Lmgc90 project

F. Dubois

Laboratoire de Mécanique et Génie Civil
Université de Montpellier 2 - CNRS

Cal@mi-team

F. Dubois ?

F. Dubois ?

- Engineer (1989)
- PhD (1994)
- UPC (~1992)
- CNRS research engineer (1994)

F. Dubois ?

- Engineer (1989)
- PhD (1994)
- UPC (~1992)
- CNRS research engineer (1994)

- Solid Mechanics
- Contact
- Numerical Analysis

F. Dubois ?

- Engineer (1989)
- PhD (1994)
- UPC (~1992)
- CNRS research engineer (1994)

- Solid Mechanics
- Contact
- Numerical Analysis

- Fortran formatted
- software architecture
- scientific computing
- high performance computing

Scope of lmgc90

- Centered on the simulation of divided media:
  - granular materials
  - masonry
  - fractured media
  - etc
- Provide a framework to model the behavior of a collection of interacting entities
- Multi-physics: thermal effects, fluids, etc

Beginning of lmgc90

- the «nightmare» has started in 2001

Goals:

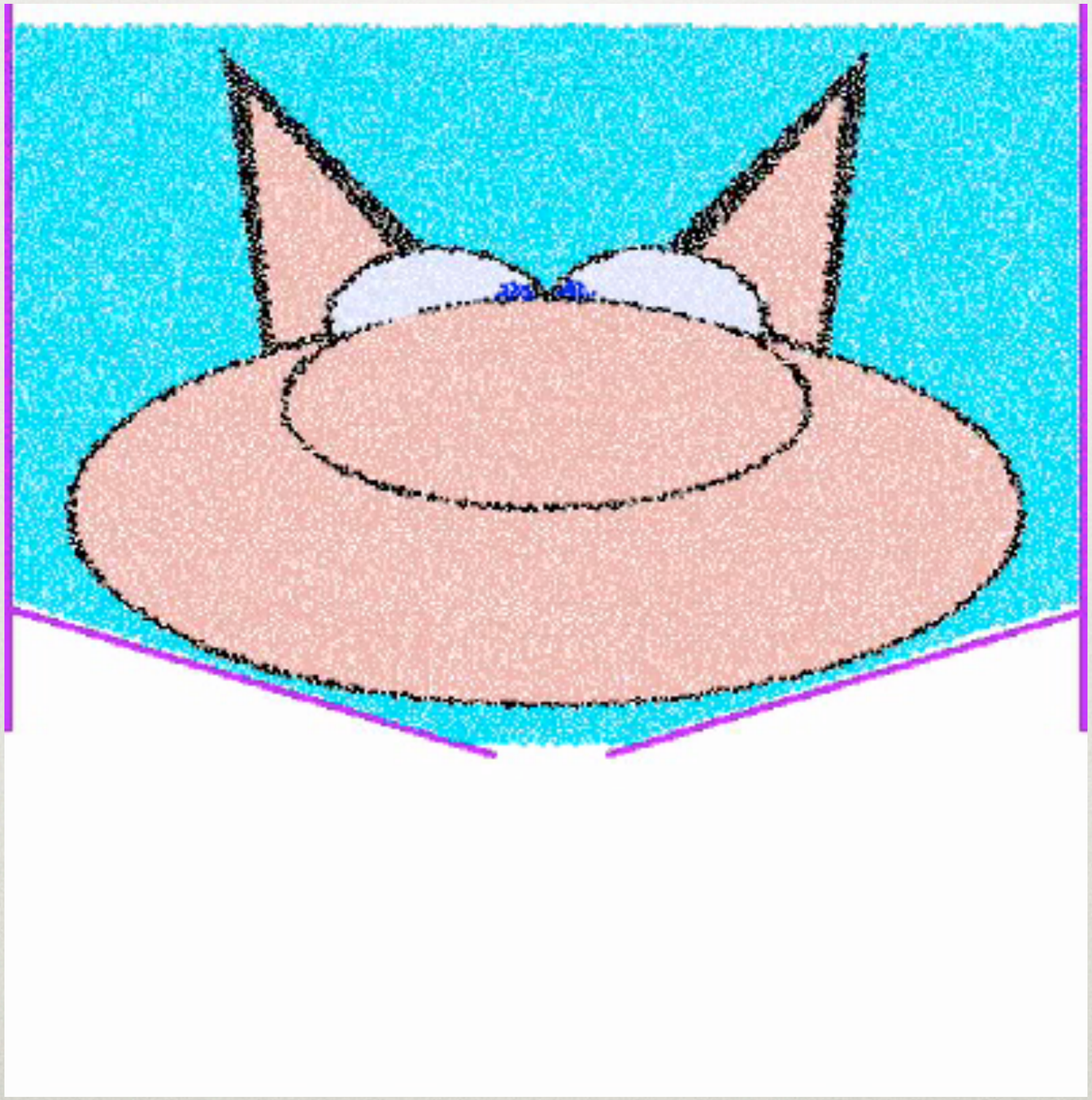
- development of an open platform for the modeling of divided materials through DEM
- make perennial some existing developments
- provide a framework to build new modeling strategies, etc
- build a community (users *and developers*)

Beginning of lmgc90

Scientific aspects

- modeling:
  - bulk model: 2D rigid, 2D deformable, 3D rigid
  - shapes: disk, polygon, sphere, polyhedron, etc
  - interaction: contact, friction, cohesion, etc
- numerical strategy:
  - smooth DEM (rigid models)
  - non smooth DEM (rigid and deformable models)
- technical tools
  - contact solver (NLGS, CGP, et)
  - shared memory / /
  - contact detection

