

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

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#### Typical programmer's CV

#### **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, J2EF, HTML, TCP/IP, REST, SOAP, Akana, Visual Studio .Net, Eclipse, SQL, MS SQL Server, MySQL, JUnit, JQuery, C, 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



### Modern challenges

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



## Modern challenges of mathematical modelling

#### Requirements to modern models (challenges of 4 M-s):

- Multidisciplinary (Междисциплинарные)—The involvement of different physical phenomena of distinct nature in one model
- Multiscale (Многомасштабные)—The account for presence of time and space scales with several order of magnitude difference in value
- Scalable (Масштабируемые)—The ability to run on different computational platform and to achieve results in reasonable time
- Multidimensional (Многомерные)—3 dimensions in space, 1 dimension in time, plus n dimensions in physical properties or geometry



## What does an Open-Source Software offer?

- OSS can be regarded as an construction set
- Usage of open source sofrware 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



#### OSS as an construction set

- 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



#### Finite volume analysis, I

Open∇FOAM

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

The Open Source CFD Toolbox

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



#### Finite volume analysis, II



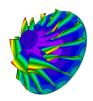


Free Software program for the solution of partial differential equations on adaptive Cartesian meshes, published under GNU GPL license http://basilisk.fr/

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



#### Finite element analysis, I



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



## Finite element analysis, II



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

## **ISP**RAS









#### Finite element analysis, III

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 under GPL of structure, released 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 Simulation Multiphysics Object-Oriented Environment — An open-source, parallel finite element framework, released under GNU LGPL https://github.com/idaholab/moose



#### Finite element analysis, IV



Sparselizard is is an efficient, multiphysics, hp-adaptive, open source C++ finite element library running on Linux, Mac and Windows, licensed under GNU GPLv2+ https://github.com/halbux/sparselizard



## Finite difference/AMR analysis



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

IBAMR

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

**SAMRAI** 



#### Code suites:

- AMReX-Astro astrophysical applications
- AMReX-Combustion simulation of combustion problems
- AMReX-FHD stochastic hybrid models

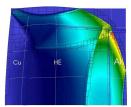
#### Individual codes:

- Castro adaptive mesh, astrophysical radiation/MHD/hydrodynamics
- IAMR variable-density incompressible Navier Stokes solver
- MAESTROeX low Mach number stellar hydrodynamics code
- MFIX-Exa multi-phase flow simulation tool for the exascale
- Nyx cosmological hydrodynamics simulation code
- WarpX exascale computing platform for beam-plasma simulations
- PeleLM simulation code for low Mach number reacting flows
- PeleC compressible hydrodynamics code for reacting flows

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



## ISP RAS

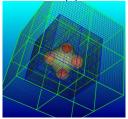


ALE-AMR multi-material detonation front calculation

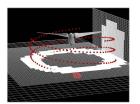


Three-dimensional AMR simulation of cardiac fluid dynamics in the human heart

#### SAMRAI Applications



An electronic structure calculation of Be4 cluster



simulation of The use of AMR to resolve tip vortices of e human heart an isolated V-22 rotor



## Lagrangian methods, I







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



#### Lagrangian methods, II



C++/CUDA/OpenMP based Smoothed Particle Hydrodynamics (SPH) Solver, released under GNU LGPL, 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



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









#### Lagrangian methods, III

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

free implementation of meshless methods C++ library for solving PDEs with an intuitive syntax. The library released under the MIT License http://e6.ijs.si/medusa/



## Lagrangian methods, IV



Yade is a discrete numerical models with focus on Discrete Element Method. https://yade-dem.org/



## High order analysis







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 GPLv.3.0 https://github.com/flexi-framework/flexi

## **ISPRAS**





#### Mixed methods libraries, I

is a software platform for development of parallel numerical models on general meshes. It is a supplimentary tool for supercomputer INMOST 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 highorder 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/



#### Mixed methods libraries, II



**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



### 1D analysis

System analysi
Open Source Multi-physics Simulation Engine projectchron finite elements, multi-body, collisions, vehicle simulations. It is published under the BSD-3 license.

https://projectchrono.org/

Open WAM

OpenWAM is a free, open source 1-dimensional gas-dynamic code. It is published under GPL. https://www.cmt.upv.es/OpenWam.aspx



OpenModelica is an environment based on the Modelica modeling language for modeling. simulating, optimizing and analyzing complex dynamic systems. It is published under GPL. https://openmodelica.org/



the integrated multidisciplinary simulation of multibody, multiphysics systems, including nonlinear mechanics of rigid and flexible bodies https://www.mbdyn.org/ It is published under GPL.



#### Uncertainty analysis



An Open source initiative for the Treatment of Uncertainties, Risks'N Statistics. It is published under LGPL. http://www.openturns.org/



### Optimization software, I



open M D A O

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





 ${\sf BlenderFOAM}$ 

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. GNU is published under **GPL** v.3.0. https: //nathanrooy.github.io/posts/2019-03-05/ blenderfoam-aerodynamic-shape-optimization/



#### OpenFOAM+Blender+Python

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):





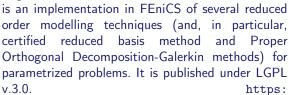


#### Model reduction

**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



//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





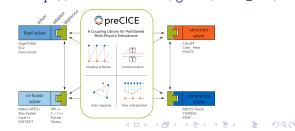




O-Palm

Coupling software

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 OpenPALM is a software allowing the concurrent execution and the intercommunication of programs based on in-house as well as commercial codes. It is published under GPL v.3.0. http://www.cerfacs.fr/globc/PALM\_WEB/





## Meshing software, I



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.



