Introduction to the 4C Multiphysics Framework @UKACM & GACM Autumn School 2025

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Reminder

- Please **download** the **virtual box**, if not yet already done.
- Detailed instructions available in the course material at link to PREPARATION .

Introduction to the 4C Multiphysics Framework

- **What is 4C Multiphysics?**
- Capabilities of 4C Multiphysics
- How to build 4C Multiphysics
- The input file
- Tips and tricks to create a 4C input file

What is 4C Multiphysics?

- Modular, parallel, and open-source simulation environment
- Solves single- and multiphysics real-world problems
  - Described by differential equations (meso and macro scale)
  - Focus on finite element and particle methods
  - Applied in engineering, science, and biomedicine
  - Ready to use applications/solvers
- Extensible framework for methods development and new applications (C++)
  - Single fields
  - Coupling algorithms (surface-to-surface, volume-to-volume, (non-)matching grids)
  - Linear Algebra/Solvers/Preconditioners

What is 4C Multiphysics?

- Not yet heard of 4C Multiphysics?
  - Open source since 10/2024 under LGPL-v3.0-or-later
    https://github.com/4C-multiphysics/4C
  - Roots date back >20 years, > 50 PhD theses, > 400 papers
- Ca. active 35 developers
- Quarterly release, latest v2025.3.0

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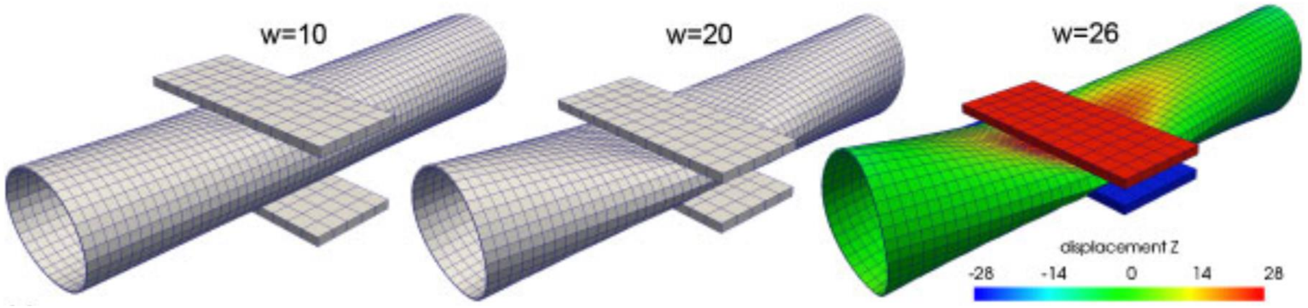
Solid mechanics

- 3D solids (EAS, Fbar), 2D (plane strain, plane stress), shells, beams
- Small / finite deformations
- Explicit / implicit time integration
- Various material models
    - (Hyper-)elasticity
    - Viscosity
    - Plasticity
    - Fiber reinforced materials
- Contact formulations:
    - Penalty, Lagrange Multipliers, Nitsche
    - node-to-segment, segment-to-segment (mortar)
- Example 1: Large-scale dynamic contact analysis of thin-walled pipe (continuum shell)
- Example 2: Dynamic failure of steel ropes modelled on the scale of individual wires based on Cosserat continua employing a beam formulation



A. Popp, M. Gitterle, M. W. Gee, W. A. Wall (2010). A dual mortar approach for 3D finite deformation contact with consistent linearization. *Int. J. Num. Meth. Engng. 83(11)*

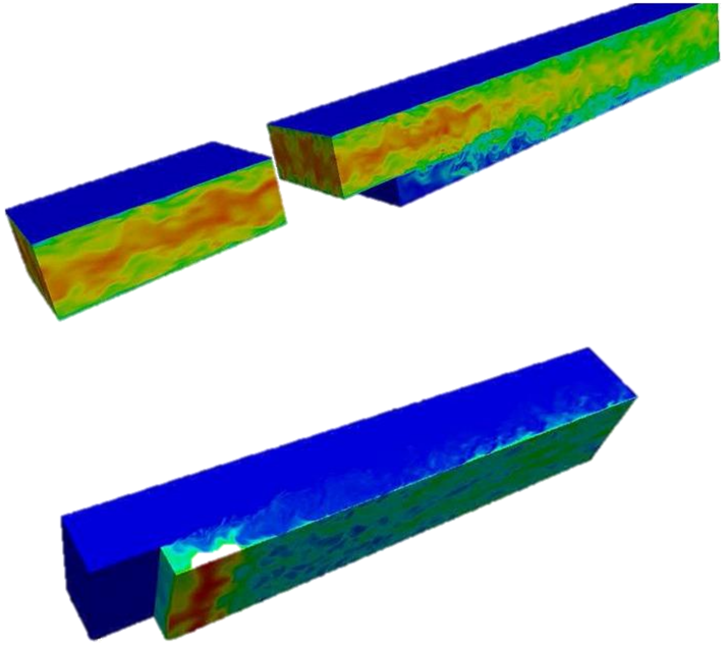
C. Meier, W. A. Wall, A. Popp (2017). A unified approach for beam-to-beam contact. *Comput. Methods Appl. Mech. Engrg., 315*

Fluid mechanics / Turbulence / Heat

- 2D / 3D fluid flow solver based on finite elements
  - Incompressible Navier-Stokes equations
  - Weakly compressible variable-density low-Mach number flows
  - with Eulerian or Arbitrary Langrangian-Eulerian (ALE) observer (mesh motion)
  - Monolithic solution approach

- Turbulence modeling via Large-eddy simulation (LES) with different turbulence models
  - Dynamic Smagorinsky
  - Dynamic Vreman
  - Multifractal Subgrid Scales