Beginning of lmgc90

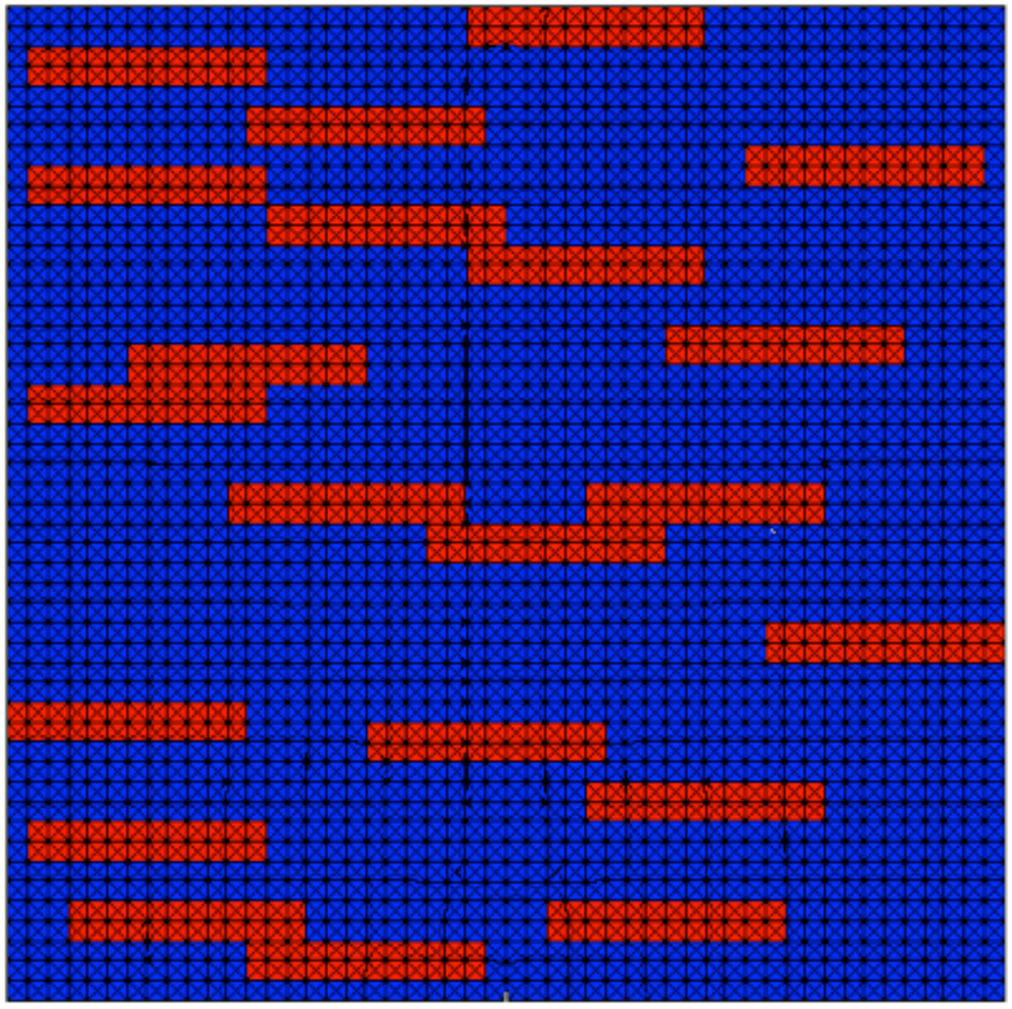


M. Renouf

Beginning of lmgc90

G. Saussine

Beginning of lmgc90



Beginning of lmgc90

Technical aspects

- fortran community

=> Fortran9x

- scientific computing

=> specifications are always changing

- potential developers are (future) scientists

=> limit side effects using modules + set()/get()

