



# eFlows4HPC

## Innovative HPC workflows for industry Reduced Order Models

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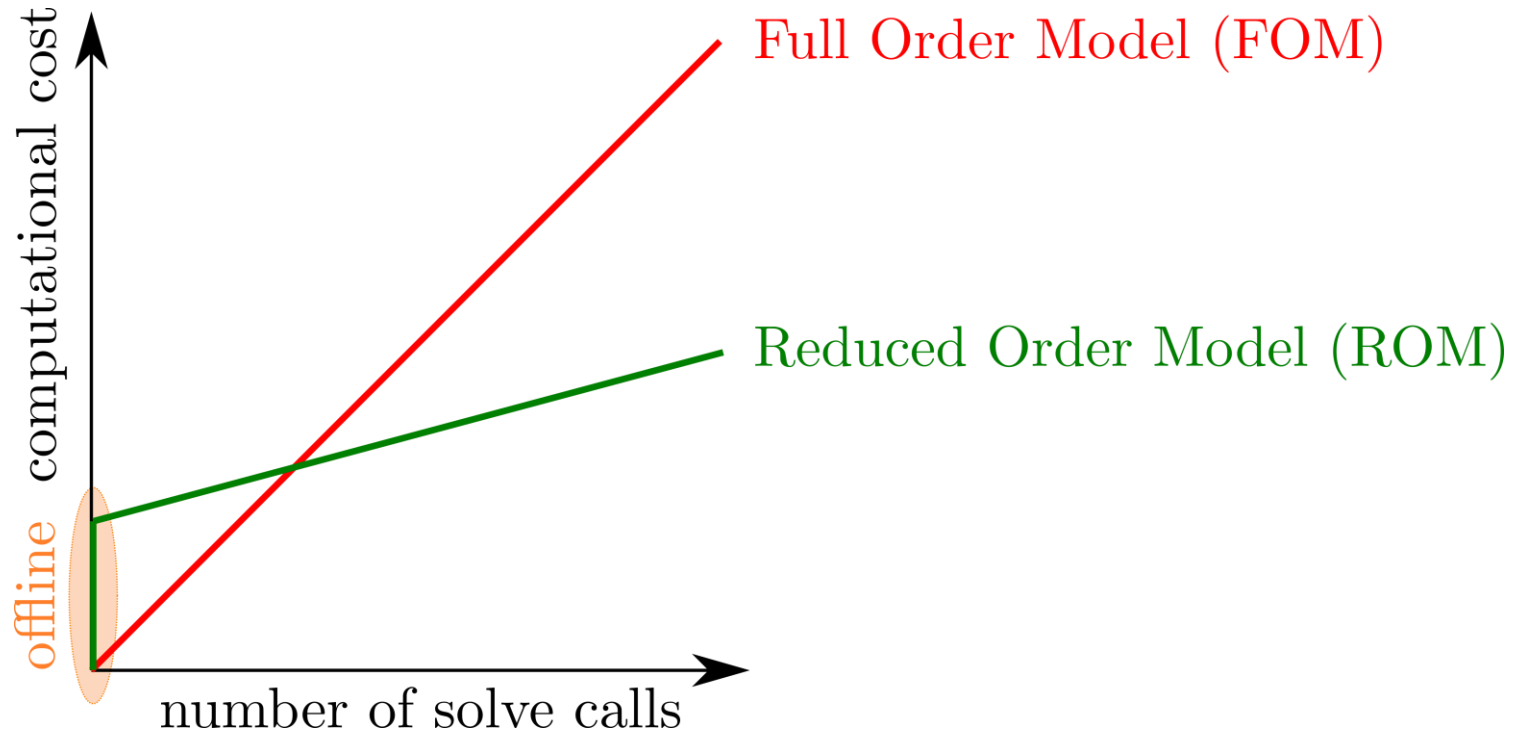
- **ROM Theory**
  - **Motivation**
  - **Parametrized Problem**
  - **Approximation Space (Parametric Exploration)**
  - **Reduced Order Basis**
  - **System Projection**
  - **Hyper-reduction**
- **Demo**
- **eFlows4HPC Use Case**
  - **HPC Workflow**
  - **Results**
- **HPCWaaS Small Demo**



# ROM THEORY



# Motivation



# Parametrized Problem

**Convection-Diffusion Equation:**

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u - D \nabla^2 u = 0$$

**Variational Formulation:**

$$\int_{\Omega} w \left( \frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) \right) dx + \int_{\Omega} \nabla w \cdot (D \nabla u) dx = 0$$

**Semi-Discrete Problem:**

$$M_C \frac{du}{dt} = (K - L)u$$

# Parametrized Problem

State Variable at Time  $t$ :

$$\mathbf{u}_t = \mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_t$$

Adapted Time Discretization:

$$[M_C - \theta \Delta t (K - L)] (\mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_{t+1}) = [M_C + (1 - \theta) \Delta t (K - L)] (\mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_t)$$

Residual:

$$\mathbf{R}_t(\mathbf{u}_t) = \mathbf{R}(\mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_t(t; \boldsymbol{\mu}), t; \boldsymbol{\mu})$$

Given:

$$\mathbf{R}_t(\mathbf{u}_t) = [M_C - \theta \Delta t (K - L)] (\mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_{t+1}) - [M_C + (1 - \theta) \Delta t (K - L)] (\mathbf{u}_{\text{ref}} + \Delta \mathbf{u}_t)$$

# Parametrized Problem

Residual:

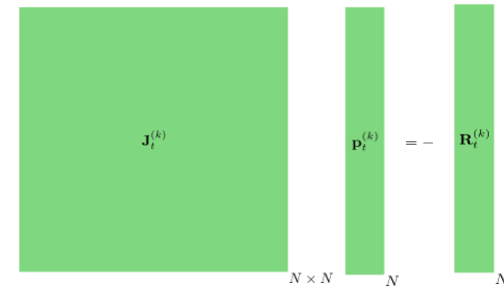
$$\mathbf{R}_t(\mathbf{u}_t) = \mathbf{R}(\mathbf{u}_{\text{ref}} + \Delta\mathbf{u}_t(t; \boldsymbol{\mu}), t; \boldsymbol{\mu})$$

Jacobian (Derivative of Residual):

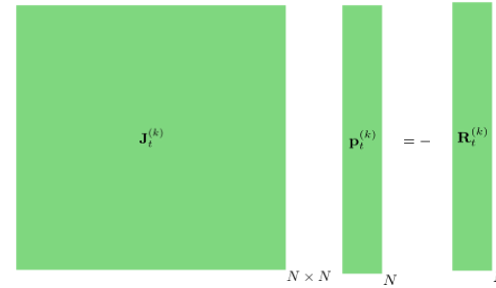
$$J_t = \frac{\partial \mathbf{R}_t}{\partial \mathbf{u}_{t+1}} = M_C - \theta \Delta t (K - L)$$

Newton-Raphson Iteration

$$\begin{aligned} \mathbf{J}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu}) \mathbf{p}_t^{(k)} &= -\mathbf{R}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu}) \\ \Delta\mathbf{u}_t^{(k+1)} &= \Delta\mathbf{u}_t^{(k)} + \alpha_t^{(k)} \mathbf{p}_t^{(k)} \\ \mathbf{u}_t^{(k+1)} &= \mathbf{u}_t^{(k)} + \Delta\mathbf{u}_t^{(k+1)}, \end{aligned}$$



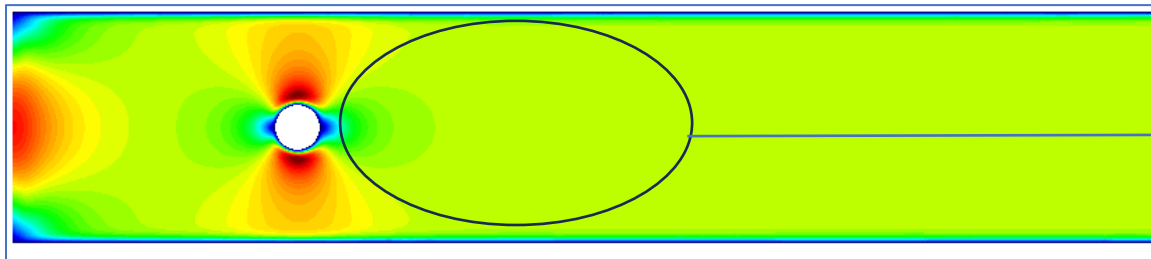
# Parametrized Problem



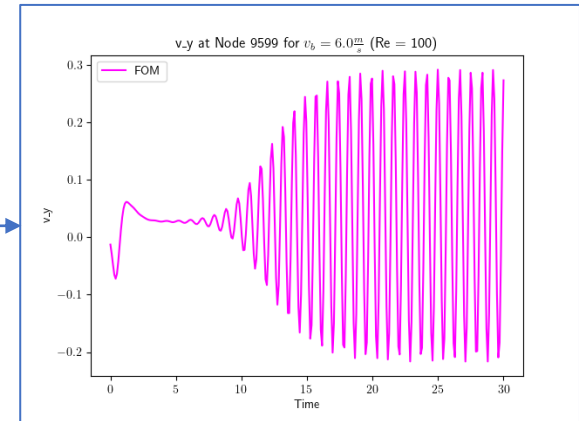
FOM Assembling:

$$\begin{aligned}
 \mathbf{J}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu}) \mathbf{p}_t^{(k)} &= -\mathbf{R}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu}) \\
 \Delta \mathbf{u}_t^{(k+1)} &= \Delta \mathbf{u}_t^{(k)} + \alpha_t^{(k)} \mathbf{p}_t^{(k)} \\
 \mathbf{u}_t^{(k+1)} &= \mathbf{u}_t^{(k)} + \Delta \mathbf{u}_t^{(k+1)},
 \end{aligned}$$

$$\mathbf{R}_t = \sum_{e=1}^L \mathbf{L} e^T \mathbf{R}_t^e$$



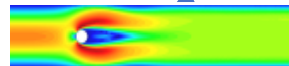
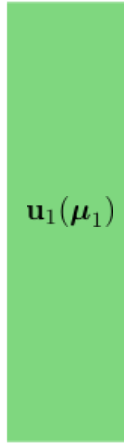
68298 elements





