

Open Source Software as a construction set for complex digital models of technical systems.

Matvey Kravoshin

Ivannikov ISP RAS Open Conference — 2019

6 December, 2019

- ① Introduction
- ② Finite volume analysis
- ③ Finite element analysis
- ④ Finite difference/AMR analysis
- ⑤ Lagrangian methods
- ⑥ High order analysis
- ⑦ Mixed methods libraries
- ⑧ Optimization software
- ⑨ Model reduction
- ⑩ Coupling software
- ⑪ Meshing software
- ⑫ Visualization
- ⑬ Integration platforms
- ⑭ Problem-oriented libraries
- ⑮ OpenFOAM forks
- ⑯ Demanded skills
- ⑰ Conclusions

AMY JONES

Sometown, CA 94172 | 555-555-5555 | aj@somedomain.com | LinkedIn URL

Software Engineer

Object-Oriented Analysis ■ Design and Development ■ Relational Database Systems

- **Innovative software engineer** offering experience in the full software development lifecycle – from concept through delivery of next-generation applications and customizable solutions.
- **Expert in advanced development methodologies**, tools and processes contributing to the design and rollout of software applications.
- **Known for excellent troubleshooting skills** – able to analyze code and engineer well-researched, cost-effective and responsive solutions.

Technical Tools

Java, JavaScript, .Net, XML, J2EE, HTML, TCP/IP, REST, SOAP, Akana, Visual Studio .Net, Eclipse, SQL, MS SQL Server, MySQL, JUnit, jQuery, C, C++, Apache Tomcat and Maven, Spring Framework, Hibernate, JDeveloper, WebLogic, IIS, Google Apps and more

Professional Experience

Software Engineer, 1/14 to Present – ABC COMPANY, Sometown, CA

Provide object-oriented software (OOS) design for one of the construction industry's leading project- management platforms. Develop and customize software for diverse client base. **Achievement Highlights:**

- Contributed software engineering expertise in the development of products through

The majority of today's industrial & scientific problems are:

- Multiscale
- Multiphysical
- Resource-consuming (computational, human, time)
- Not solved only experimentally or analytically
- Interdisciplinary

Proprietary software:

- High costs
- Slow development cycle
- A sink of expertise from customer to developer

Alternative: Open-Source software

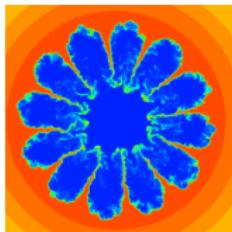
What does an Open-Source Software offer?

- OSS can be regarded as an construction set
- Usage of open source software from prosperous developers acts as a source of knowledge and experience
- Source code could be literally regarded as natural language
- Conservation (capitalization) of experience inside the team

- Which models are present now?
- How could they be used?
- Which demands are imposed on the competences of engineer?



- Unsorted list: <https://github.com/unicfdlab?tab=stars>
- Categorized list: <https://www.cfd-online.com/Wiki/Codes>

Open ∇ FOAM*The Open Source CFD Toolbox***SU2**

General-purpose FVM unstructured CFD code, GPL v.3

<https://github.com/OpenFOAM>

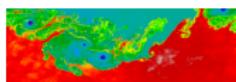
A generalized unstructured massively parallel low Mach flow code, Apache License v.2.0,
<https://github.com/NaluCFD/Nalu>

An Open-Source Suite for Multiphysics Simulation and Design, LGPL v.2.1
<https://github.com/su2code/SU2>

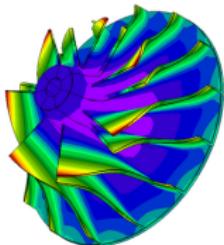
A fundamentally research platform for R & D in the field of high-fidelity (WENO) Computational Fluid Dynamics under GPL v.3.0
<https://github.com/ucns3d-team/UCNS3D>



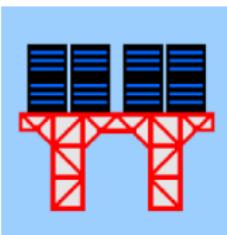
Free Software program for the solution of partial differential equations on adaptive Cartesian meshes, published under GNU GPL license
<http://basilisk.fr/>