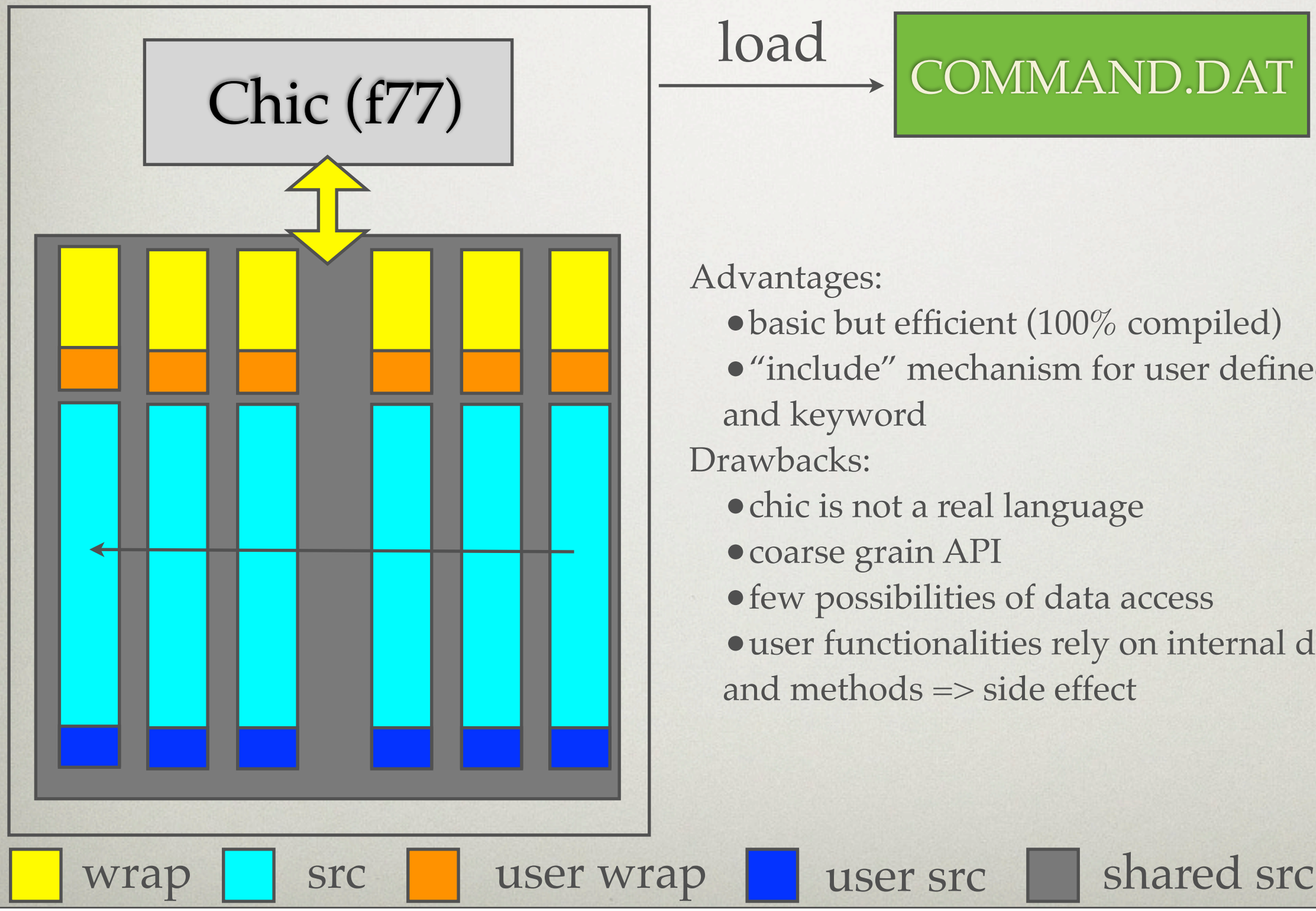
- end-user are scientists

=> keyword/script driven simulation instead of a monolithic «main»

- propose

Beginning of LMGC90

- LMGC90v1 : collection of modules+Chic



Advantages:

- basic but efficient (100% compiled)
- "include" mechanism for user defined functionalities and keyword

Drawbacks:

- chic is not a real language
- coarse grain API
- few possibilities of data access
- user functionalities rely on internal data structures and methods => side effect

Beginning of lmgc90

Technical aspects

- tools: cvs, mailing list, make, robodoc (for keyword documentation)
- needed libraries: lapack, matlib (material), Pelicans (FEM)
- visualization: gmv, gmsh

- developper version and user version

Beginning of lmgc90

Resources

- man power:
  - 2 stable developers F. Dubois & M. Jean
  - PhD students (lmgc, ema, lma, etc)

- funding:
  - SNCF: ballast modeling
  - IRSN: fracture of heterogeneous material
  - European project SICONOS: use lmgc90 has a modeling tool

Beginning of lmgc90

Assessment (developer)

- After few iterations the whole design choices seemed to be relevant (everything is handled in the same way),
- the adhoc design is difficult to understand which reduces the number of developers,
- the paranoiac design allows parallel developments, but leads to redundant code (+bug , -maintainability)
- the supervisor is not build on a language and is not suitable to handle data

Beginning of lmgc90

Assessment (user)

- functional code (2D/3D, etc)
- lack of documentation
- «smart» simulations need some development

Remarks:

- «Open source license + web site + mailing list + training course» necessary to create a «user community»,
- «code complexity» helps to protect the done work but inhibit the creation of a «developer community»