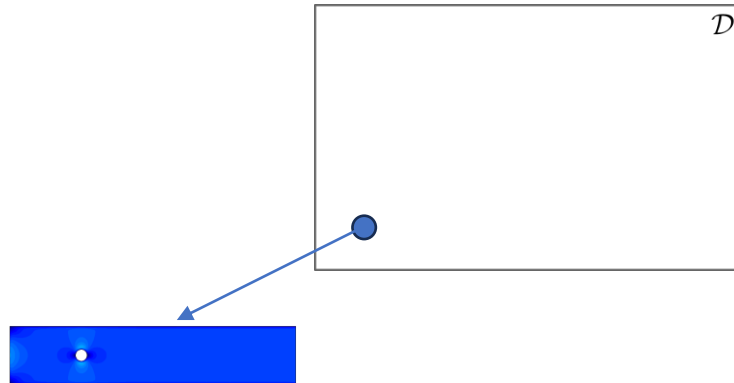
# Approximation Space (Parametric Exploration)

$$\mathbf{A}^u = \mathbf{u}_1(\mu_1)$$



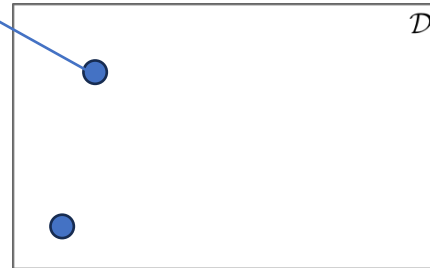
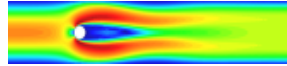
# Approximation Space (Parametric Exploration)

$$\mathbf{A}^u = \mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1)$$



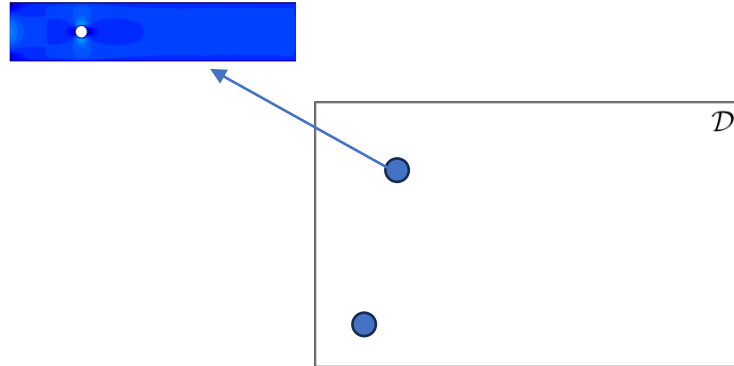
# Approximation Space (Parametric Exploration)

$$\mathbf{A}^u = \mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1), \mathbf{u}_1(\boldsymbol{\mu}_2)$$



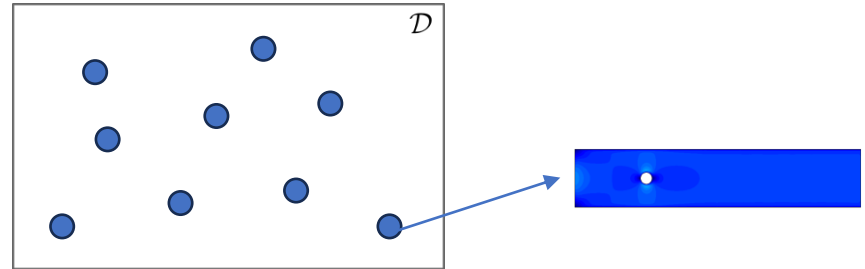
# Approximation Space (Parametric Exploration)

$$\mathbf{A}^u = \mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1) \mid \mathbf{u}_1(\boldsymbol{\mu}_2), \mathbf{u}_2(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_2)$$



# Approximation Space (Parametric Exploration)

$$\mathbf{A}^u = \mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1) \mid \mathbf{u}_1(\boldsymbol{\mu}_2), \mathbf{u}_2(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_2) \mid \dots, \mathbf{u}_T(\boldsymbol{\mu}_P)$$



# Right Reduced Order Basis (ROB)

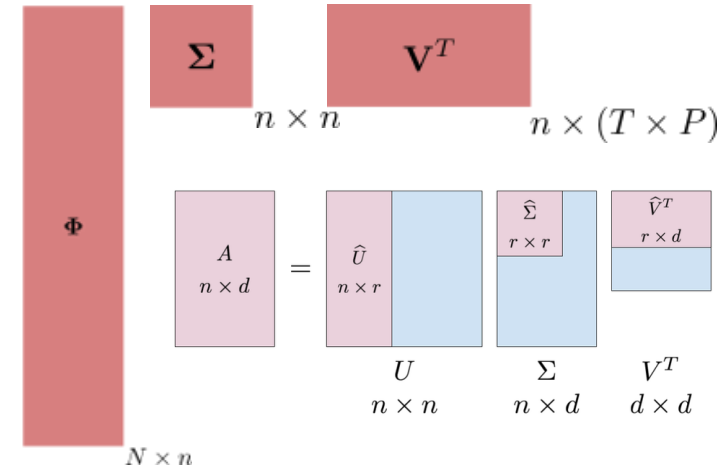
$$\mathbf{A}^u = [\mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1), \mathbf{u}_1(\boldsymbol{\mu}_2), \mathbf{u}_2(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_P)]$$

$N \times (T * P)$

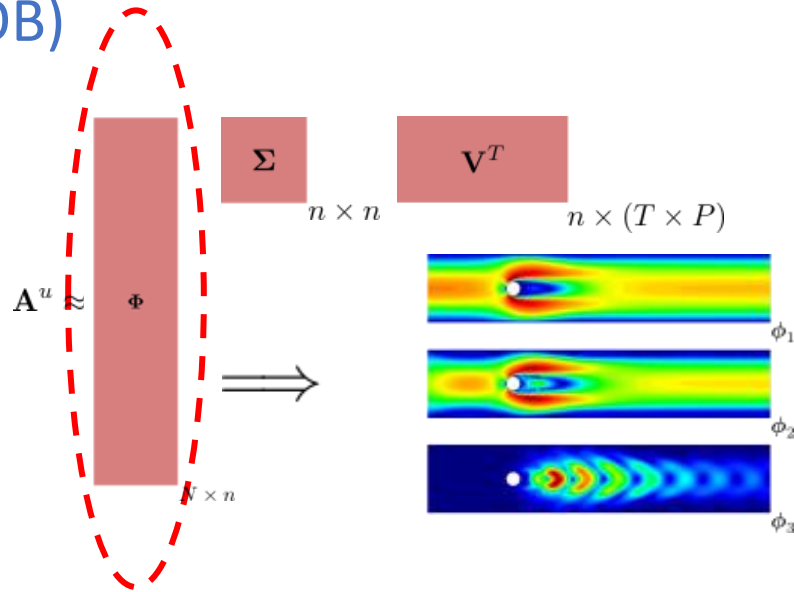
# Right Reduced Order Basis (ROB)

$$\mathbf{A}^u = [\mathbf{u}_1(\boldsymbol{\mu}_1), \mathbf{u}_2(\boldsymbol{\mu}_1), \dots, \mathbf{u}_T(\boldsymbol{\mu}_1), \mathbf{u}_1(\boldsymbol{\mu}_2), \mathbf{u}_2(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_2), \dots, \mathbf{u}_T(\boldsymbol{\mu}_P)]$$

Singular Value Decomposition:



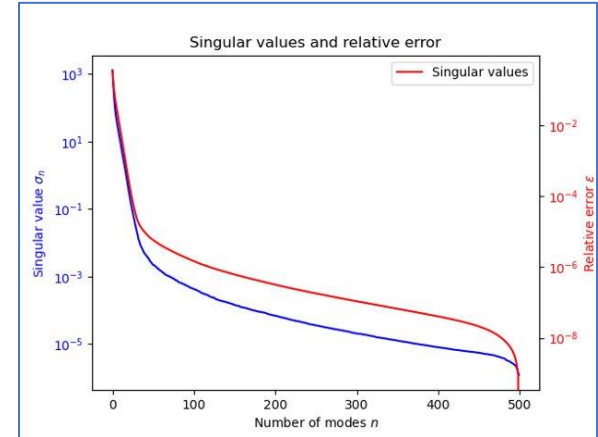
# Right Reduced Order Basis (ROB)