The fast Finite Volume simulator with UQ support, published under GNU GPL v.3.0 license
<https://github.com/alsvinn/alsvinn>



CalculiX is a package designed to solve field problems using finite element method. It is published under GPL license.
<http://www.calculix.de/>



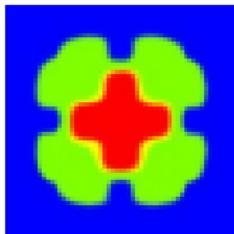
Parallel finite element unstructured meshes general purpose library, published under BSD-3-Clause
<https://github.com/SCOREC/core>



General Purpose Finite Element Embedded Language and Library in C++, published under LGPL
<https://github.com/feelpp/feelpp>



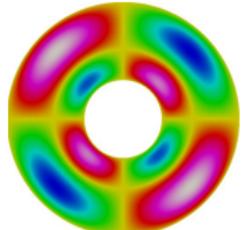
Fluidity is an open source, general purpose, multiphase computational fluid dynamics FEM code, published under LGPL v.2.1
<https://github.com/FluidityProject/fluidity>



A C++ software library supporting the creation of finite element codes and an open community of users and developers, published under LGPL v.2.1
<https://github.com/dealii/dealii>



A set of computational tools that enables research & numerical analysis in fluid dynamics employing asynchronous parallel programming, published under own license
<https://github.com/quinoacomputing/quinoa>

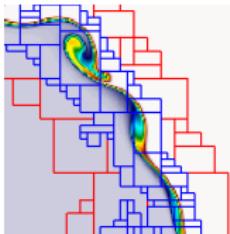
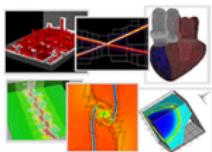


Elmer is the computational FEM tool for multi-physics problems developed by CSC in collaboration with Finnish universities, research laboratories and industry, licensed under GPL
<https://github.com/ElmerCSC/elmerfem>

General-purpose FEM code for mechanical, vibroacoustical and termal analysis of structure, released under GPL
https://github.com/ralic/Code_Aster

is an implicit, unstructured grid, finite element code for the solution and analysis of multiphysics problems, released under own OSS license
<https://github.com/SNLComputation/Albany>
Multiphysics Object-Oriented Simulation Environment — An open-source, parallel finite element framework, released under GNU LGPL
<https://github.com/idaholab/moose>

Finite difference/AMR analysis

**IBAMR****SAMRAI**

AMReX is a software framework containing all the functionality to write massively parallel, block-structured adaptive mesh refinement (AMR) applications
<https://github.com/AMReX-Codes/amrex>

is a distributed-memory parallel implementation of the immersed boundary (IB) method with support for Cartesian grid adaptive mesh refinement (AMR), published under it's own license
<https://github.com/IBAMR/IBAMR>

Structured Adaptive Mesh Refinement Application Infrastructure, published under GNU LGPL
<https://github.com/LLNL/SAMRAI>

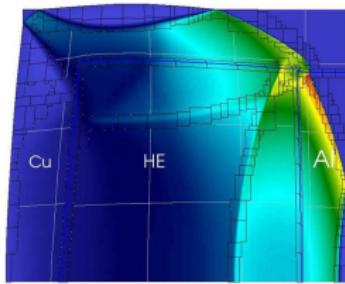
Code suites:

- AMReX-Astro
- AMReX-Combustion
- AMReX-FHD

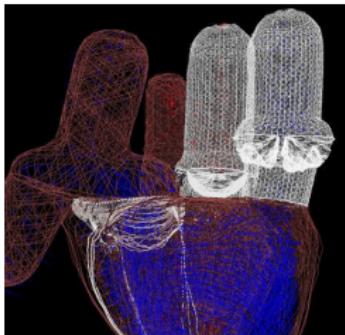
Individual codes:

- Castro
- IAMR
- MAESTROeX
- MFIX-Exa
- Nyx
- WarpX
- PeleLM
- PeleC

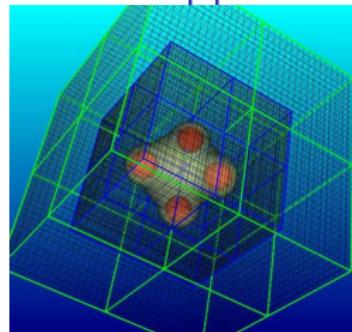
<https://amrex-codes.github.io/>



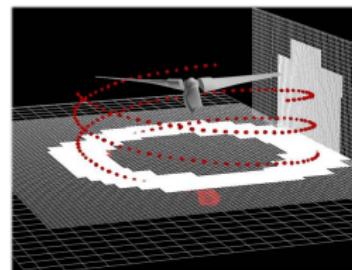
ALE-AMR multi-material detonation front calculation



Three-dimensional AMR simulation of cardiac fluid dynamics in the human heart



An electronic structure calculation of Be₄ cluster



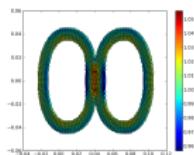
The use of AMR to resolve tip vortices of an isolated V-22 rotor



Open-source implementation of vortex method for computational hydrodynamics of viscous incompressible fluid, GNU GPL v.3.0
<https://github.com/vortexmethods/VM2D>

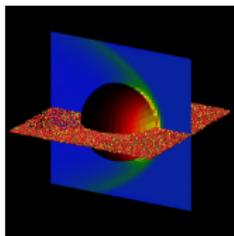
Discrete Element Method Particle Simulation Software. It can be used for the simulation of particulate materials, and aims to for applications it to industrial problems, GNU GPL v.2.0
<https://github.com/CFDEMproject/>

LIGGGHTS-PUBLIC
is Open Source software for particle-based numerical modelling, implementing the Discrete Element Method (DEM), for modelling processes involving large deformations, granular flow and/or fragmentation, Apache Licence
<https://launchpad.net/esys-particle>

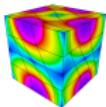
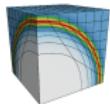


C++/CUDA/OpenMP based Smoothed Particle Hydrodynamics (SPH) Solver, released under GNU GPL,
<https://github.com/DualSPHysics/DualSPHysics>

PySPH is a framework for Smoothed Particle Hydrodynamics (SPH) simulations implemented in Python and the performance critical parts are implemented in Cython and PyOpenCL, released under own license
<https://github.com/pypr/pysph>

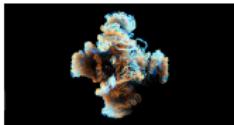
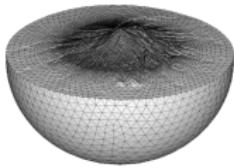


SPARTA stands for Stochastic PArallel Rarefied-gas Time-accurate Analyzer and is a Direct Simulation Monte Carlo (DSMC) code designed to run efficiently on parallel computers.
<https://github.com/sparta/sparta>



a fully-featured Monte Carlo particle transport code based on modern methods: constructive solid geometry, continuous-energy transport code and HDF5 format support, released MIT License
<https://github.com/openmc-dev/openmc>

LAGrangian High-Order Solver solves the transient Euler equations of compressible gas dynamics in a moving Lagrangian frame using unstructured high-order finite element spatial discretization, released under BSD-2 License
<https://github.com/CEED/Laghos>

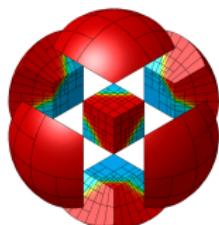


A scientific software for the numerical simulation of seismic wave phenomena and earthquake dynamics, released BSD 3-Clause "New" or "Revised" License
<https://github.com/SeisSol/SeisSol>

A generalized unstructured massively parallel low Mach flow code, Apache License v.2.0,
<https://github.com/NaluCFD/Nalu>

Flexi offers a powerful framework, which is tailored for high-fidelity (Discontinuous-Galerkin) time-dependent simulations in HPC environments, published under GPLv3.0
<https://github.com/flexi-framework/flexi>