LMGC90 TODAY

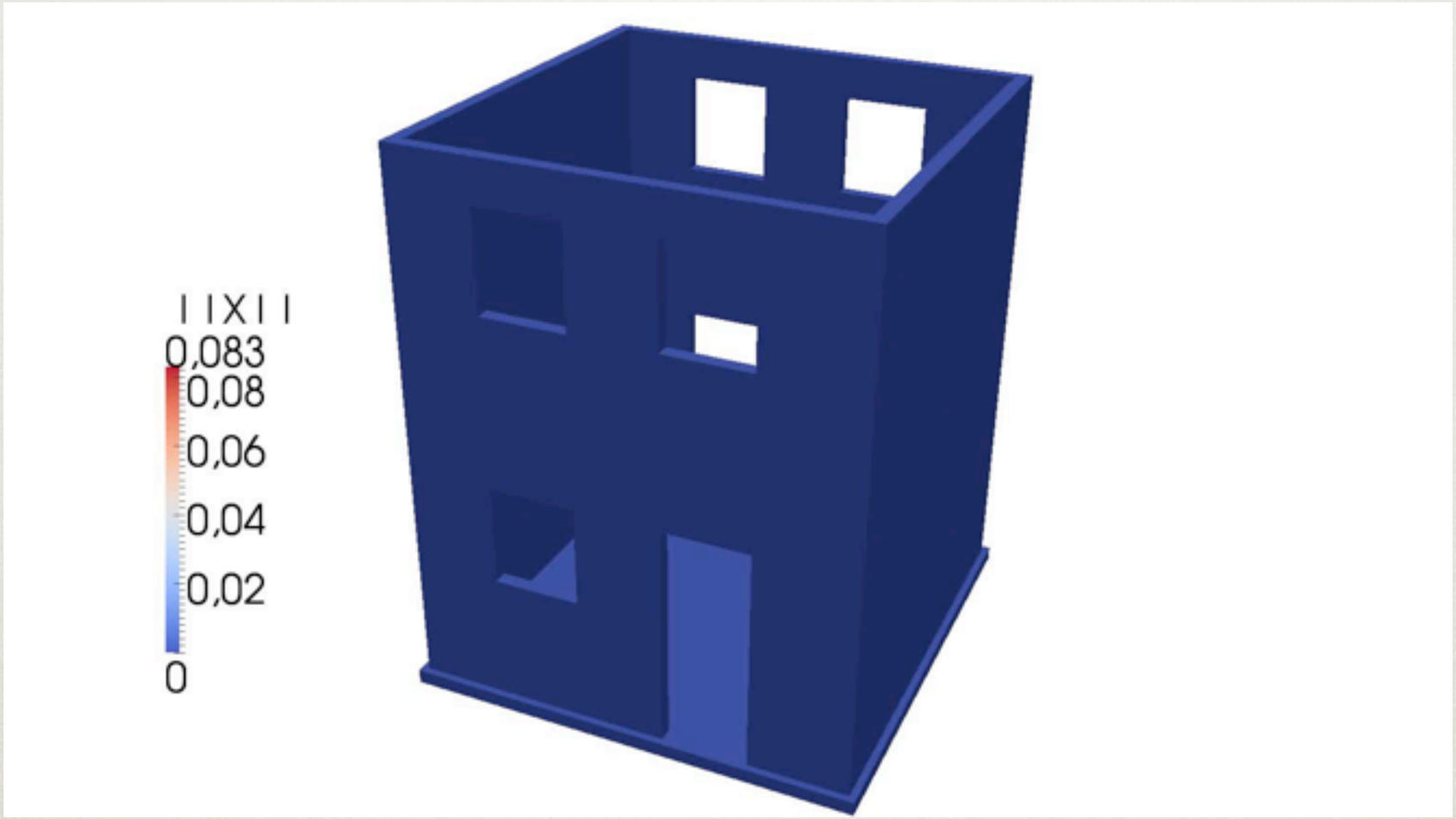
Scientific Aspects

- various improvements:
  - modeling: bulk models, shapes, interaction, multi-model representation + switch
  - numerical strategies
  - technical tools: DDM, contact detection, field projection, etc
- multi-physics
  - thermal effects, electrical
  - gaz-grains, fluid-grains coupling