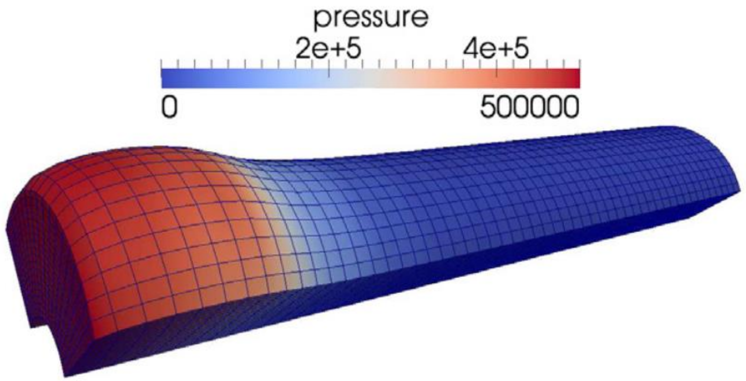
- Example: LES fluid flow through channel heated from the bottom



U. Rasthofer, G. C. Burton, W. A. Wall, V. Gravemeier (2010). An algebraic variational multiscale-multigrid-multifractal method (AVM4) for large-eddy simulation of turbulent variable–density flow at low Mach number. *Num. Methods in Fluids, 76*

Porous media

- Darcy & Darcy-Brinkmann flows
- Finite deformation formulation
- Monolithic solution approach
- Multiphase variant with several fluid phases



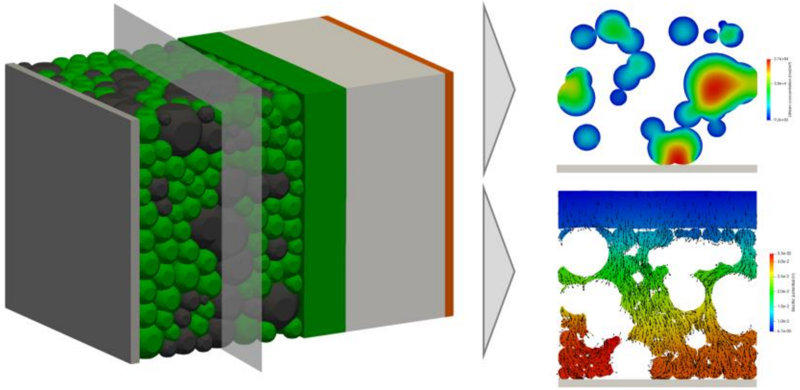
- Example:
  - Darcy–Brinkman flow through a quarter of a hollow cylinder
  - Pressure wave travels through the porous media

A.-T. Vuong, C. Ager, W.A. Wall (2016). Two finite element approaches for Darcy and Darcy–Brinkman flow through deformable porous media—Mixed method vs. NURBS based (isogeometric) continuity. *Comput. Methods Appl. Mech. Engrg. 305*

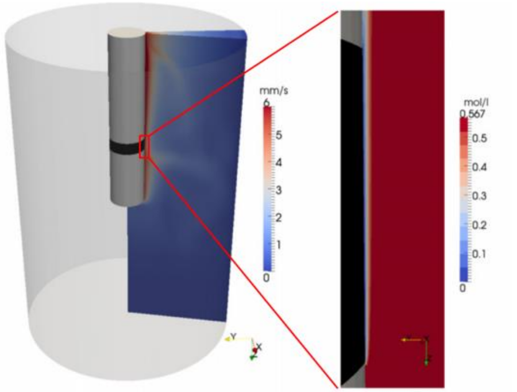
Electrochemistry

- Analysis of solid state batteries
- Interaction of solid mechanics, electrochemistry, and optionally temperature effects
- Inelastic expansion due to charge/temperature changes
- Contact mechanics at electrode-electrolyte interface (delamination phenomena)
- Concentration fields governed by convection-diffusion equation

- Example 1:
  - solid-state battery, structured from left to right with a current collector, a composite cathode, a solid electrolyte separator, a lithium metal anode, and another current collector.
  - Visualization of the lithium concentration distribution in the active material and the electric potential, including local flux visualization, within the composite cathode of a solid-state battery.
- Example 2:
  - Rotating cylinder electrode: interplay of natural convection with forced convection in the electrolyte due to the rotating cylindrical Copper cathode. (left: velocity field, right: Copper concentration boundary layer close to the cathode)



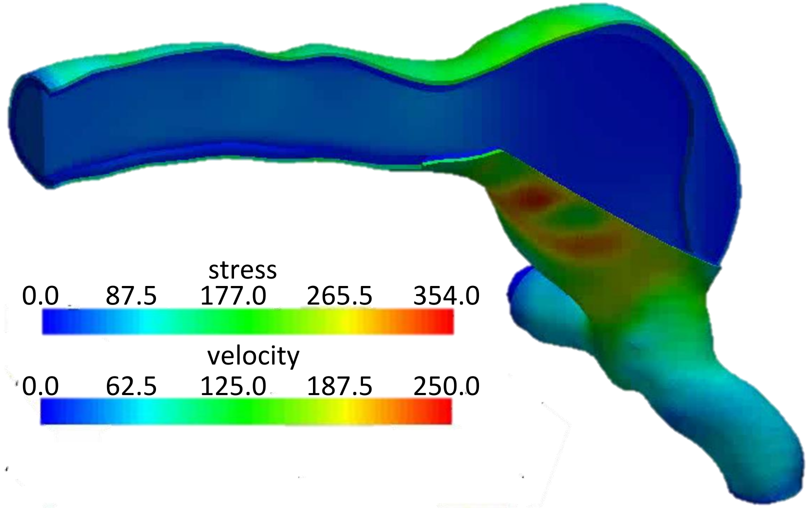
C.P. Schmidt, S. Sinzig, V. Gravemeier, W.A. Wall (2023). A three-dimensional finite element formulation coupling electrochemistry and solid mechanics on resolved microstructures of all-solid-state lithium-ion batteries. *Comput. Methods Appl. Mech. Engrg., 417*