INMOST



Mixed methods libraries, I
is a software platform for development of parallel numerical models on general meshes.
It is a supplementary tool for supercomputer numerical mathematical models characterized by a maximum generality of supported computational meshes, BSD 3-Clause License
<https://github.com/INMOST-DEV/INMOST>
is a free, lightweight, scalable C++ library for finite element methods, arbitrary high-order finite element meshes and spaces with conforming and nonconforming adaptive mesh refinement, published under GNU LGPL
<https://github.com/mfem-mfem>



general-purpose (but mainly for research and scientific studies) open-source computing platform for solving partial differential equations, published under GNU LGPL v.3.0
<https://fenicsproject.org/>

**ENigMA**

general-purpose multiphysics computational platform developed by Von Karman Institute. It is published under the LGPL v3.0. <https://github.com/andrealani/COOLFluiD> is an object-oriented C++ template library which aim is to provide multi-physics simulation in a multi-domain environment : FDM, FVM, FEM, SPH, BEM, etc. It is published under GPLv2. <https://github.com/bjaraujo/ENigMA>



Explore and predict with confidence.

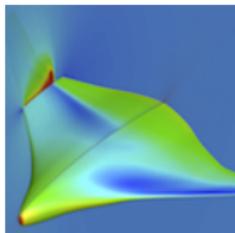


state-of-the-art research and robust, usable software for optimization and UQ. It is published under the LGPL.
<https://dakota.sandia.gov>

is an open-source high-performance computing platform for efficient optimization, focused on supporting gradient-based optimization with analytic derivatives. It is published under the Apache License, Version 2.0.
<https://openmdao.org/>

is a parametric aircraft geometry tool and allows the user to create a 3D model of an aircraft defined by common engineering parameters. It is published under the NASA Open Source Agreement.
<https://github.com/OpenVSP/OpenVSP>

Optimization software, II



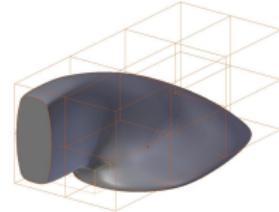
BlenderFOAM

DAFoam contains a suite of discrete adjoint solvers for OpenFOAM and supports design optimizations for a wide range of disciplines such as aerodynamics, heat transfer, structures, hydrodynamics, and radiation. It is published under GNU GPL v.3.0.
<https://github.com/mdolab/dafoam>

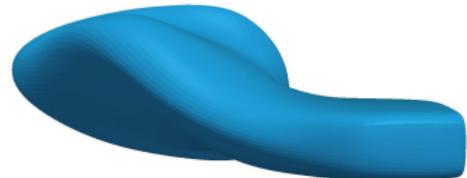
OpenAeroStruct is a lightweight tool that performs aerostructural optimization using OpenMDAO. It couples a vortex-lattice method (VLM) and a 6 degrees of freedom 3-dimensional spatial beam model. It is published under Apache License 2.0.
<https://github.com/mdolab/OpenAeroStruct>

Open-source Fluid Based Shape Optimization. It is published under GNU GPL v.3.0. <https://nathanrooy.github.io/posts/2019-03-05-blenderfoam-aerodynamic-shape-optimization/>

Simple optimization toolkit BlenderFOAM with geometry parametrization using Blender, OpenFOAM for simulation and Python for coupling. The toolkit is exemplified with the problem of the Formula Ford airbox shape optimization:



The optimization procedure produced the next shape of airbox (left – old, right – new):



libROM



is a library to compute proper orthogonal decomposition-based reduced order models (POD-based ROMs). It is published under Apache License 2.0.

<https://github.com/LLNL/libROM>

is an implementation in FEniCS of several reduced order modelling techniques (and, in particular, certified reduced basis method and Proper Orthogonal Decomposition-Galerkin methods) for parametrized problems. It is published under LGPL v.3.0.

