passing parallelism behind unique interface with implementations (MPI, multi-thread, hybrid…)
  - Tested up to 60,000 cores on CEA super-calculator.
  - Integrates dynamic load balancing (for all Arcane distributed objects: mesh, groups, variables…)

- **Multi-platform support**
  - Linux (workstation and cluster) / Windows (workstation)

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**a multi-layer architecture for HPC simulators**
ArcGeoSim™?

IFPEN project for **Innovation** and **Rationalization** in software development for new geosciences simulators

Co-developed with **Arcane for Geosciences Simulation**

For a new generation from basin to reservoir simulators

Since 2007, 10+10 FTE human resources by IFPEN and CEA in an active collaboration
ArcGeoSim™

HPC framework for new generation of geosciences scientific softwares

Geosciences development platform for parallel applications

- Basin Modeling
  - TemisFlow & DionisosFlow
- Reservoir simulation & CO₂ management
  - PumaFlow
  - CooresFlow

External Links
- Linear Solvers, XML, HDF5
- Reservoir simulation & CO₂ management
- EOR CO₂ Numerical Lab initiative

HPC Simulator development parallel platform

- Advanced methods
  - Numerical schemes, AMR, (Non-)Linear Solvers
- Common utilities
  - Mesh, I/O, //
- Environment & Productivity
  - Documentation, Training, Daily Tests, Code Analysis...

Optimized library
- R & I
- Prospective R&D
- External Links, Unix Solves, XML, HDF5...

Generic / multi-purpose library
- CATS
- ArcTem
- CAMEL
- ArcDES
- Puma
- Coores
- Geoxim
- COTS
- ArcGeoSim™
The life of a framework

How to lead framework development

What’s first?

- Request from business applications
  - Usually requested for “yesterday”
- Low level concepts / optimizations
  - May be intrusive and requiring prototypes
- Architectural design
  - Ok for the integration of a new concept
  - But not seen as a functional enhancement
  - “When it works, why changing something?”
  - To see beyond the “functionalities”
    - Long time project
    - To be ready to unexpected evolutions!
Tools for a sustainable HPC framework

And IFPEN illustrations

- **Proactive analysis**
  - Be ready before the business requirements
  - “Innovation distinguishes between a leader and a follower”

- **Unify local cases into a larger framework**
  - Unified Linear Algebra Framework
  - Unified mesh format
  - Towards a new generation of distributed mesh in Arcane

- **Don’t let it wild**
  - ComTech, a multi-headed conscience
  - Continuous Integration (DailyTests, Jenkins, coverity*)
  - Internal parts *may* be tricky but external interfaces *must* be easy
  - Have an “Orthogonalization staff”
    - A new feature may come to be able to mix others
Tools for a sustainable HPC framework

And IFPEN illustrations

- Continuous (Non-) Linear solvers
  - Adaptive criteria, AMG, DDM, multi/many-cores
- Domain Specific Languages (in house & ∇-Nabla)
- Application Dataflow Analysis
- Automatic Differentiation / Code Generation (XSD/C#)
- Backend independent task based programming
- Numerical schemes

Mesh Free, Dimensional

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