A. Ehrl, G. Bauer, V. Gravemeier, W.A. Wall (2013). A computational approach for the simulation of natural convection in electrochemical cells. *J. Comput. Phys.., 235*

Fluid-structure interaction (ALE)

- Monolithic/partitioned (iterative) FSI (2D / 3D)
- **Moving mesh approach** for the fluid (Arbitrary Langrangian Eulerian formulation)
- Fluid described by incompressible Navier-Stokes equations
- Lagrangean description for solid (various material models)



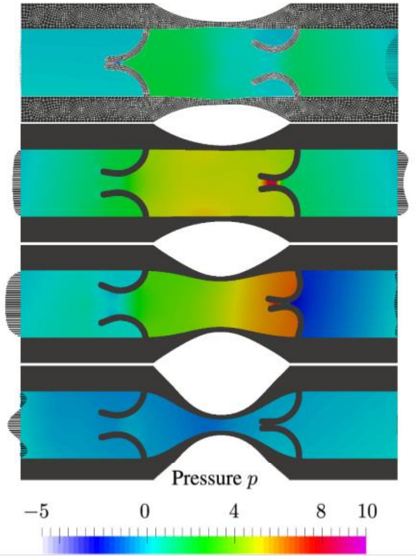
- Example: Blood flow through abdominal aorta including aneurysm

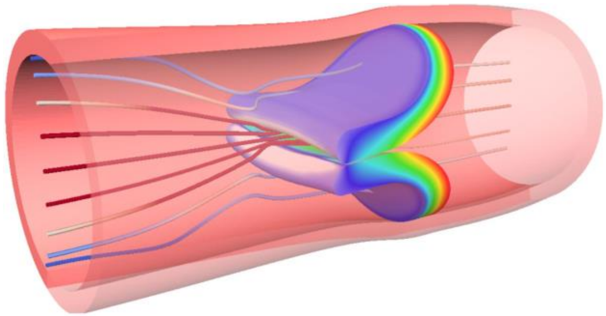
A. Maier, et al (2010). A comparison of diameter, wall stress, and rupture potential index for abdominal aortic aneurysm rupture risk prediction. *Annals of biomedical engineering*, *38*(10)

Fluid-structure interaction (CutFEM)

- Monolithic FSI (2D / 3D)
- **CutFEM approach** for the fluid (**fixed grid**)
- Fluid described by incompressible Navier-Stokes equations
- Lagrangean description for solid (various material models)
- Solids may collide

- Example: Fluid flow through double-leafed valve with poroelastic leaflets in an elastic tube
  - Color scale: velocity of fluid streamlines, pressure on leaflets' surface
  - Opening and closing of the valves includes contact



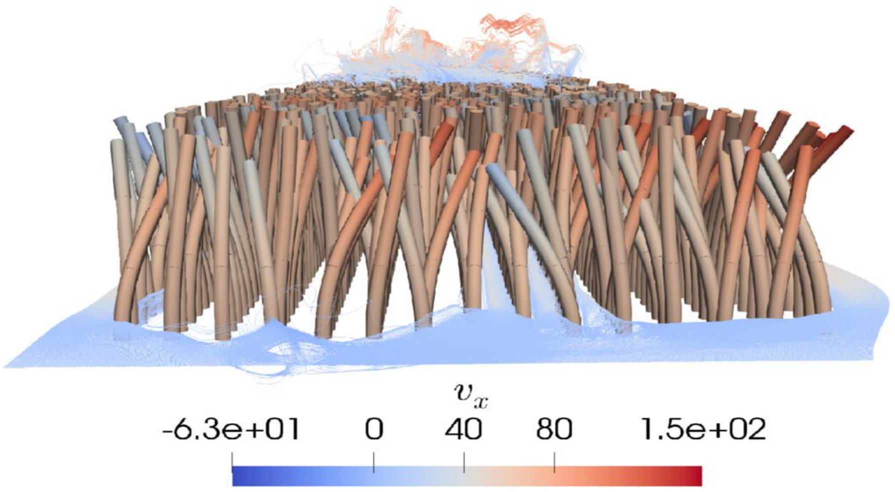


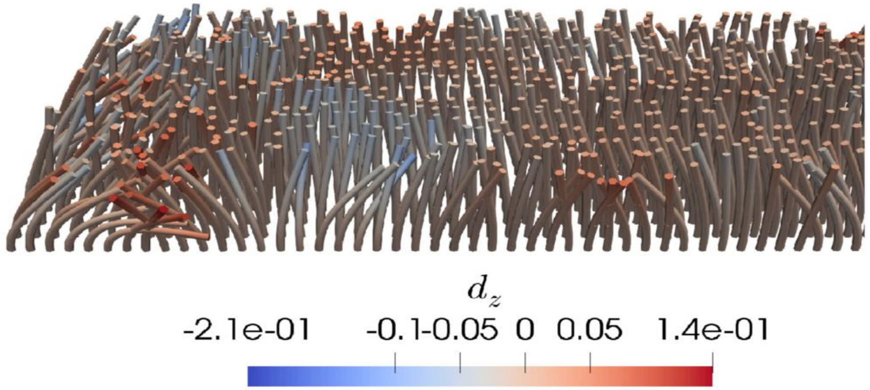
C. Ager, et al. (2021): A consistent and versatile computational approach for general fluid-structure-contact interaction problems. *Int. J. Num. Meth. Engng., 122(19)*

Fluid-structure interaction (mixed-dimensional)