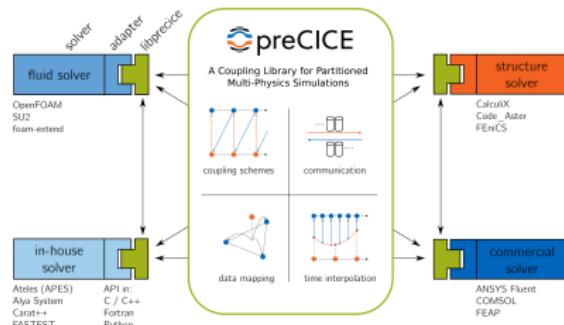
<https://github.com/mathLab/RBniCS>



In real Time Highly Advanced Computational Applications for Finite Volumes - ROMs for OpenFOAM. Versions for DGM and SEM are available. It is published under LGPL v.3.0.
<https://github.com/mathLab/ITHACA-FV>



precICE stands for Precise Code Interaction Coupling Environment. Its main component is a library that can be used by simulation programs to be coupled together in a partitioned way, enabling multi-physics simulations, such as fluid-structure interaction. It is published under LGPL v.3.0. <https://github.com/precice/precice>





Netgen/NGSolve

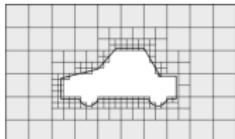


Ani3D provides portable libraries for each step in the numerical solution of systems of PDEs with variable tensorial coefficients: (1) unstructured adaptive mesh generation, (2) metric-based mesh adaptation, (3) finite element discretization and interpolation, (4) algebraic solvers. It is published under LGPL v.2.0.

<https://sourceforge.net/projects/ani3d/>

is a high performance multiphysics finite element software. It is published under LGPL v.2.1.
<https://github.com/NGSolve/netgen>

the open source system for processing and editing 3D triangular meshes. It is published under GNU GPL v3.0.
<https://github.com/cnr-isti-vclab/meshlab>



TetWild

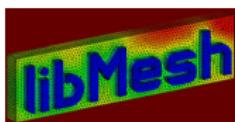


Meshing software, II

The `snappyHexMesh` utility is a part of OpenFOAM and generates 3-dimensional meshes containing hexahedra (hex) and split-hexahedra (split-hex) automatically from triangulated surface geometries, or tri-surfaces, in Stereolithography (STL) or Wavefront Object (OBJ) format. It is published under GNU GPL v3.0.
<https://www.openfoam.com/>

is a library for tetrahedral mesh generation. It is published under GNU GPL v3.0.
<https://github.com/Yixin-Hu/TetWild>

PyGeM is a python library using Free Form Deformation, Radial Basis Functions and Inverse Distance Weighting to parametrize and morph complex geometries. It is ideally suited for actual industrial problems, since it allows to handle 1) Computer Aided Design files (in .iges and .stl formats); 2) Mesh files (in .unv and OpenFOAM formats) 3) Output files (in .vtk format) 4) LS-Dyna Keyword files (.k



Meshing software, III

G+Smo (pronounced gismo or gizmo) is a C++ library for isogeometric analysis (IGA). Geometry plus simulation modules aims at the seamless integration of Computer-aided Design (CAD) and Finite Element Analysis (FEA). It is published under Mozilla Public License 2.0.
<https://github.com/gismo/gismo>

The library provides a framework for the numerical simulation of partial differential equations using arbitrary unstructured discretizations on serial and parallel platforms. A major goal of the library is to provide support for adaptive mesh refinement (AMR) computations in parallel. It is published under LGPL v2.1.
<https://github.com/libMesh/libmesh>

mimmo is a open source C++ library for mesh manipulation and morphing developed by Optimad Engineering Srl. It is published under LGPL v3.0.
<https://github.com/optimad/mimmo>



Gmsh is an open source 3D finite element mesh generator with a built-in CAD engine and post-processor. It is published under GNU GPL v2.0.
<http://gmsh.info/>

cfMesh is an open-source library for mesh generation using the OpenFOAM® framework. The library supports generation of meshes of arbitrary cell types. It is published under GNU GPL v3.0.
<https://cfmesh.com/cfmesh/>



ParaView is an open-source, multi-platform data analysis and visualization application. It is published under BSD 3-clause License.
<https://github.com/Kitware/ParaView>

VisIt is an open-source interactive parallel visualization and graphical analysis tool for viewing scientific data. It is published under BSD 3-clause License.
<https://github.com/visit-dav/visit>

3D scientific data visualization and plotting in Python. Mayavi strives to be a reusable tool that can be embedded in your applications in different ways. It is published under BSD License.
<https://github.com/enthought/mayavi>