LMGC90 TODAY

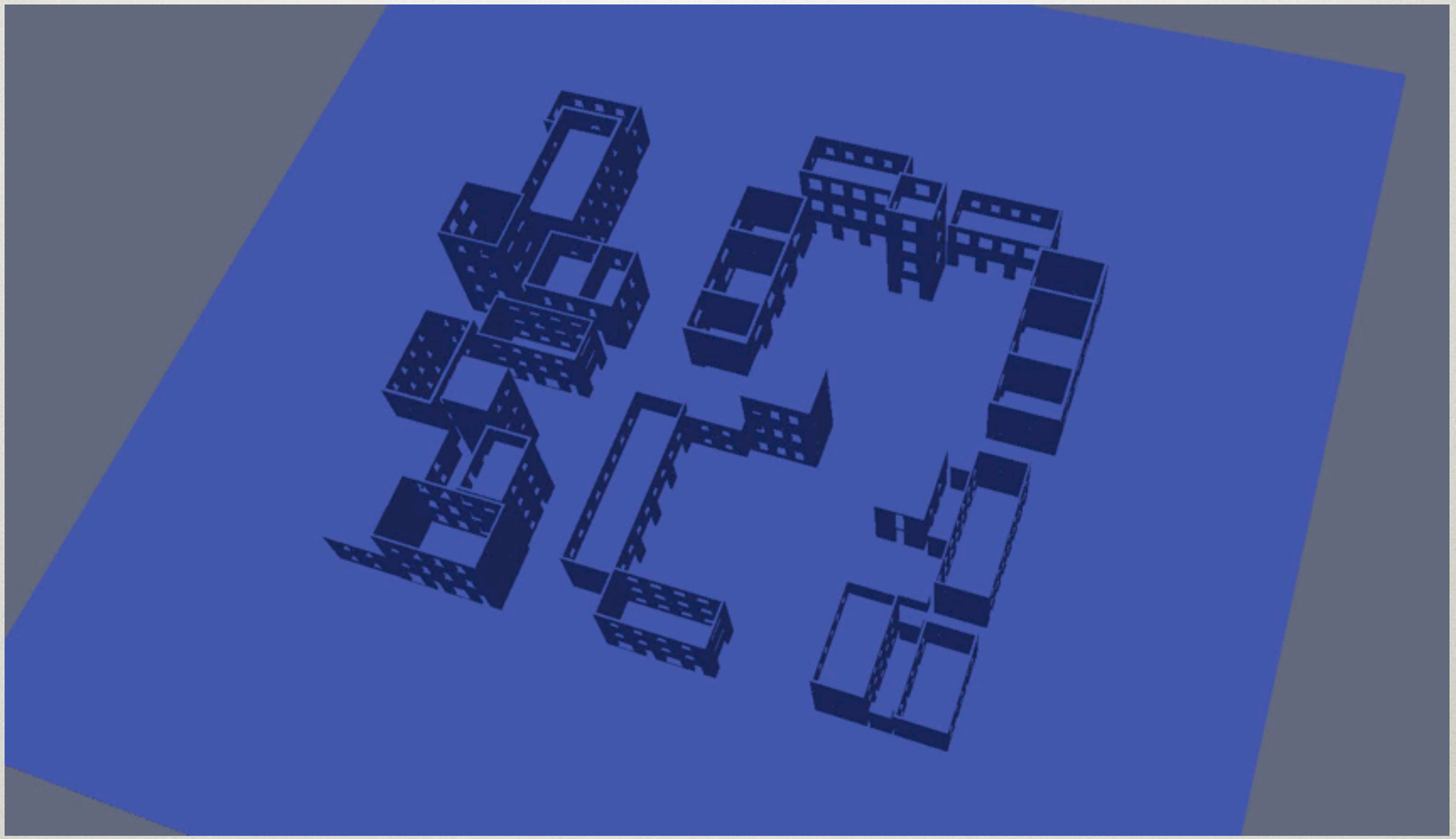
P. Taforel

LMGC90 TODAY



P. Taforel

LMGC90 TODAY

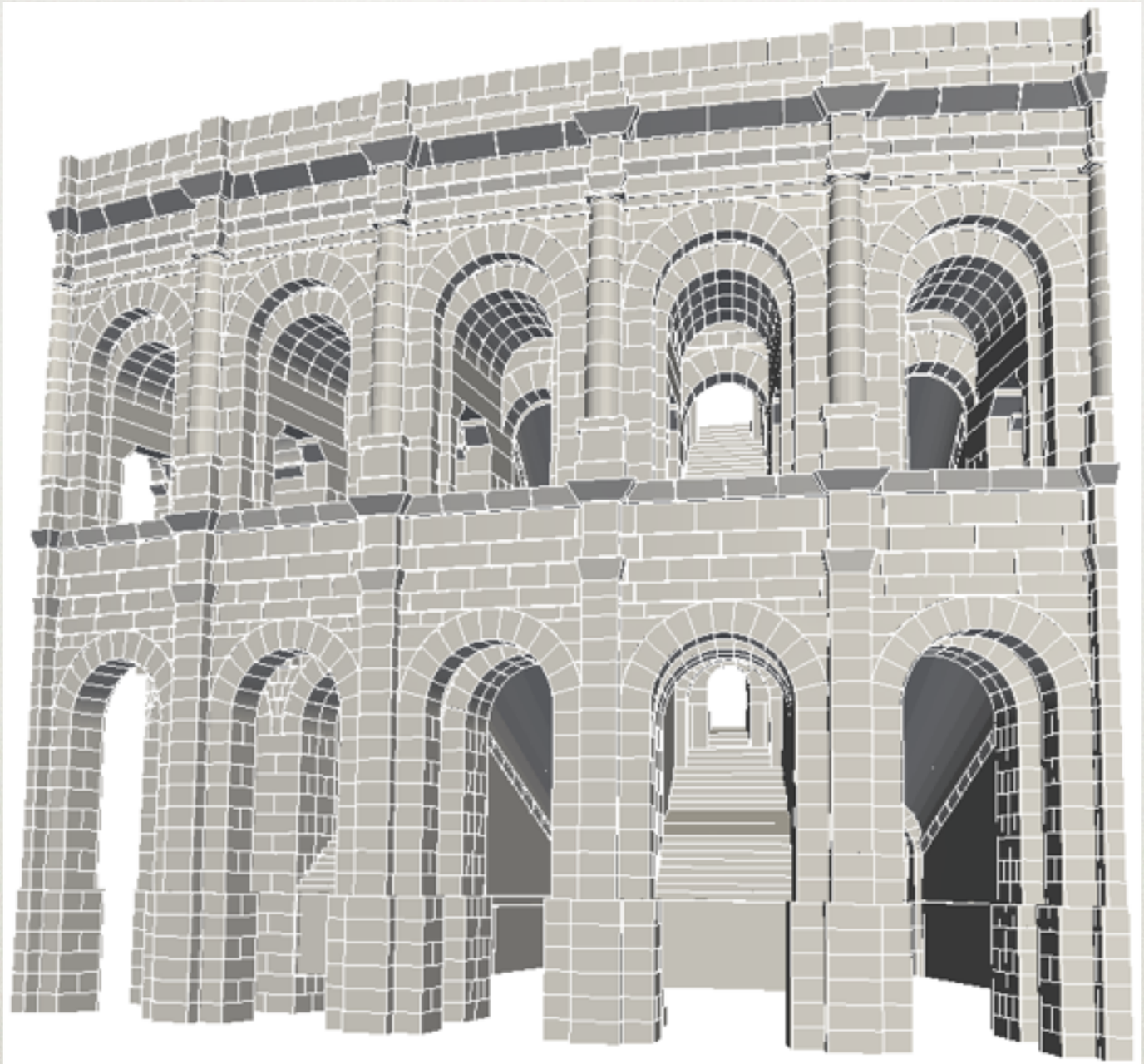


P. Taforel