- Two-way partitioned mixed-dimensional coupling
- Fibers: Slender one-dimensional (1D) fibers based on geometrically exact nonlinear beam theory
- Flow: 3D incompressible Navier-Stokes equations
- Regularized mortar-type finite element discretization

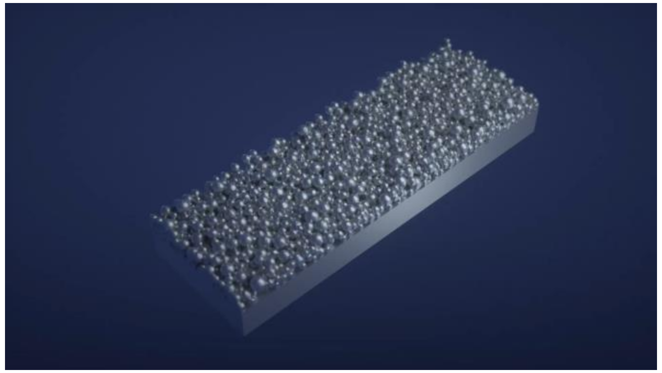
- Example: submersed vegetation canopy



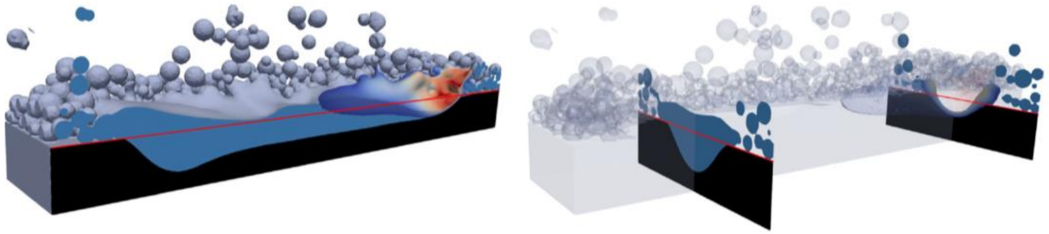


N. Hagmeyer, M. Mayr, A. Popp (2024).
A fully coupled regularized mortar-type finite element approach for embedding one-dimensional fibers into three-dimensional fluid flow. *Int. J. Num. Meth. Eng., 125*

Fluid-structure interaction (SPH)



- Available interaction types
  - DEM (also in combination with elastic solids)
  - SPH
  - Peridynamics (WIP)
- Fluid-structure interaction
  - Solids
    - mobile but undeformable of arbitrary shape
    - Can collide
  - Fluid with different phases
  - Optionally thermal conduction
  - Optionally reversible phase changes

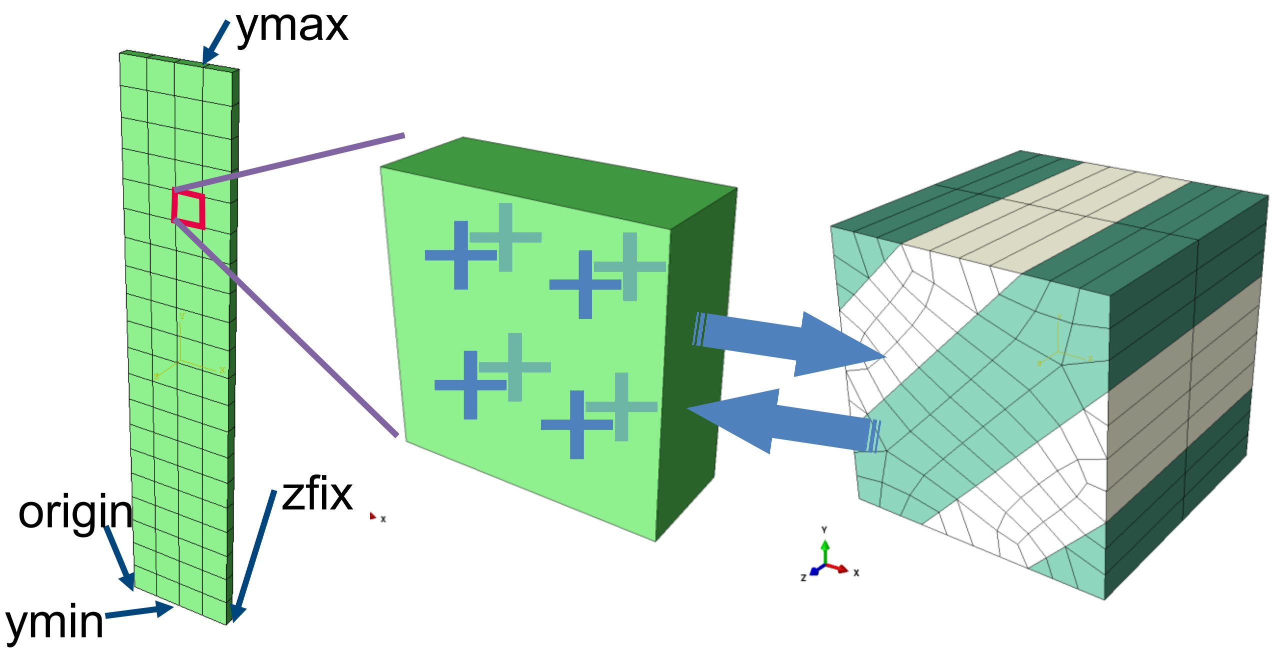


- Example: Highly dynamic particle simulation of powder bed fusion in additive manufacturing. Metal powder particles are heated using a laser beam moving along. Eventually, the particles melt and combine with the underlying substrate. ($17e^6$ SPH particles, $5e^5$ time steps)

S.L. Fuchs, et al. (2022): A versatile SPH modeling framework for coupled microfluid-powder dynamics in additive manufacturing: binder jetting, material jetting, directed energy deposition and powder bed fusion. *Engineering with Computers (https://doi.org/10.1007/s00366-022-01724-4)*