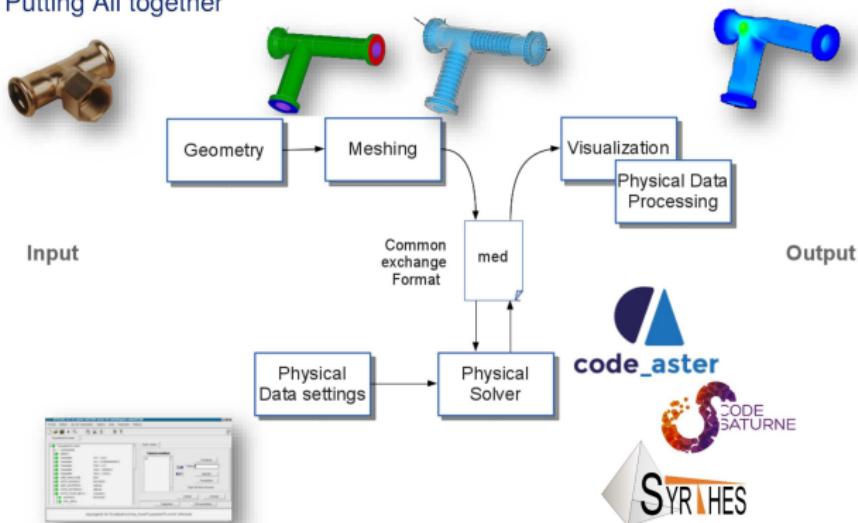
FreeCAD is a general-purpose parametric platform for 3D CAD/CAE based on Open Cascade Technology. It is published under LGPL v.2.
<https://github.com/FreeCAD/FreeCAD>

SALOME is an open-source software that provides a generic Pre- and Post-Processing and coupling platform for numerical simulation. It is based on an open and flexible architecture made of reusable components and is published under LGPL v.2.1
<https://www.salome-platform.org>

Blender is the free and open source 3D creation suite. It supports the entirety of the 3D pipeline—modeling, rigging, animation, simulation, rendering, compositing and motion tracking, even video editing and game creation and is published under GNU GPL.
<https://github.com/blender/blender>



Putting All together



QGDsolver

libAcoustics

OpenNOSE

rheoTool

SOWFA

ExaWind

AMR-Wind

Energyplus

MACH-Aero

AeroSandBox

CfdOF

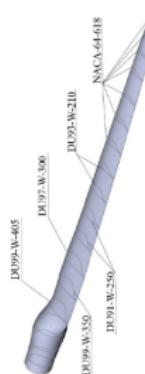
Problem-oriented libraries, I

- OpenFOAM implementation of regularized gas- and hydrodynamics equations <https://github.com/unicfdlab/QGDsolver>
- open-source (OpenFOAM) library for the far-field acoustics <https://github.com/unicfdlab/libAcoustics>
- an open-source (OpenFOAM) procedure for the simulation of nasal aerodynamics <https://home.aero.polimi.it/quadrio/it/Tesi/pesci/tesi-pesci.pdf>
- Toolbox to simulate GNF and viscoelastic fluid flows in OpenFOAM <https://github.com/fppimenta/rheoTool>
- Toolbox (OpenFOAM) for the windplant simulation <https://github.com/NREL/SOWFA>
- ECP library for precise simulation of windplants <https://www.exawind.org/>
- AMReX based library for wind-turbine simulations <https://github.com/Exawind/amr-wind>
- Open-source toolbox for simulation of house energy balance <https://github.com/NREL/EnergyPlus>
- The aerodynamic shape optimization library based on OpenMDAO, Python, OpenFOAM <https://github.com/mdolab/MACH-Aero>
- Aircraft design optimization, fully-coupled viscous/inviscid 3D aerodynamics, and reverse-mode automatic differentiation <https://github.com/peterdsharpe/AeroSandbox>
- Computational Fluid Dynamics (CFD) for FreeCAD based on OpenFOAM solver <https://github.com/jaheyns/CfdOF>