//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









### Meshing software, II

The snappyHexMesh utility is a part of OpenFOAM and generates 3-dimensional meshes containing hexahedra (hex) and splithexahedra (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 tetrahderal 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) dLS-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



## Meshing software, IV



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 $\circledR$  framework. The library supports generation of meshes of arbitrary cell types. It is published under GNU GPL v3.0. https://cfmesh.com/cfmesh/



Discretization tools for finite volume and inverse problems. Published under MIT License. https://github.com/simpeg/discretize



### Meshing software, V



A generic programming header only C++ library for processing polygonal and polyhedral meshes. It is published under MIT License. https://github.com/mlivesu/cinolib



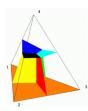
open source software for bidimensional and tridimensional surface and volume remeshing It is published under GNU LGPL. https://github.com/MmgTools

	Mesh	adaptation		library
MAdLib	Published	under	LGPL	License.
	https://sites.uclouvain.be/madlib/			
MeshAdapt	General hr-version tetrahedral mesh adaptation.			

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## Meshing software, VI



A Quality Tetrahedral Mesh Generator and a 3D Delaunay Triangulator. It is publishedGNU Affero General Public License. http://wias-berlin.de/software/tetgen/

# CGAL

is a software project that provides easy access to efficient and reliable geometric algorithms in the form of a C++ library It is published under dual GNU GPL/LGPL. http://www.cgal.org/

#### VoroCrust

is the first provably correct algorithm for conforming Voronoi meshing of nonconvex and non-manifold domains Published under VoroCrust 1.0 non-exclusive license. https://vorocrust.sandia.gov/



#### Visualization







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 Vislt 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



### **GUI & Integration**







FreeCAD is an 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 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



### SALOME Integration platform



**ISP RAS QGDsolver libAcoustics** 

## Problem-oriented libraries, I

OpenFOAM implementation of regularized gas- and hydrodynamuics 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

OpenNOSE nasal aerodynamics https://home.aero.polimi.it/quadrio/it/ Tesi/pesci/tesi-pesci.pdf

Toolbox to simulate GNF and viscoelastic fluid flows in OpenFOAM

rheoTool https://github.com/fppimenta/rheoTool

Toolbox (OpenFOAM) for the windplant simulation https://github. **SOWFA** com/NREL/SOWFA

ECP library for precise simulation of windplants https://www.

**ExaWind** exawind.org/

AMReX based library for wind-turbine simulations https://github. AMR-Wind

com/Exawind/amr-wind

Open-source toolbox for simulation of house energy balance https: Energyplus

//github.com/NREL/EnergyPlus

The aerodynamic shape optimization library based on OpenMDAO, MACH-Aero

Python, OpenFOAM https://github.com/mdolab/MACH-Aero

Aircraft design optimization, fully-coupled viscous/inviscid 3D AeroSandBox aerodynamics, and reverse-mode automatic differentiation https:

//github.com/peterdsharpe/AeroSandbox

Computational Fluid Dynamics (CFD) for FreeCAD based on **CfdOF** 

OpenFOAM solver https://github.com/jaheyns/CfdOF

# ISP RAS

MOM6

peridigm

**OPM** 

### Problem-oriented libraries, II

a scientific software for the numerical simulation of seismic SeisSol wave phenomena and earthquake dynamics https://github.com/SeisSol/SeisSol

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

a finite element code for the solution of dynamic and quasi-static PyLith tectonic deformation problems https://github.com/geodynamics/

pylith

an open-source computational peridynamics code developed at Sandia National Laboratories for massively-parallel multi-physics simulations

https://github.com/peridigm/peridigm

The Open Porous Media (OPM) initiative encourages open innovation and reproducible research for modeling and simulation of porous media

processes https://opm-project.org/

The object-oriented HPC platform for CFD, plasma and multi-physics COOLFluiD 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



### Problem-oriented libraries, III

An open-source implementation of Quadrature-Based Moment **OpenQBMM** 

Methods https://www.openqbmm.org/

OpenFOAM library for the simulation of multispecies evolving aerosols AeroSolved

https://github.com/pmpsa-cfd/aerosolved

ODS Studio allows rapid design and analysis of commercial and

ODS residential building design (OpenFOAM+Blender+Radiance) https:

//www.ods-engineering.com/tools/ods-studio/

DLR parametric aircraft geometry modeller https://dlr-sc.github. TiGI

io/tigl/

The library for numerical simulation of viscous compressible hybridCentralSolvers flows, developed by ISP RAS Unicfd group https://github.com/

unicfdlab/hybridCentralSolvers

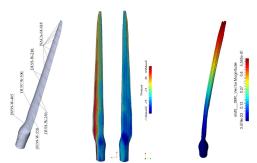


### Application to real problems

- 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



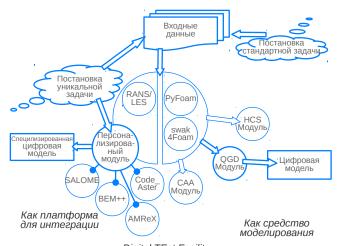






### OpenFOAM forks

- 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







- Research Gate
- Zenodo (DOI for sources, articles, data)
- GitHub
- OpenTeams



- 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 sofrware 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!