Multiscale modeling

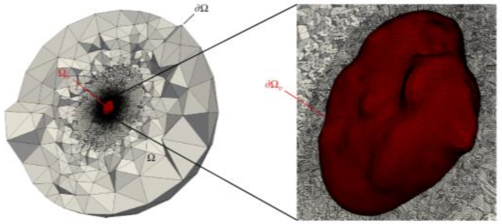
- FE^2 approach
- Microstructure
  - is calculated at each macro Gauss point
  - can be different in each macro element
  - can be run in parallel, with additional processes for the microstructure
- Simulation time increases exponentially



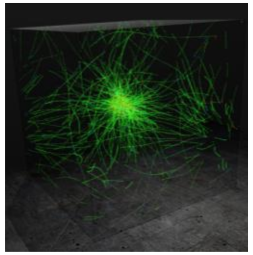
- Example
  - Tensile bar with laminar microstructure
  - Instead of 80 elements, the model comprises 80 x 8 x 176 = 112.640 elements

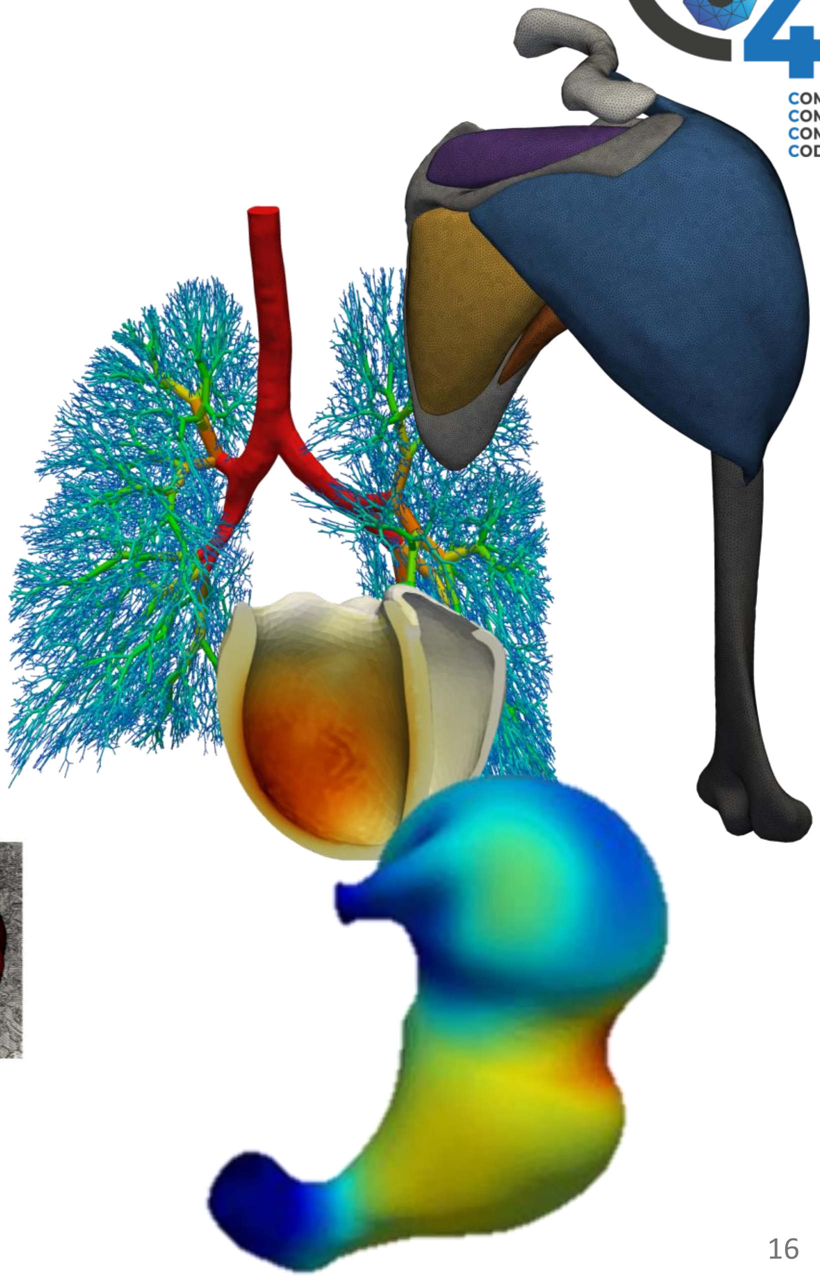
Biomechanics applications
(https://4c-multiphysics.org/publications/)

- Lung modeling: Mixed dimensionial modeling (0D, 1D, 3D)
  - Roth, C.J. Ismail, M., Yoshihara, L., Wall, W.A. (2016) Numer. Meth. Biomed. Eng. 33(1)
- Musculoskeletal systems
  - Engelhardt, L., Sachse, R., Burgkart, R., & Wall, W. A. (2025) Int. J. Num. Meth. Biomed Eng. 41(4)
- Heart
  - Gebauer, A., Pfaller, M., Bräu, F., Cyron, C., Wall, W. (2023) Biomech Model Mechanobiol 1-20
- Stomach
  - Henke, M. S., Brandstaeter, S., Fuchs, S. L., Aydin, R. C., Gizzi, A., Cyron, C. J. (2025): submitted for publication, preprint: arXiv:2509.02486
- Tumor / Cancer modeling
  - Kremheller, J., Brandstaeter, S., Schrefler, B.A., Wall, W.A. (2021) Int J Numer Method Biomed Eng



- Cellbiology
  - Müller, K.W., Cyron, C.J., Wall, Proc. Roy. Soc. A 471 (2182)





