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Cast3M, a problem-solving software for structural and fluid analysis

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May 31, 2024 version





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Outline

- 1 What is Cast3M?
- 2 Examples
- 3 Feature focus
- 4 Development model, openness
- 5 Future





What is Cast3M?

- Matlab(R) for the Finite Element Method (generalized rule of three);
- 40 years old;
- Integrated problem-solving environment:
 - User's programming language **Gibiane** and a developer's programming language Esope;
 - Inline full documentation (french and english);
 - Meshing, computation, post-treatment.
- Focus on non-linear implicit computational mechanics problems (vibration, plasticity, large deformation, contact-friction, fluids) from the nuclear industry;
- Some figures: ≈ 100 developers-users (5 at CEA currently), 1500 **test cases**, 9000 Google Scholar hits (Cast3M, Castem), 1.5M lines of code (Esope, half are comments), 170kloc (Gibiane), 170kloc (inline doc), 30Mo compressed (bzip2) executable.





Gibiane

- Interactive REPL (read-eval-print loop);
- Domain-Specific Language? Rather domain-specific objects: maillage (mesh), rigidite (matrix), modele (physical model), chpoint (fields on vertices), chamelem (fields on elements);
- Programming paradigm: **functional programming** (follow the maths) and referential transparency;
- Programming principles: **simplicity**, documentation, regularity, testing;
- Goals: correctness, quality.

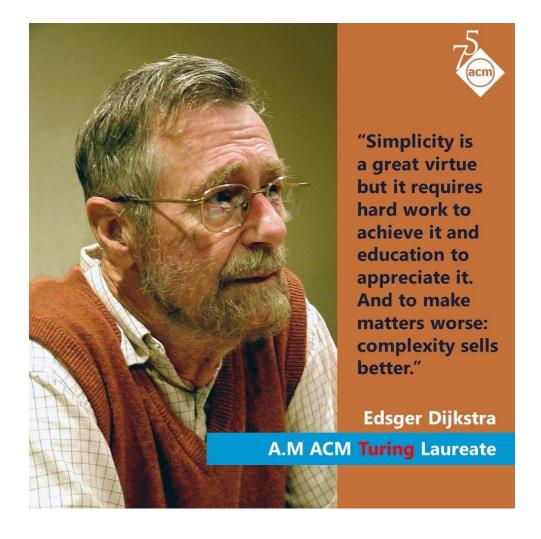
Almost no syntax:

- operators: objr = OPERATOR obj1 ... objn ;
- statements: STATEMENT obj1 ... objn ; (Warning: side-effects!).





Simplicity?

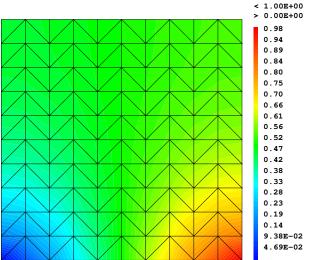






Simple example

```
* Hello world FEM-style
* General options
OPTI DIME 2 ELEM TRI3 DENS 0.1;
* Mesh
p0 = 0.0.; p1 = 1.0.;
                              POINT
bot = DROI p0 p1 ;
                              MESH
msh = TRAN bot (0. 1.);
                              MESH
* Problem
mod = MODE msh THERMIQUE ; MODEL
mat = MATE \mod K \ 3.14;
                       ELEMENTWISE FIELD
* Matrices
cnd = COND mod mat ;
                              MATRIX
mbl = BLOQ T bot ;
                              MATRIX
vbl = NOMC T (COOR 1 bot); NODAL FIELD
fbl = DEPI mbl vbl ;
                              NODAL FIELD
* Solve
mtot = cnd ET mbl ;
                              MATRIX
ftot = fbl :
                              NODAL FIELD
sol = RESO mtot ftot ;
                              NODAL FIELD
* Plot
TRAC sol msh;
```

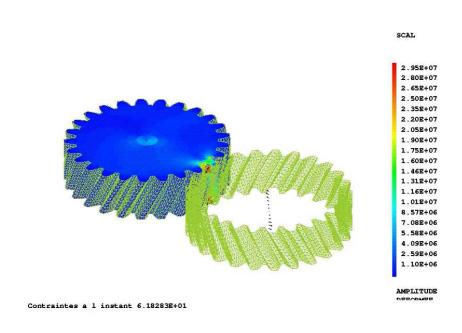


- Few objects (≈ 40);
- Many operators (≈ 500).