Note that:

Where:

$$\mathbf{A}^u = \Phi_n \Sigma_n \mathbf{V}_n^T + \mathbf{E} \quad n \ll N$$





# Right Reduced Order Basis (ROB)

Reconstruct each solution field with only few coefficients.

$$\mathbf{A}^u \approx \Phi \hat{\mathbf{P}}_t^{(k)}$$

$N \times n$

$$\mathbf{A}^u = [\mathbf{u}_1(\mu_1), \mathbf{u}_2(\mu_1), \dots, \mathbf{u}_T(\mu_1), \mathbf{u}_1(\mu_2), \mathbf{u}_2(\mu_2), \dots, \mathbf{u}_T(\mu_2), \dots, \mathbf{u}_T(\mu_P)]$$

Note that:

$$\mathbf{A}^u = \Phi_n \Sigma_n \mathbf{V}_n^T + \mathbf{E}$$

Where:

$$n \ll N$$

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Note that:

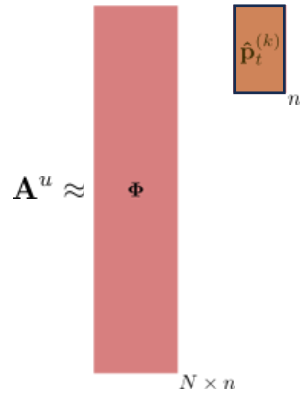
$$\mathbf{A}^u = \Phi_n \Sigma_n \mathbf{V}_n^T + \mathbf{E}$$

Where:

$$n \ll N$$

# Right Reduced Order Basis (ROB)

Reconstruct each solution field with only few coefficients.



$$\mathbf{A}^u = [\mathbf{u}_1(\mu_1), \mathbf{u}_2(\mu_1), \dots, \mathbf{u}_T(\mu_1), \mathbf{u}_1(\mu_2), \mathbf{u}_2(\mu_2), \dots, \mathbf{u}_T(\mu_2), \dots, \mathbf{u}_T(\mu_P)]$$

Note that:

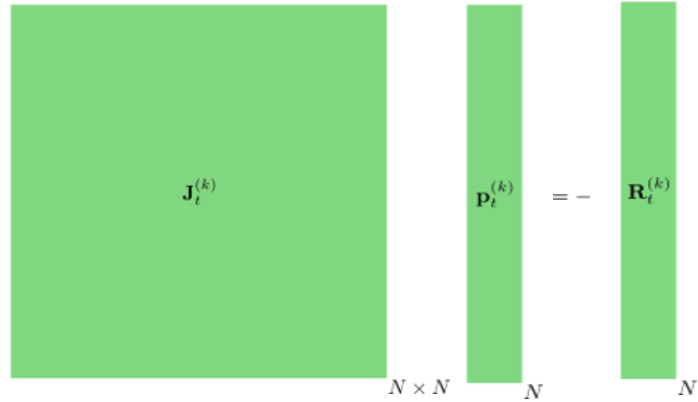
$$\mathbf{A}^u = \Phi_n \Sigma_n \mathbf{V}_n^T + \mathbf{E}$$

Where:

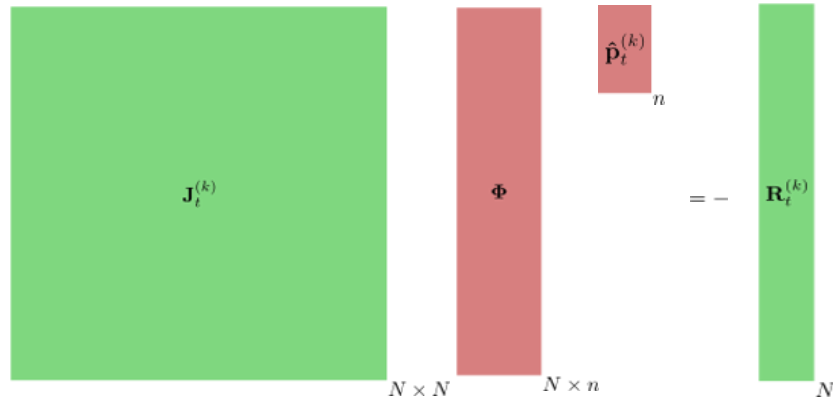
$$n \ll N$$

# FOM Newton-Raphson

$$\mathbf{J}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu}) \mathbf{p}_t^{(k)} = -\mathbf{R}_t^{(k)}(\mathbf{u}_t^{(k)}; \boldsymbol{\mu})$$
$$\Delta \mathbf{u}_t^{(k+1)} = \Delta \mathbf{u}_t^{(k)} + \alpha_t^{(k)} \mathbf{p}_t^{(k)}$$
$$\mathbf{u}_t^{(k+1)} = \mathbf{u}_t^{(k)} + \Delta \mathbf{u}_t^{(k+1)},$$



# FOM Newton-Raphson



The diagram illustrates the Newton-Raphson equation for FOM. It consists of four main components arranged horizontally from left to right:

- A large green square representing the Jacobian matrix  $\mathbf{J}_t^{(k)}$ , with the dimension  $N \times N$  written below it.
- A red vertical rectangle representing the parameter vector  $\Phi$ , with the dimension  $N \times n$  written below it.
- A red vertical rectangle representing the parameter vector  $\hat{\mathbf{P}}_t^{(k)}$ , with the dimension  $n$  written below it.
- A green vertical rectangle representing the residual vector  $\mathbf{R}_t^{(k)}$ , with the dimension  $N$  written below it.

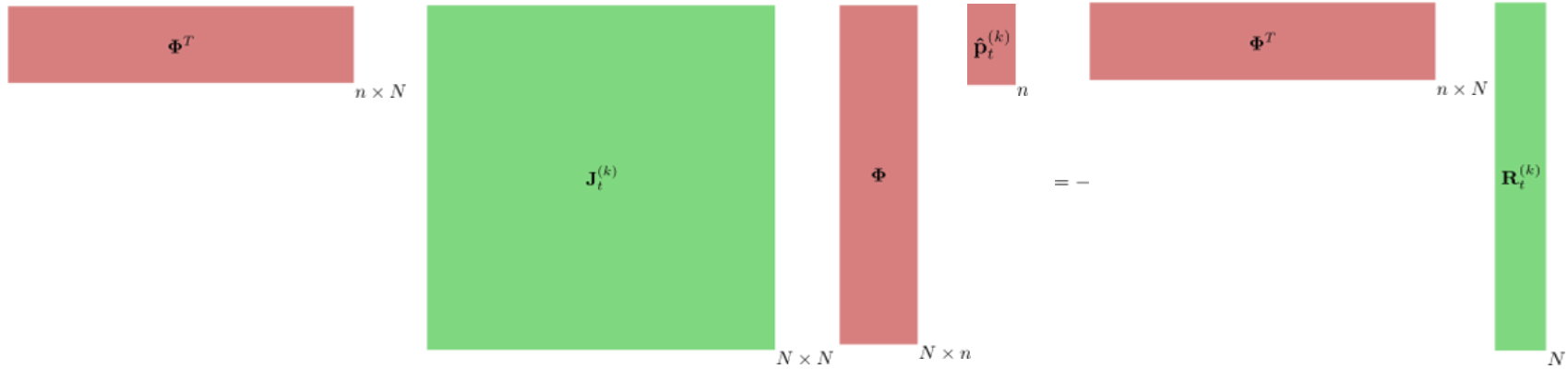
The equation is represented as  $\mathbf{J}_t^{(k)} \Phi = - \hat{\mathbf{P}}_t^{(k)} \mathbf{R}_t^{(k)}$ . The minus sign is placed between the parameter vector  $\hat{\mathbf{P}}_t^{(k)}$  and the residual vector  $\mathbf{R}_t^{(k)}$ .