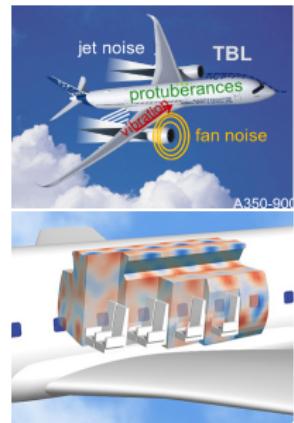
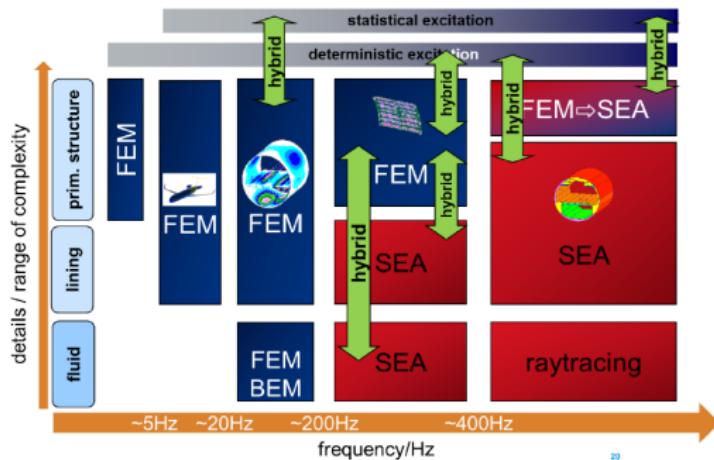
Problem-oriented libraries, II

SeisSol	a scientific software for the numerical simulation of seismic wave phenomena and earthquake dynamics https://github.com/SeisSol/SeisSol
MOM6	a next-generation open-source ocean model that combines the best of GOLD (http://code.google.com/p/gold-omod/) and MOM5 (https://mom-ocean.github.io/) https://github.com/NOAA-GFDL/MOM6
WRF	the Weather Research and Forecasting (WRF) model https://github.com/wrf-model/WRF
PyLith	a finite element code for the solution of dynamic and quasi-static tectonic deformation problems https://github.com/geodynamics/pylith
peridigm	an open-source computational peridynamics code developed at Sandia National Laboratories for massively-parallel multi-physics simulations https://github.com/peridigm/peridigm
OPM	The Open Porous Media (OPM) initiative encourages open innovation and reproducible research for modeling and simulation of porous media processes https://opm-project.org/
COOLFluiD	The object-oriented HPC platform for CFD, plasma and multi-physics simulations developed at the Von Karman Institute for Fluid Dynamics, https://github.com/andrealani/COOLFluiD
enrico	Exascale Nuclear Reactor Investigative COde with coupling to Nek5000 open-source code, https://github.com/enrico-dev/enrico

- Study of rocket lift-off processes: OpenFOAM+AMReX+...
- The integrated platform for fluid-structure interaction simulation and design variation: OpenFOAM+Code_Aster+SALOME
- *Full-scale simulation of vibrations and acoustics inside an aircraft*



«Full frequency vibro-acoustic simulation in the aeronautics industry» by A. Peiffer, Airbus Group Innovations, Vibroacoustics and Dynamics