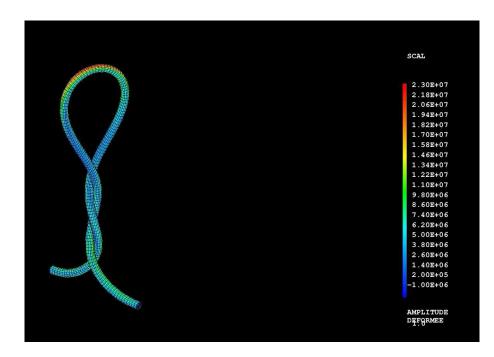




Contact-friction example (P. Verpeaux)



Gears mechanical simulation (local, web)

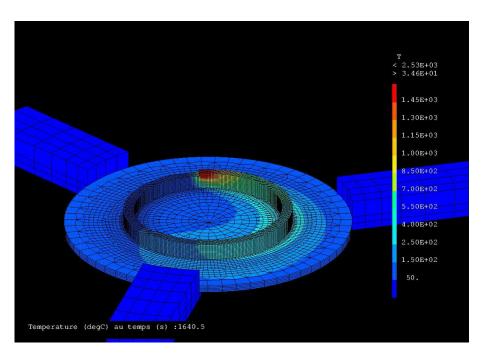


Torsion of an unstretched rope (local, web)

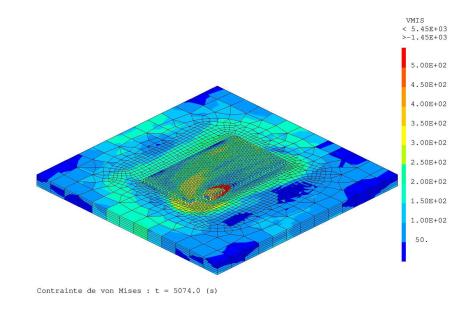




Additive Manufacturing (AM) example (S. Pascal)



Thermal simulation of an AM-ed pipe (video)



Mechanical simulation of an AM-ed 316L layer (Von Mises) (video)





SCAL

1.73E+03

1.70E+03

1.67E+03

1.57E+03

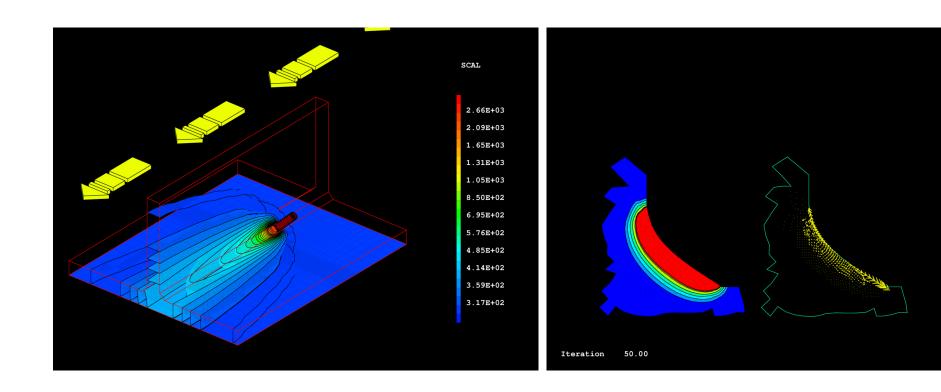
1.47E+03

1.37E+03

1.27E+03

UX UY UZ

Multiphysics Arc Welding simulation



Tee-like geometry Tungsten Inert Gas (TIG) Arc welding (local, web)





Lagrange multipliers everywhere

Generic **simple** method for prescribing linear(ized) constraints: Dirichlet boundary conditions, periodicity, mortar, contact, incompressibility.

- + **Functional programming**: just assemble terms in the matrix and the RHS $\begin{pmatrix} A & B^t \\ B & 0 \end{pmatrix} \begin{pmatrix} u \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$;
- + **physical meaning** of the Lagrange multipliers λ (reaction, flux, pressure, **conservation**);
- more unknowns;
- saddle-point structure (stability, indefiniteness, no optimal algebraic solver);
- hard work in the (linear) solver:
 - constraint elimination (static condensation);
 - double Lagrange multiplier method (factor without pivoting).