# Galerkin Projection

$$\Psi_t^{T(k)} \mathbf{J}_t^{(k)}(\tilde{\mathbf{u}}_t^{(k)}; \mu) \Phi \hat{\mathbf{p}}_t^{(k)} = -\Psi_t^{T(k)} \mathbf{R}_t^{(k)}(\tilde{\mathbf{u}}_t^{(k)}; \mu)$$

$$\Delta \hat{\mathbf{u}}_t^{(k+1)} = \Delta \hat{\mathbf{u}}_t^{(k)} + \alpha_t^{(k)} \hat{\mathbf{p}}_t^{(k)}$$

$$\tilde{\mathbf{u}}_t^{(k+1)} = \tilde{\mathbf{u}}_t^{(k)} + \Phi \Delta \hat{\mathbf{u}}_t^{(k+1)},$$



# Galerkin HROM

$$\Phi^T \mathbf{J}_t^{(k)} \Phi \quad \hat{\mathbf{p}}_t^{(k)} = - \Phi^T \mathbf{R}_t^{(k)}$$

$n \times n$     $n$     $n$

ROM Assembling:

$$\Phi^T \mathbf{R}_t = \sum_{e=1}^L \Phi^{eT} \mathbf{R}_t^e$$

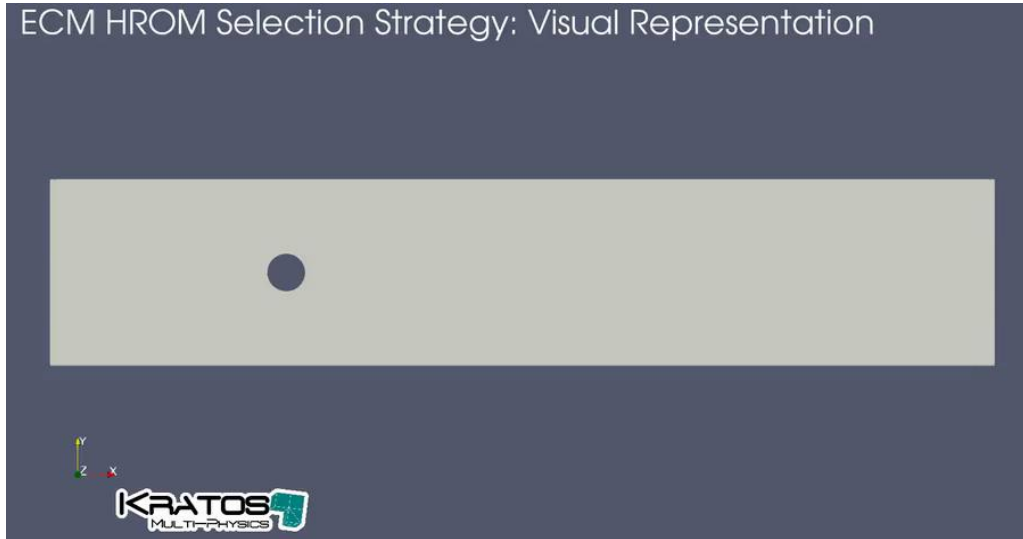
HROM Assembling:

$$\sum_{e \in \mathbf{z}} \omega^e \Phi_t^{eT} \mathbf{R}_t^e = \mathbf{0}.$$

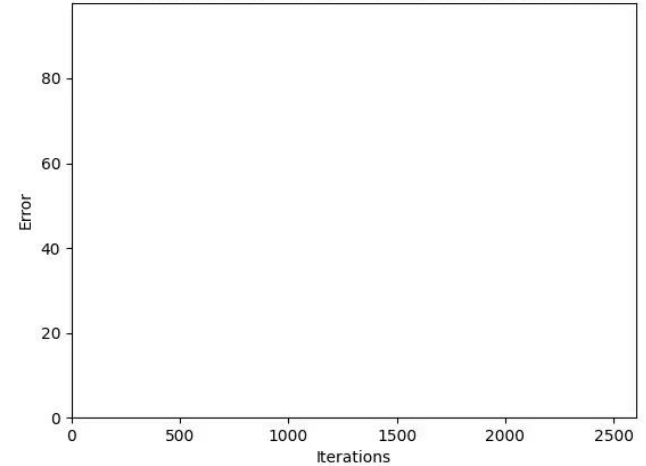
# Galerkin HROM

$$\sum_{e \in \mathbf{z}} \omega^e \Phi_t^{eT} \mathbf{R}_t^e = \mathbf{0}.$$

## ECM HROM Selection Strategy: Visual Representation



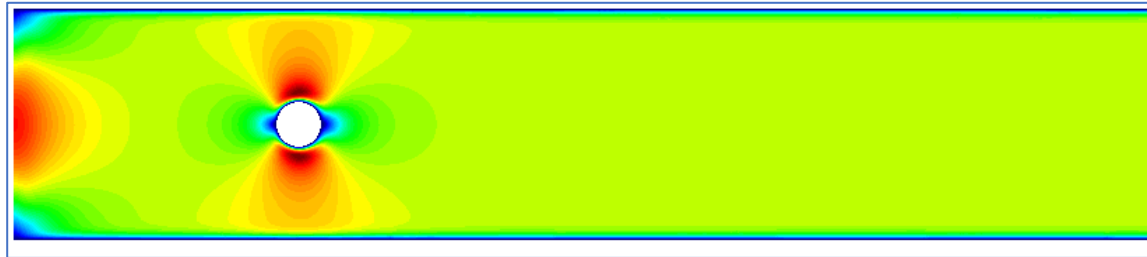
## ECM HROM Selection Strategy: Error Evolution



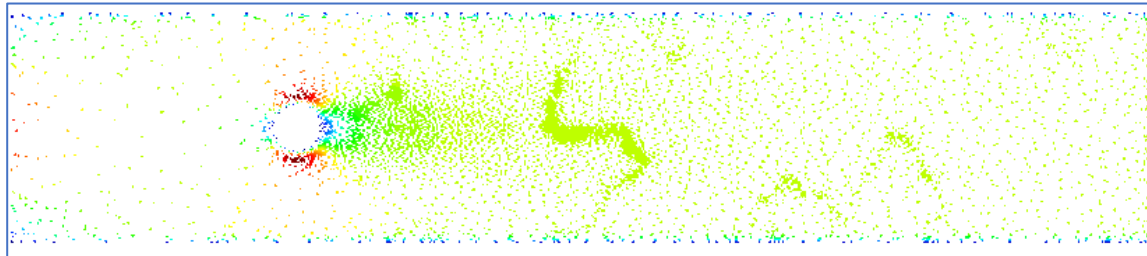
J.A. Hernández, A multiscale method for periodic structures using domain decomposition and ECM-hyperreduction, *Comput. Methods Appl. Mech. Engrg.* 368 (2020).



# ROM vs HROM



68298 elements – Speed up: 4.04



6216 elements – Speed up: 49

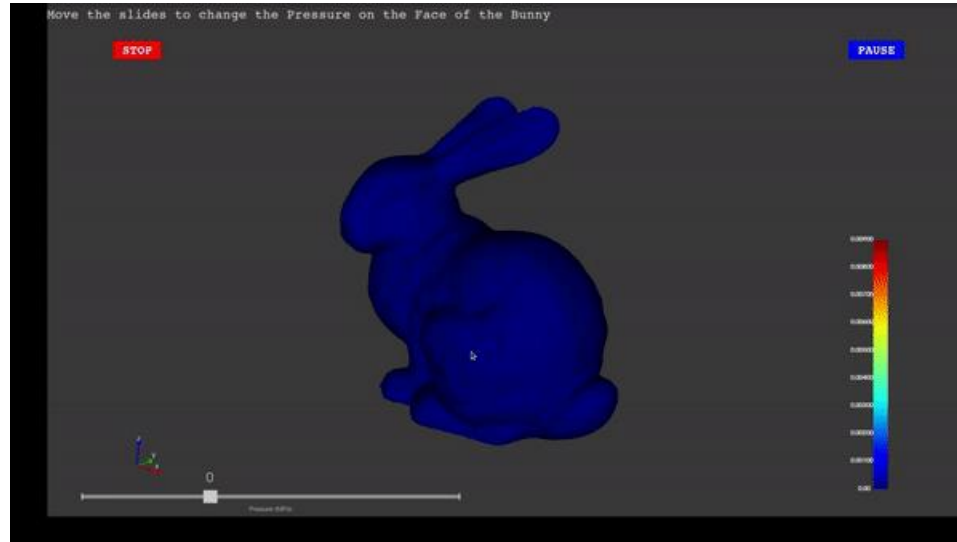


# Real Time Results



**SIEMENS**

# Real Time Results



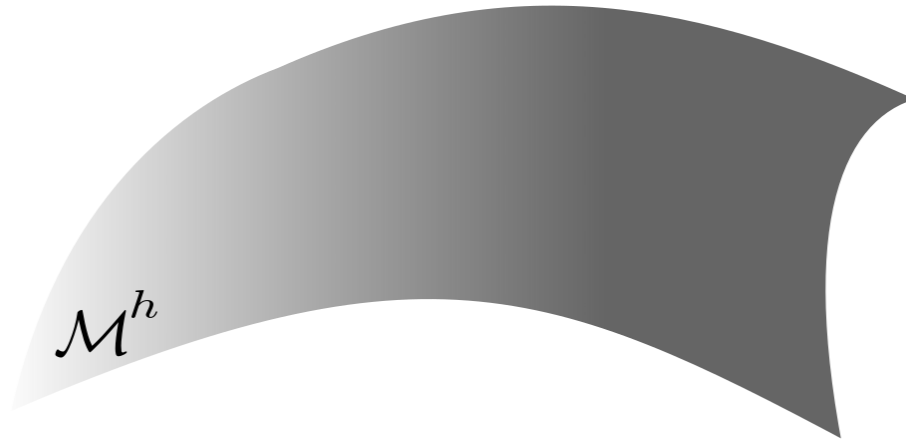


# NONLINEAR REDUCTION



# Manifold

$$\mathcal{M}^h = \{\mathbf{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P}\} \subset \mathbb{R}^{N_{\text{dofs}}}$$