LMGC90 TODAY

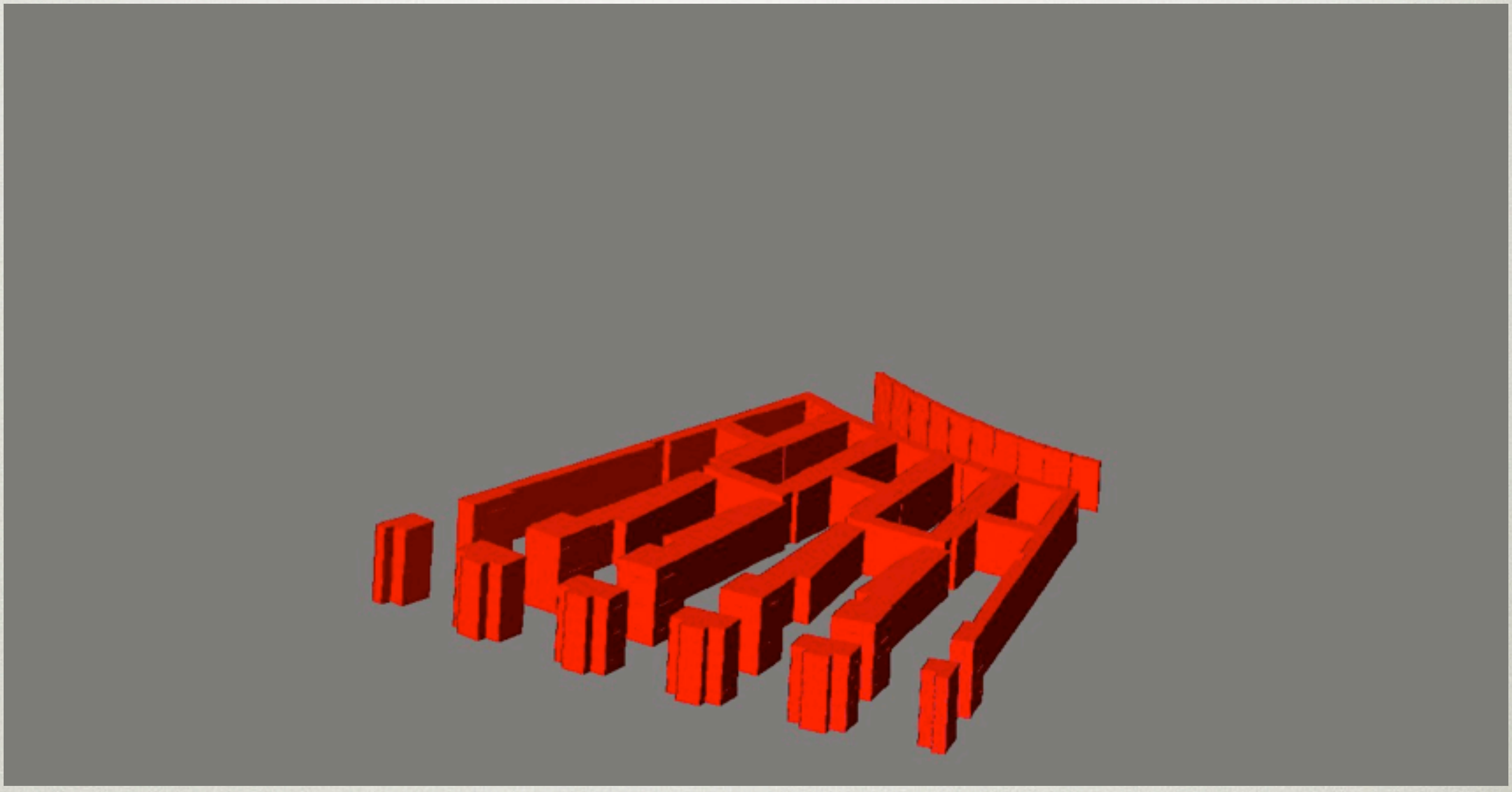
M. Bagneris

LMGC90 TODAY



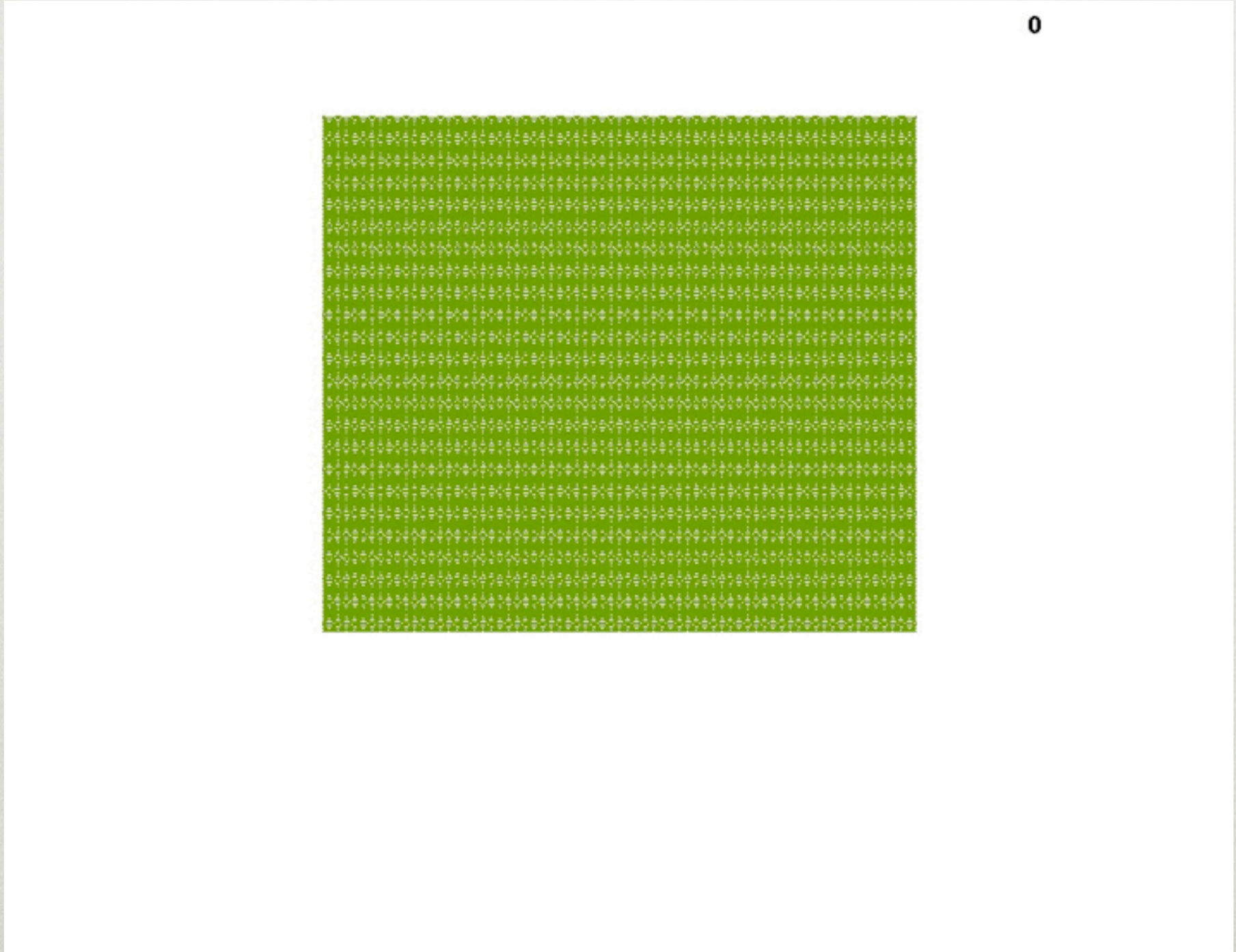
M. Bagneris

LMGC90 TODAY



M. Bagneris