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Build & run 4C (Docker Image)

- Docker image with pre-built 4C executable
  https://github.com/4C-multiphysics/4C/tree/main/docker/prebuilt_4C

- Start the docker image
  docker run --interactive --tty ghcr.io/4c-multiphysics/4c:latest
- Run simulation
  - Serial: *path/to/4C path/to/<input-file.4C.yaml> output-prefix*
  - Parallel: Prepend *mpirun –np <numProcs>*

Build & run 4C (manual build)

- Clone the repo: https://github.com/4C-multiphysics/4C
- Here is the installation: https://4c-multiphysics.github.io/4C/documentation/installation/installation.html
- Install dependencies
- Create build folder, therein
  - *cmake --preset=<name-of-preset> <4C_source_dir>*
  - *ninja -j <numProcs>*

Build & run 4C (manual build)

- Dependencies
  - https://github.com/4C-multiphysics/4C/blob/main/docker/dependencies/Dockerfile (Ubuntu 24.04)
  - C++ compiler with C++20 compatibility
  - MPI / CMake / Ninja
  - TPLs (most important)
    - Trilinos
    - Suitesparse, SuperLUDist
    - BLAS, LAPACK
    - Metis, ParMETIS
    - HDF5
    - Several install scripts: https://github.com/4C-multiphysics/4C/tree/main/dependencies/

```
apt-get update && apt-get install -y \
  doxygen \
  graphviz \
  texinfo \
  lcov \
  libblas-dev \
  libboost-all-dev \
  libcln-dev \
  libhdf5-dev \
  libhdf5-openmpi-dev \
  libnetcdf-dev \
```

- For code development, integration with CLion and Visual Studio Code is documented, see https://4c-multiphysics.github.io/4C/documentation/installation/installation.html#set-up-your-ide

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4C input file

- ASCII file in yaml format **.4C.yaml*
- Further files can be referenced
  - Linear/nonlinear solver
  - Mesh
  - Include other yaml files
- Two parts are necessary in a 4C input file
  - Parameter/header block
  - Mesh block

4C input file (header block)

- PROBLEMTYPE → 40 different “applications”
- DYNAMIC section(s) → for each field and many interaction types
- IO → mostly VTK runtime output
- SOLVER
  - References to xml files
  - Templates
    - Iterative linear solvers
    - Preconditioners
    - https://github.com/4C-multiphysics/4C/blob/main/tests/input_files/xml

```
SOLVER 2:
  SOLVER: "Belos"
  AZPREC: "Teko"
  AZREUSE: 10
  SOLVER_XML_FILE: "xml/linear_solver/iterative_gmres_template.xml"
  TEKO_XML_FILE: "xml/block_preconditioner/thermo_solid.xml"
```

- MATERIALS
  - https://4c-multiphysics.github.io/4C/documentation/materialreference.html
  - https://4c-multiphysics.github.io/4C/documentation/analysis_guide/materials.html (to be extended)

4C input file (header block)

COMPREHENSIVE
COMPUTATIONAL
COMMUNITY
CODE

- FUNCT
  - Functions of space and time (interpolation and symbolic math)
  - https://4c-multiphysics.github.io/4C/documentation/furtherreference.html#functions-reference
- Boundary conditions
  - Dirichlet bc → prescribe from scalar to FUNCT
  - Neumann bc → in reference and spatial configuration (“orthopressure”)
  - Periodic bc
  - Many more (e.g., coupling conditions, initial conditions, constraints, …)
  - https://4c-multiphysics.github.io/4C/documentation/conditionreference.html

4C input file (mesh block)

- Variant 1
  - Reference mesh file containing node sets, node coordinates, and element connectivity
  - Supported file formats
    - *.e/*.exo (EXODUS II from Cubit)
    - *.vtu
    - *.msh (GMSH – to come soon)

```yaml
STRUCTURE GEOMETRY:
  FILE: "/tmp/pw_m3.exo"
  SHOW_INFO: "summary"
  ELEMENT_BLOCKS:
    - ID: 1
      ELEMENT_NAME: SOLID
      ELEMENT_DATA: "MAT 2 KINEM nonlinear TECH eas_full"

FLUID GEOMETRY:
  FILE: "/tmp/pw_m3.exo"
  SHOW_INFO: "detailed"
  ELEMENT_BLOCKS:
    - ID: 2
      ELEMENT_NAME: FLUID
      ELEMENT_DATA: "MAT 1 NA ALE"
```

4C input file (mesh block)

COMPREHENSIVE
COMPUTATIONAL
COMMUNITY
CODE

- Variant 2
  - Node sets (DNODE/DLINE/DSURF/DVOL–NODE TOPOLOGY)
  - NODE COORDS
    - Unique numbering
  - ELEMENTS
    - Different element types within one file possible
    - Individual material per element
    - Several fields within one file possible for multiphysics, e.g., STRUCTURE ELEMENTS, FLUID ELEMENTS, TRANSPORT ELEMENTS, …

```
  - "NODE 7 DVOL 1"
  - "NODE 4 DVOL 1"
NODE COORDS:
  - "NODE 1 COORD 0.00236432494005
  - "NODE 2 COORD 0.09009273926518
  - "NODE 3 COORD -0.0711680774560
```