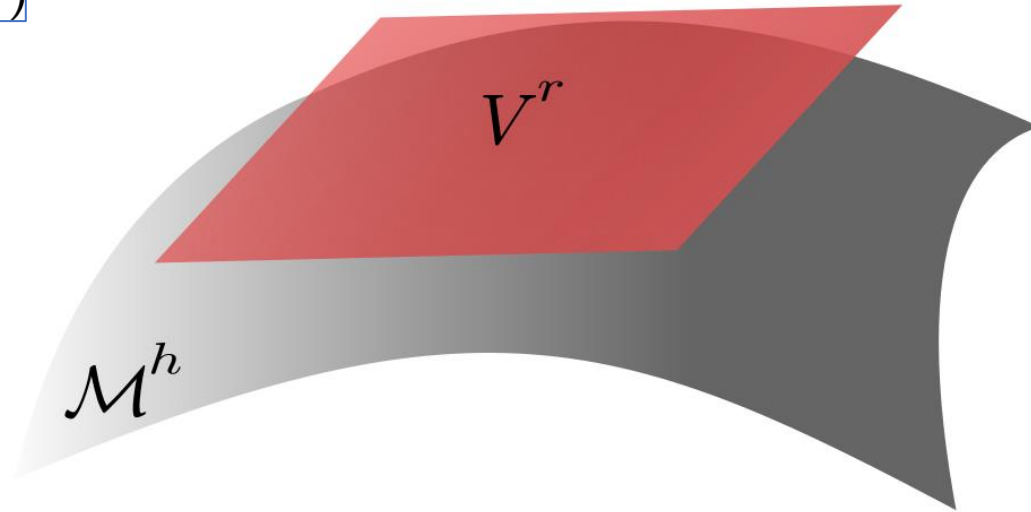


# Manifold: Linear Approximation

$$\mathcal{M}^h = \{\mathbf{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P}\} \subset \mathbb{R}^{N_{\text{dofs}}}$$

$$\tilde{\mathbf{u}} \approx \mathbf{D}(\hat{\mathbf{p}}) = \boldsymbol{\Phi} \hat{\mathbf{p}}$$

$$V^r := \text{col}(\boldsymbol{\Phi})$$

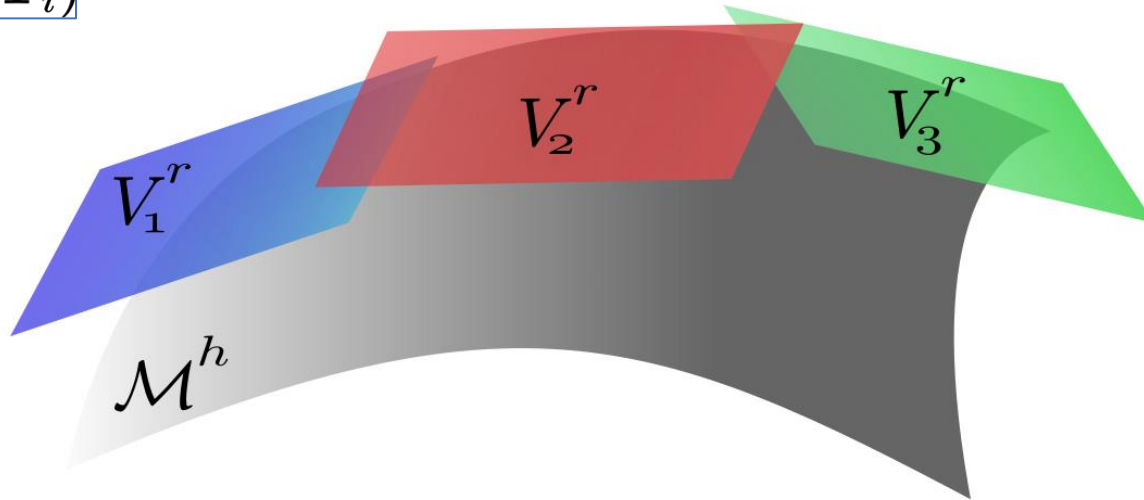


# Manifold: Local Linear Approximation (Non-linear)

$$\mathcal{M}^h = \{\mathbf{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P}\} \subset \mathbb{R}^{N_{\text{dofs}}}$$

$$\tilde{\mathbf{u}} \approx \mathbf{D}(\hat{\mathbf{p}}) = \Phi_i \hat{\mathbf{p}}$$

$$V_i^r := \text{col}(\Phi_i)$$



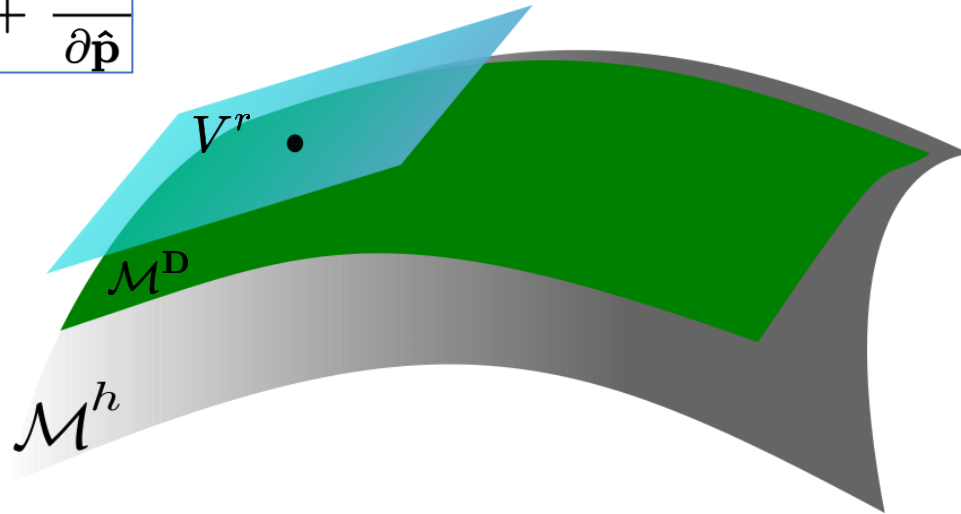


# Manifold: Quadratic Approximation (Non-linear)

$$\mathcal{M}^h = \{\mathbf{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P}\} \subset \mathbb{R}^{N_{\text{dofs}}}$$

$$\tilde{\mathbf{u}} \approx \mathbf{D}(\hat{\mathbf{p}}) = \boldsymbol{\Phi} \hat{\mathbf{p}} + \mathbf{H} \hat{\mathbf{p}} \otimes \hat{\mathbf{p}}$$

$$\mathbf{V}^r := \frac{\partial \mathbf{D}}{\partial \hat{\mathbf{p}}} = \boldsymbol{\Phi} + \frac{\partial \mathbf{H}}{\partial \hat{\mathbf{p}}}$$

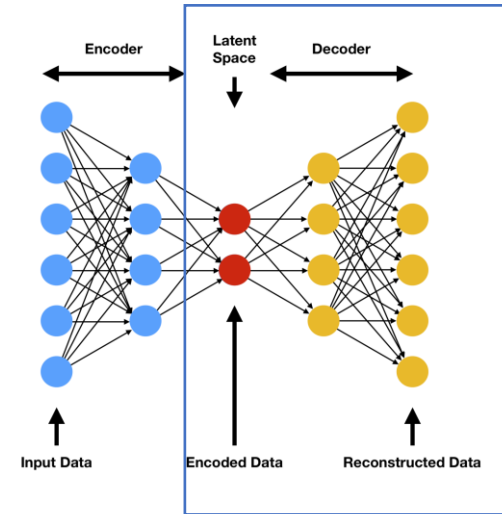
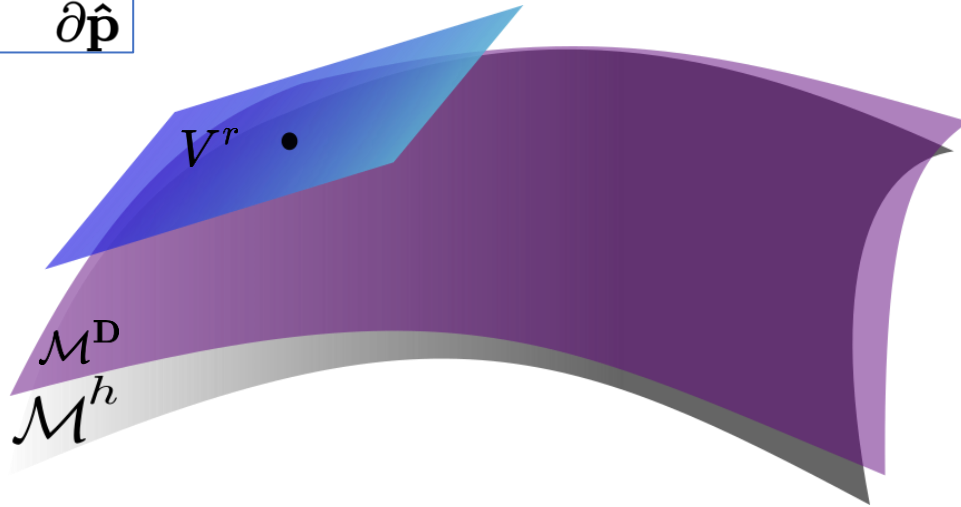


# Manifold: Neural Networks (Non-linear)

$$\mathcal{M}^h = \{\mathbf{u}(\boldsymbol{\mu}) \mid \boldsymbol{\mu} \in \mathcal{P}\} \subset \mathbb{R}^N$$