Saving and Loading

A simple way of saving your objects (your work!) at any time: OPTI SAUV filename; SAUV;

- portable binary or ASCII format;
- full or selective;
- incremental: just call SAUV; multiple times;
- release memory for saved objects: FANT statement.

Loading is symmetric: OPTI REST filename; REST;

- at a given checkpoint in an incremental save;
- should load any savefile from older versions of Cast3M (quality requirement for safety studies).





Development strategy

- 1. Monthly developer's meeting (was weekly at the beginning of the project):
 - discuss only the formal specification (documentation) of an operator, not the implementation: objr = NEW_OPERATOR obj1 ... objn ;
 - Do not document the code, code the documentation!
- 2. Program a test case for the new operator (user's language Gibiane);
- 3. Program the new operator (Gibiane and/or Esope);
- 4. Integrate it in nightly version of Cast3M (continuous integration).

Traceability of developments since 1988 (web).

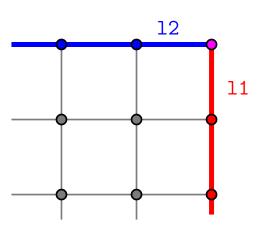




Error Handling

- Quality requirement: an unhandled error is a bug;
- An example of error handling in the RESO solver:

```
bloq1 = BLOQ T <u>l1</u>; bloq2 = BLOQ T <u>l2</u>;
fbl1 = DEPI bloq1 0.;
fbl2 = DEPI bloq2 0. or 1.; REDUNDANT or INCOMPATIBLE
sol = RESO (mat ET bloq1 ET bloq2) (fbl1 ET fbl2);
```



- Cast3M warns and continues in the first case and exits on error in the second case;
- Linear algebra libraries generally won't handle this case gracefully,
- Cast3M uses few external libraries (fxdr, X11, openGL, pthread, MPI, med) for quality reasons: license, longevity, portability, testing, non-regression and error handling. Numerical libraries are preferably included (BLAS, LAPACK, ARPACK).





Openness

- License: free for educational or research purposes, small fee for industry users;
- Windows, Linux and MacOS (arm) yearly version with bundled source code;
- Website: http://www-cast3m.cea.fr/
- Yearly user's meeting (last friday of November): free lunch for attendees and free polo for speakers!
- Free yearly **training sessions**: structural mechanics beginner and advanced (e-learning, english or at Université Paris-Saclay, french), additive manufacturing (classroom, french), developer (classroom, french). Training slides on the website;
- Integration of external developments done by CEA (ex: topological optimization, biomechanics of tumoral cells);
- Free Hotline.





Conclusion

Conclusion

- Ease of use of an integrated "white box" problem-solving language;
- Keep simplicity with useful generic tools: Lagrange multipliers, save-load feature, error handling;
- Document, test, code, integrate.

Future

- Battle the curse of complexity;
- Handle more complex applications;
- Have fun formalizing and solving problems!





The End

Questions?





Optimization

The real problem is that programmers have spent far too much time worrying about efficiency in the wrong places and at the wrong times; premature optimization is the root of all evil (or at least most of it) in programming.

Donald E. Knuth (1974)

Computer Programming as an Art:

ACM Turing Award Lecture



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The bad and the ugly?

- No nodes object: shared and hidden (but a configuration object exists);
- Operator syntax is in french;
- Lack of regularity on the developer's side (duplication of utilities and of an object);
- Operators are ordinary objects (character string) and can be overloaded, name scoping is global in procedures;
- Very ambitious parallelism model (multiple operators-multiple objects).





Automatic parallelism

Asynchronous shared-memory parallelism

```
• result = ASSI iassi OPERATOR obj1 ... objn ;;
```

Single instruction multiple data:

```
objp = PART mesh or modele ;
result = ASSI TOUS OPERATOR objp ...;
```

- Automatic user-level parallelism: OPTI PARA vrai ;;
- Internal parallelism for some operators (RESO) with pthreads;

Distributed-memory parallelism

- COLL ENVOYER i obj1 ... objn ; and obj1 ... objn = COLL RECEVOIR i ;
- Synchronous operator by default but asynchronous with ASSI;
- Quite similar to save-load functionality;
- Not automatic!