2 styles possible

```
"DVOL-NODE TOPOLOGY": [
  "NODE 6 DVOL 1",
  "NODE 1 DVOL 1",
  "NODE 4 DVOL 1",
  "NODE 2 DVOL 1",
  "NODE 7 DVOL 1",
  "NODE 5 DVOL 1",
  "NODE 3 DVOL 1",
  "NODE 8 DVOL 1"
],
"NODE COORDS": [
  "NODE 1 COORD  0.0023643 0.0023643 0.0023643",
  "NODE 2 COORD  0.0900927 1.0900927 0.0900927",
  "NODE 3 COORD -0.0711680 -0.0711680 0.9288319",
  "NODE 4 COORD  0.0897298 1.0897298 1.0897298",
  "NODE 5 COORD  0.9623662 -0.0376337 -0.0376337",
  "NODE 6 COORD  0.9846652 0.9846652 -0.0153347",
  "NODE 7 COORD  1.0655405 0.0655405 1.0655405",
  "NODE 8 COORD  0.9818398 0.9818398 0.9818398"
],
"STRUCTURE ELEMENTS": [
  "1 SOLID HEX8 1 5 6 2 3 7 8 4 MAT 1 KINEM nonlinear TECH eas_full FIBER1 0.707106 0.707106 0.0"
]
```

4C input file (mesh block)

- Variant 3
  - Rectangular grid internally created
  - VOLUME / SIDE / EDGE / CORNER keywords for boundary conditions
  - Supported element types
    - HEX8 / HEX20 / HEX27
    - WEDGE6 / WEDGE15

```
DESIGN SURF NEUMANN CONDITIONS:
  - E: 2
    NUMDOF: 3
    ONOFF: [1, 0, 0]
    VAL: [1, 0, 0]
    FUNCT: [0, 0, 0]
DNODE-NODE TOPOLOGY:
  - "CORNER structure x- y- z- DNODE 1"
DSURF-NODE TOPOLOGY:
  - "SIDE structure x- DSURFACE 1"
  - "SIDE structure x+ DSURFACE 2"
STRUCTURE DOMAIN:
  bottom_corner_point: [0.0, 0.0, 0.0]
  top_corner_point: [4.0, 4.0, 4.0]
  subdivisions: [3, 3, 3]
  rotation_angle: [45.0, 0.0, 30.0]
  auto_partition: false
  elements:
    SOLID:
      HEX8:
        MAT: 1
        KINEM: linear
```

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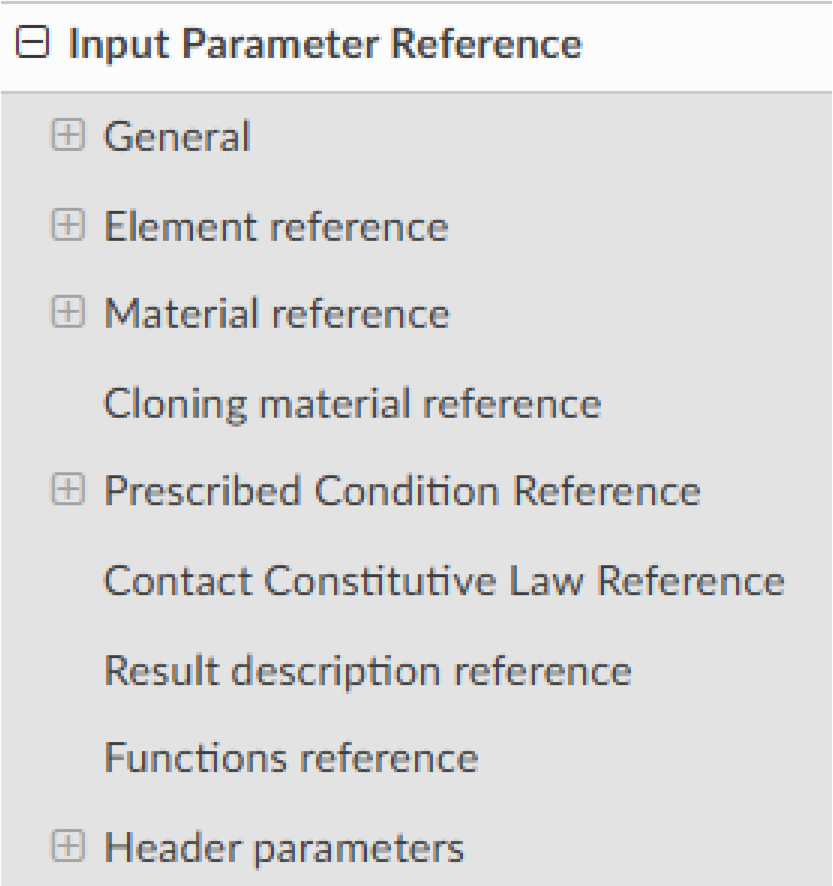
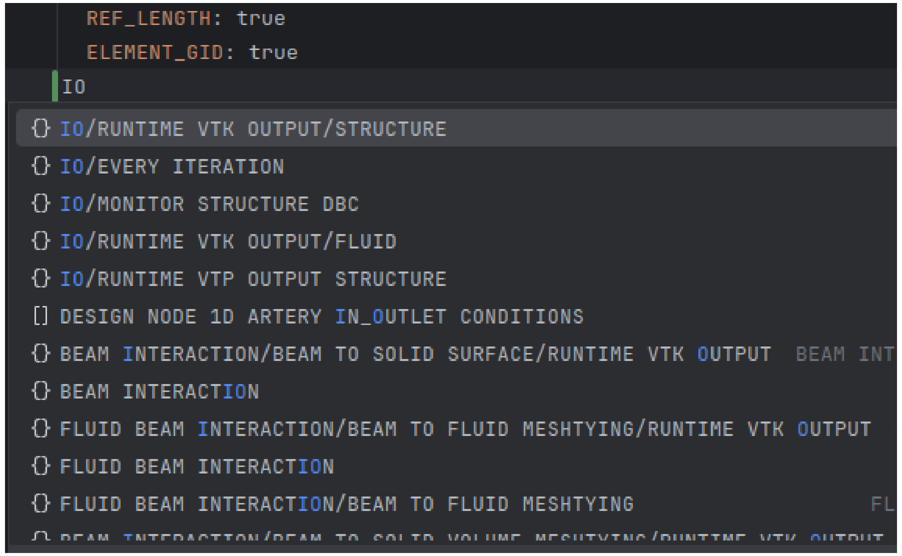
Input file creation