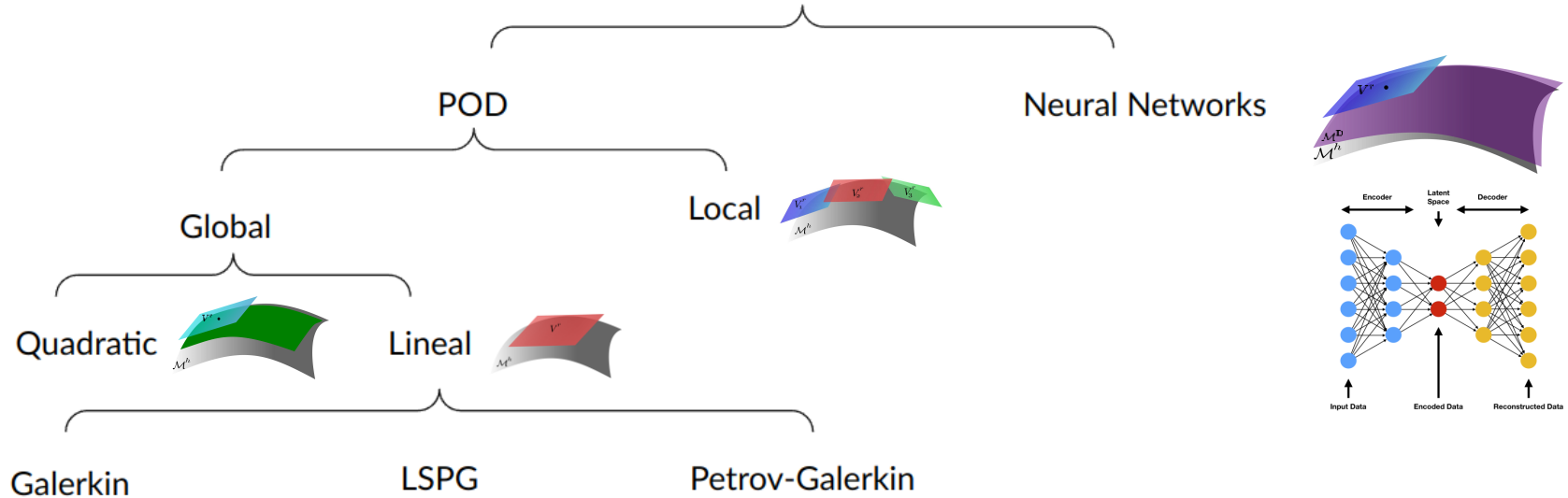
$$\tilde{\mathbf{u}} \approx \mathbf{D}(\hat{\mathbf{p}}) = \mathcal{NN}(\hat{\mathbf{p}})$$

$$V^r := \frac{\partial \mathbf{D}}{\partial \hat{\mathbf{p}}}$$



# Summary

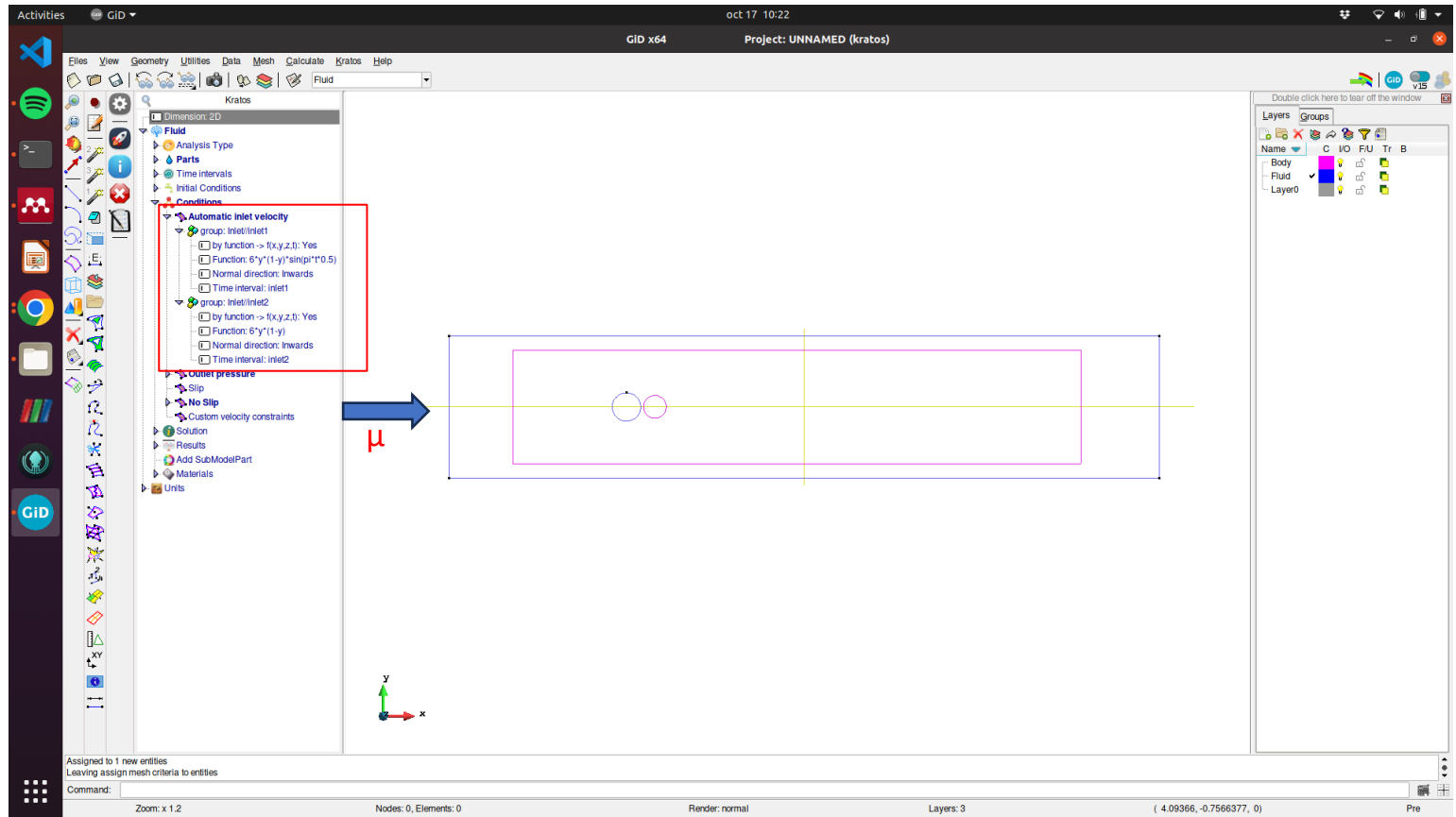
$$\tilde{\mathbf{u}} \approx \mathbf{D}(\hat{\mathbf{p}})$$