LMGC90 TODAY



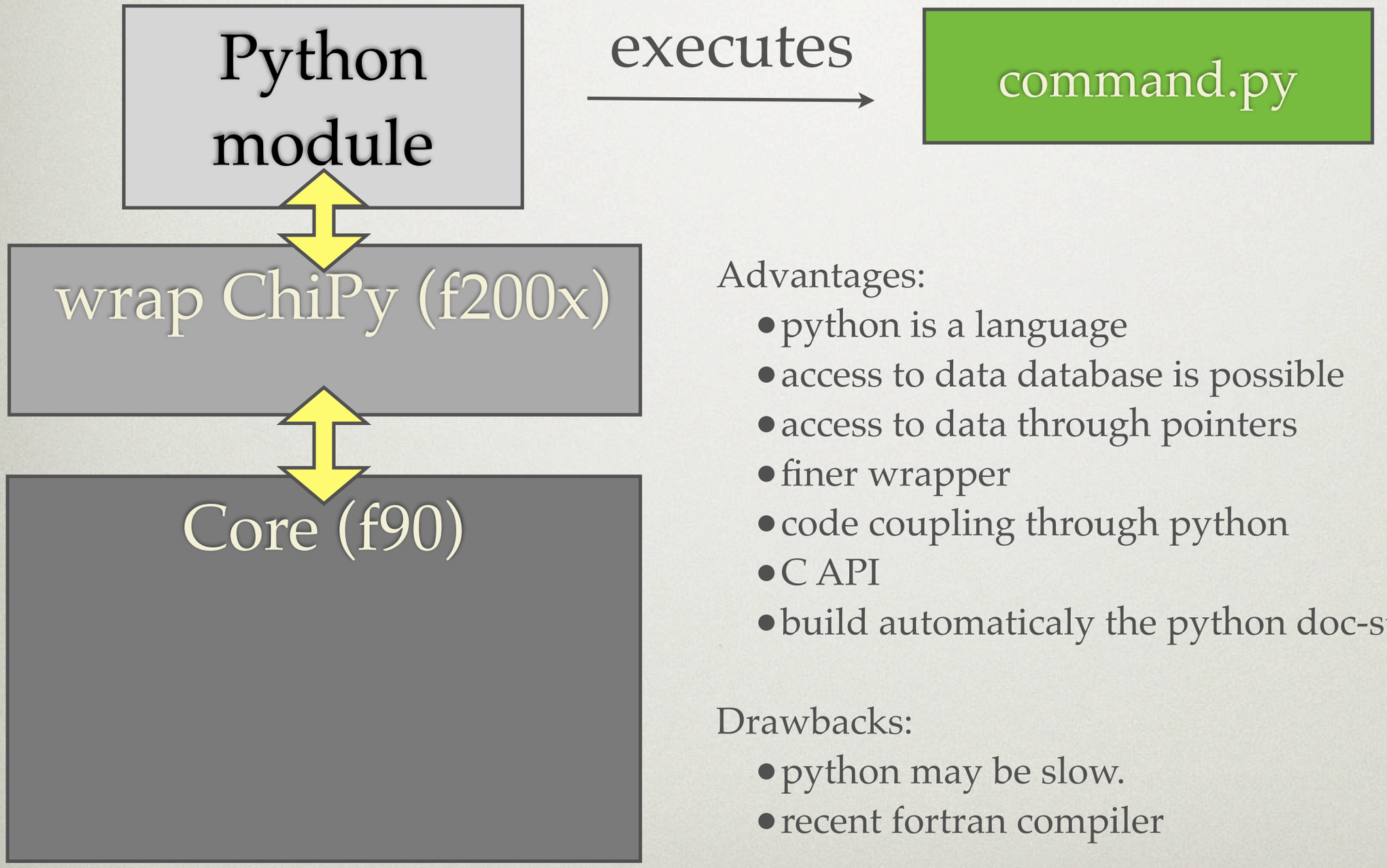
A. Martin

LMGC90 TODAY

V. Topin peligrif+lmgc90 DNS+DEM

LMGC90 TODAY

- python as supervisor (swig)



Advantages:

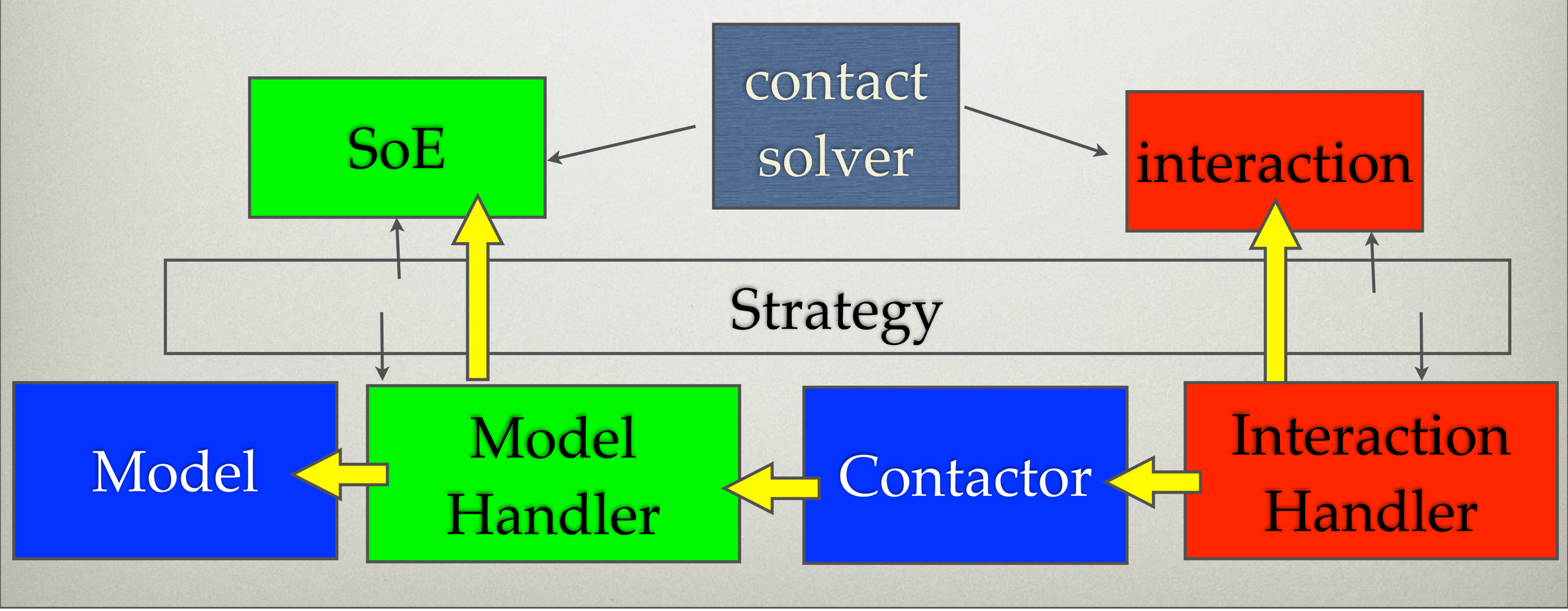
- python is a language
- access to data database is possible
- access to data through pointers
- finer wrapper
- code coupling through python
- C API
- build automaticaly the python doc-strings (doxygen)

Drawbacks:

- python may be slow.
- recent fortran compiler

LMGC90 TODAY

- Core:
  - Split modeling/simulation
  - Sets of modules are gathered into libraries



LMGC90 TODAY

Technical Aspects:

- preprocessor (python + compiled code) with support of various mesh/*cad* formats (through gmshpy)
- user wrapper and sandbox mechanism
- binding of external libraries (try to avoid direct call): linear algebra, material models, mechanical FEM, contact detection, etc
- user function to set fields, material parameters
- projection of fields
- etc

LMGC90 TODAY

Technical Aspects:

- automatic documentation: doxygen, pydoc
- subversion + trac
- cmake, ctest, cdash
- visualization: paraview (xml-vtk format)

LMGC90 TODAY

Lmgc90 as a library:

- siconos-lmgc90
- peligriff-lmgc90

Code couplings through python:

- lmgc90 - CodeAster
- lmgc90 - dg (:-)
- saladyn: python toolbox in Salome
  + lmgc90 + CodeAster + siconos +

LMGC90 TODAY

- Assessment (developer):
  - complexity increases but the python supervisor allow to do more things without programming
  - the scope of the code evolves
  - needs import maintenance effort (1 man/year)
  - review meeting are necessary to keep coherence

- Assessment (user):
  - deep improvement of functionalities
  - probably too tricky (:-(for end-user
  - organize each year a user meeting (2 days)
  - need of dedicated «for dummies» applications

LMGC90 TODAY

Resources:

- man power
  - 2.5 developers: F. Dubois, M. Renouf, M. Jean
  - PhD, postdoc
  - 3 limit term contracts: M. Bagneris, A. Martin, R. Mozul

- funding
  - ANR, Oseo-FEDER, Languedoc-Roussillon
  - EDF, ALCAN, Saint-Gobain Recherche, etc

A lot of time spend to manage projects, write reports, etc

LMGC90 TOMORROW

- Scientific aspects: so many things to do
  - multi-physics
  - multi-scale
- Technical aspects:
  - database management, post-processing, visualization
  - fields: up-scaling/down-scaling and strategy to switch between models
  - // computing
- Resources:
  - man power needed to maintain and updgrade the code has deeply increased (> 1 man/year)
  - new developments via sub-projects

LMGC90

- More informations
  http://www.lmgc.univ-montp2.fr/~dubois/LMGC90
  http://subver.lmgc.univ-montp2.fr/trac_LMGC90v2

- Next training course
  November 2011