- Where to find helpful information
  - https://4c-multiphysics.github.io/4C/documentation/input_parameter_reference/parameterreference.html
  - Existing input files (>2000)
    - *https://github.com/4C-multiphysics/4C/tree/main/tests/input_files*
    - File names are historically grown (f2 → fluid 2-dimensional, elch → electrochemistry)
    - Search for relevant keyword/input parameter in docu
    - Search for files containing the keyword
    - Start with a valid input file

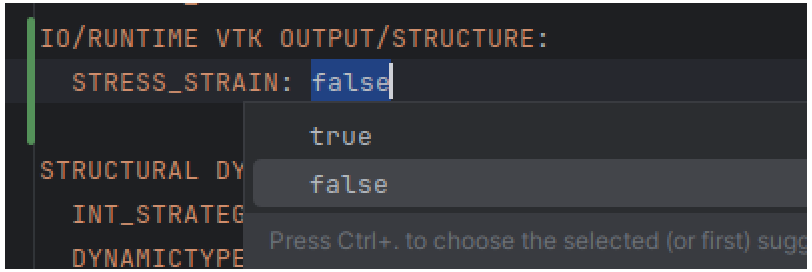


Input file creation

- Input file creation with IDE support (e.g. VS Code or CLion) using schema file
  - Auto completion (Ctrl + Space)



  - Only offers not yet set parameters
  - Shows available options and initializes with default value



Input file creation

- Reuse parts of files via inclusion

periodicCube-base.yaml

```
INCLUDES:
  - periodicCube-head.yaml
  - periodicCube-bc.yaml
  - periodicCube-geo.yaml
```

periodicCube-head.yaml

```
PROBLEM TYPE:
  PROBLEMTYPE: "Structure"
IO:
  STRUCT_STRESS: "Cauchy"
  STRUCT_STRAIN: "GL"
IO/RUNTIME VTK OUTPUT:
  INTERVAL_STEPS: 1
IO/RUNTIME VTK OUTPUT/STRUCTURE:
  OUTPUT_STRUCTURE: true
  DISPLACEMENT: true
  STRESS_STRAIN: true
```

periodicCube-bc.yaml

```
FUNCT1:
  - COMPONENT: 0
    SYMBOLIC_FUNCTION_OF_SPACE_TIME: "pull"
  - VARIABLE: 0
    NAME: "pull"
    TYPE: "linearinterpolation"
    NUMPOINTS: 2
    TIMES: [0,20]
    VALUES: [0,5]
DESIGN SURF DIRICH CONDITIONS:
  - E: 1
    NUMDOF: 3
    ONOFF: [1,0,0]
    VAL: [0,0,0]
```

periodicCube-geo.yaml

```
  - NODE    239 COORD    -3.5857860     5.0000000     1.6666670
  - NODE    240 COORD    -3.5857860     5.0000000    -1.6666670
STRUCTURE ELEMENTS:
  -       1 SOLID HEX8 70 69 239 237 4 3 6 7 MAT 1 KINEM linear
  -       2 SOLID HEX8 72 71 240 236 70 69 239 237 MAT 1 KINEM linear
  -       3 SOLID HEX8 65 66 238 235 72 71 240 236 MAT 1 KINEM linear
  -       4 SOLID HEX8 180 152 160 190 37 25 31 43 MAT 1 KINEM linear
  -       5 SOLID HEX8 176 174 180 190 36 35 37 43 MAT 1 KINEM linear
  -       6 SOLID HEX8 96 82 176 190 12 8 36 43 MAT 1 KINEM linear
  -       7 SOLID HEX8 189 95 96 190 45 13 12 43 MAT 1 KINEM linear
```

Input file creation

- https://4c-multiphysics.github.io/4C/documentation/analysis_guide/preprocessing.html

- Several ways to create mesh files
  - Coreform Cubit → *.e (EXODUS II) format
  - https://pypi.org/project/meshio/ enables mesh conversion
    - Supports widely-used mesh formats (proprietary & open) as input
    - Convert file into *.vtu (or *.msh) format for usage within 4C
    - Please stay tuned, we are currently working on a reliable and versatile solution based on meshio

Growing ecosystem around 4C Multiphysics

- Tools: https://4c-multiphysics.github.io/4C/documentation/tools/tools.html#tools
  - QUEENS (https://github.com/queens-py/queens)
    - Parameter studies
    - Sensitivity analysis
    - Uncertainty quantification
    - Parameter identification
    - Inverse analysis
  - FourCIPP (https://github.com/4C-multiphysics/fourcipp)
    - Python parser to interact with 4C input files
  - 4C-Webviewer (https://github.com/4C-multiphysics/4C-webviewer)
    - Visualize and edit 4C input
  - Several input generator scripts (BeamMe, cubitpy, …)

4C Multiphysics summary

- 4C solves challenging real-world applications
- Extensible modular C++ software structure
- Freely available under LPGL-3.0-or-later
- https://github.com/4C-multiphysics/4C
- Join the community ☺
  (photo from our this year‘s workshop July 29^{th} – 31^{st}, 2025)

4C Multiphysics @UKACM&GACM Autumn School 2025

Hands-on-sessions

- 9:30 – 11:00 (1) Solid mechanics with plasticity
- 11:15 – 12:45 (2) Contact mechanics
- 11:15 – 12:45 (3) Fluid-solid interaction
- 15:30 – 16:00 State-of-the-art research with 4C (Overview)

Tomorrow

- QUEENS
- QUEENS & 4C