**DEMO**

<https://shorturl.at/fxABR>

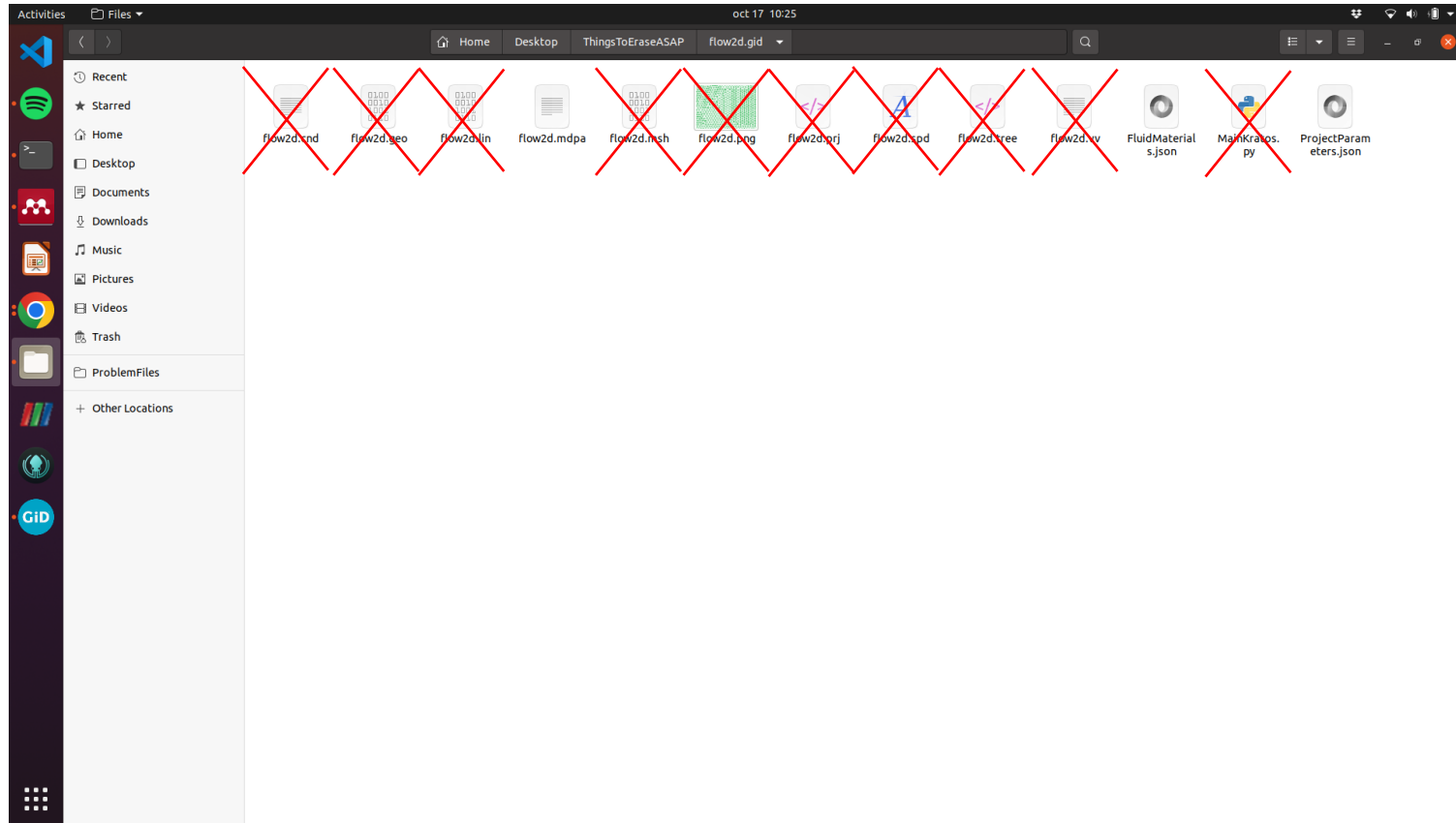


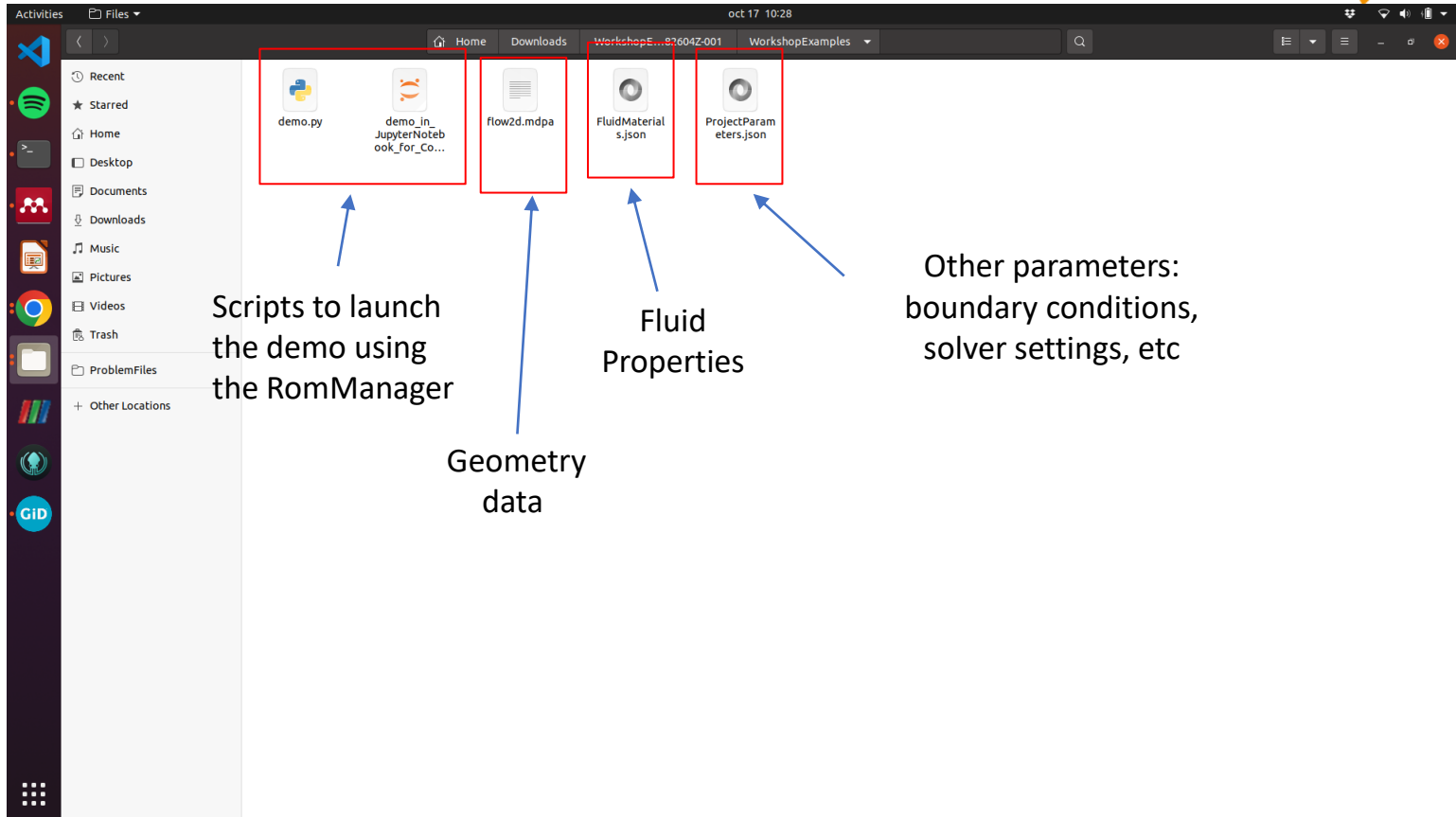
The screenshot displays the Kratos software interface for a 2D fluid simulation. The left sidebar shows a tree view of the simulation setup, with the 'Automatic inlet velocity' group highlighted in a red box. A blue arrow points from this group to a central diagram of a rectangular domain with two circular inlets. The bottom status bar shows 'Nodes: 0, Elements: 0'.

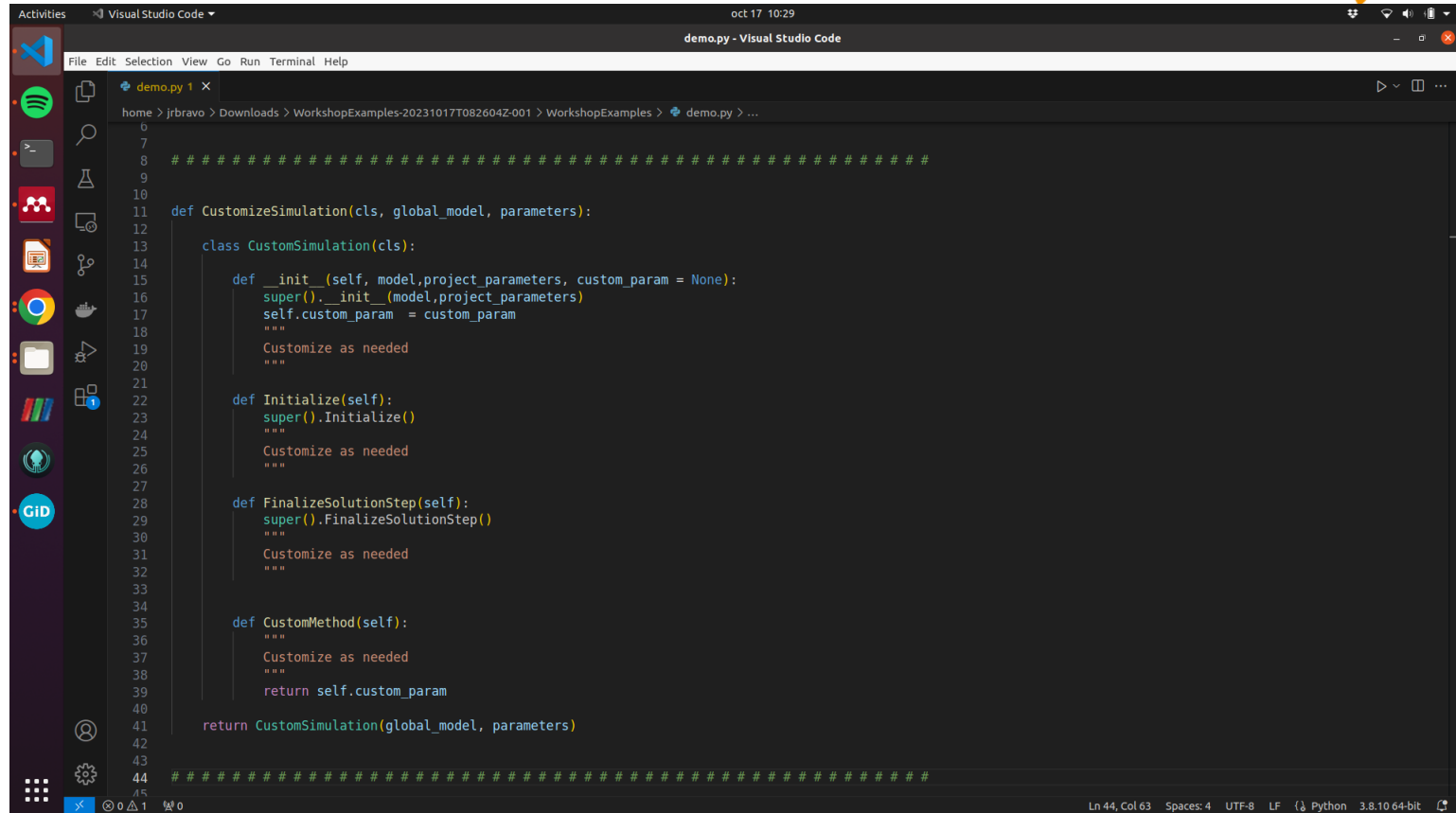
**Tree View Structure:**

- Dimension: 2D
  - Fluid
    - Analysis Type
    - Parts
    - Time Intervals
    - Initial Conditions
    - Conditions
      - Automatic inlet velocity (highlighted)
        - group: Inlet/Inlet1
          - by function -> f(x,y,z,t): Yes
          - Function:  $6 \cdot y \cdot (1 - y) \cdot \sin(\pi \cdot t \cdot 0.5)$
          - Normal direction: Inwards
          - Time interval: inlet1
        - group: Inlet/Inlet2
          - by function -> f(x,y,z,t): Yes
          - Function:  $6 \cdot y \cdot (1 - y)$
          - Normal direction: Inwards
          - Time interval: inlet2
      - Outer pressure
      - Slip
      - No Slip
      - Custom velocity constraints
    - Solution
    - Results
    - Add SubModelPart
    - Materials
    - Units