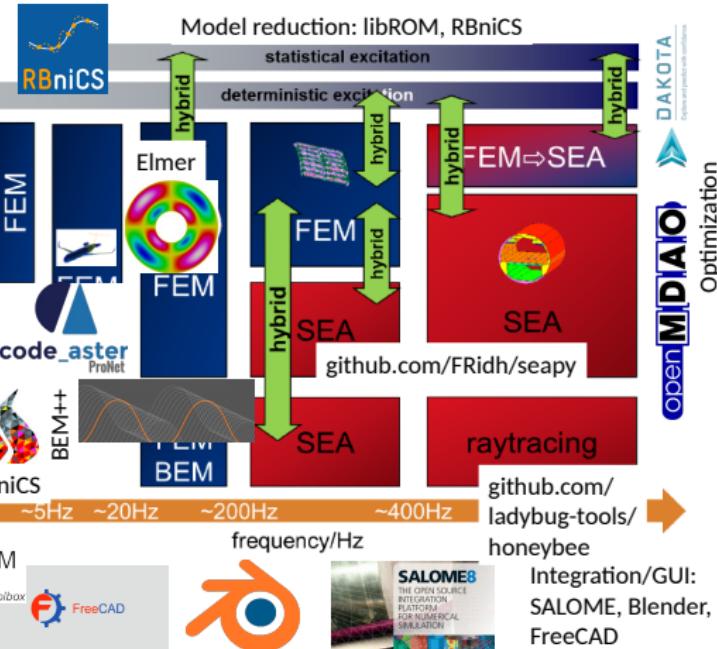
OSS solution to the problem



Data assimilation: DAPPER

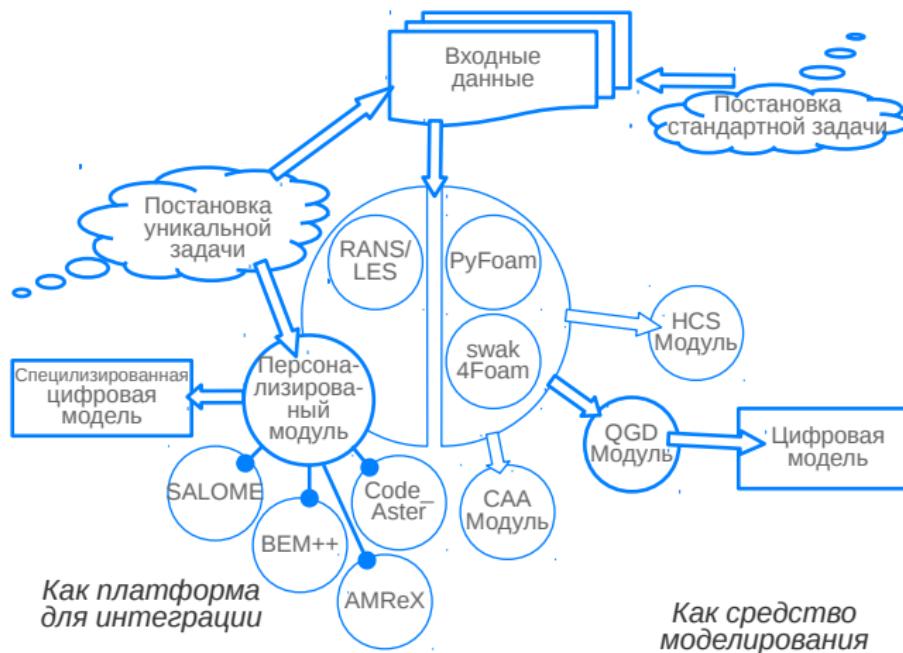
OpenFOAM
The Open Source CFD Toolbox

UCNS3D



- FEM: Code_Aster (including anisotropy of materials), Elmer (in spatial-frequency doamin), MFEM
- FEM/RKDG: MFEM, Nektar++
- Aerodynamic noise sources/CFD: OpenFOAM, AMReX
- BEM: BEM++
- Optimization: Dakota/openMDAO
- Integration/GUI: SALOME/Blender
- Model reduction: RBniCS, ITHACA
- Coupling: precICE

- blueCFD®-Core is an Windows® port of OpenFOAM®.
- RapidCFD is an OpenFOAM solvers ported to Nvidia CUDA.
- DigiTEF/OpenDTEF is an ISP RAS build of OpenFOAM



- Engineer must be well trained at the intersection of at least 3 knowledge areas:
 - Applied physics
 - Programming
 - Mathematics
- Validation and verification of algorithms & libraries
- Common libraries interfaces and methods for models coupling
- Libraries and area of their application
- High-performance computing theory and practice
- Stable application development
- Communication skills and team work

- Single-physics problems are more exception, than the rule
- Open-source software covers almost all aspects of modern engineering & science
- The idea of OSS as a construction set is used by many teams
- OSS creates new demands to engineers and developers
- Each year the coupling procedure between different libraries & codes requires less efforts and resources
- The shift of engineer's attitude to the problem solution: from "Which program" to "Which model"
- Changes in requirements to engineer's skills and education

As the conference is dedicated to open-source software, I encourage you to

- use as many OSS packages as possible and as much as possible;
- enhance existing OSS
- develop new OSS in novel areas of science & industry



Thank you for the attention!