**Status Bar:** Nodes: 0, Elements: 0







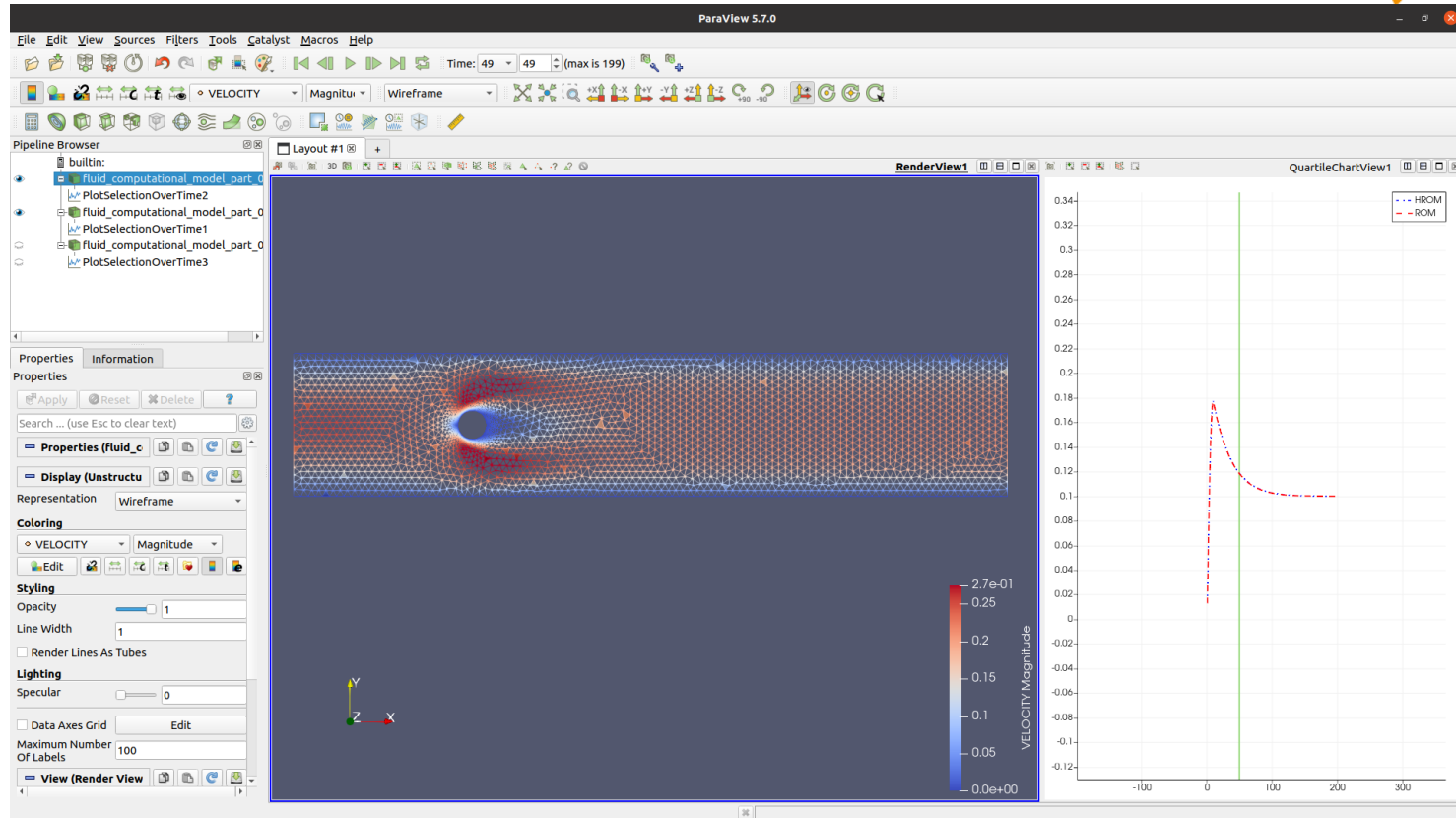
```
home > jrbravo > Downloads > WorkshopExamples-20231017T082604Z-001 > WorkshopExamples > demo.py > ...
6
7
8 #####
9
10
11 def CustomizeSimulation(cls, global_model, parameters):
12
13     class CustomSimulation(cls):
14
15         def __init__(self, model, project_parameters, custom_param = None):
16             super().__init__(model, project_parameters)
17             self.custom_param = custom_param
18             """
19             Customize as needed
20             """
21
22         def Initialize(self):
23             super().Initialize()
24             """
25             Customize as needed
26             """
27
28         def FinalizeSolutionStep(self):
29             super().FinalizeSolutionStep()
30             """
31             Customize as needed
32             """
33
34         def CustomMethod(self):
35             """
36             Customize as needed
37             """
38             return self.custom_param
39
40     return CustomSimulation(global_model, parameters)
41
42
43
44 #####
45
```



```
Activities Visual Studio Code oct 17 10:29 demo.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
demo.py 1 X
home > jbravo > Downloads > WorkshopExamples-20231017T082604Z-001 > WorkshopExamples > demo.py > ...
35     def CustomMethod(self):
36         """
37         Customize as needed
38         """
39         return self.custom_param
40
41     return CustomSimulation(global_model, parameters)
42
43
44     #####
45
46     def UpdateProjectParameters(parameters, mu=None):
47         """
48         Customize ProjectParameters here for imposing different conditions to the simulations as needed
49         """
50         parameters["processes"]["boundary_conditions_process_list"][0]["Parameters"]["modulus"].SetString(f"{str(mu[0])}*y*(1-y)*sin(pi*t*0.5)")
51         parameters["processes"]["boundary_conditions_process_list"][1]["Parameters"]["modulus"].SetString(f"{str(mu[0])}*y*(1-y)")
52
53
54         return parameters
55
56     #####
57
58     def UpdateMaterialParametersFile(material_params_file_name, mu):
59         pass
60         # with open(material_params_file_name, mode="r+") as f:
61         #     data = json.load(f)
62         #     #change the angles of 1st and 2nd layer
63         #     data["properties"][0]["Material"]["Variables"]["EULER_ANGLES"][0] = mu[0]
64         #     data["properties"][1]["Material"]["Variables"]["EULER_ANGLES"][0] = mu[1]
65         #     #write to file and save file
66         #     f.seek(0)
67         #     json.dump(data, f, indent=4)
68         #     f.truncate()
69
70     #####
71
72
73
74     def GetRomManagerParametersEvam1a1():
```

```
Activities Visual Studio Code oct 17 10:30 demo.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
demo.py 1 x
home > jrbravo > Downloads > WorkshopExamples-20231017T082604Z-001 > WorkshopExamples > demo.py > ...
162         "create_hrom_visualization_model_part" : false,
163         "echo_level" : 0
164     }
165 }
166
167     return general_rom_manager_parameters
168
169
170     #####
171
172
173
174
175
176
177 def Example1():
178     mu_train = [[1]] #[param1, param2, ..., param_p] #list of lists containing values of the parameters to use in POD
179
180     general_rom_manager_parameters = GetRomManagerParametersExample1()
181     project_parameters_name = "ProjectParameters.json"
182
183     rom_manager = RomManager(project_parameters_name,general_rom_manager_parameters,CustomizeSimulation,UpdateProjectParameters,UpdateMaterialParametersFile)
184
185     """if no list "mu" is passed, the case already contained in the ProjectParameters and CustomSimulation is launched (useful for example for a single time dependent sim
186     rom_manager.Fit(mu_train)
187     rom_manager.RunHROM(mu_train)
188     rom_manager.PrintErrors()
189
190
191
192
193
194 def Example2():
195     mu_train = [[4],[6]]#train parameters
196     mu_test = [[5],[7]] #test parameters
197
198     general_rom_manager_parameters = GetRomManagerParametersExample2()
199     project_parameters_name = "ProjectParameters.json"
200
Ln 44, Col 63 Spaces: 4 UTF-8 LF Python 3.8.10 64-bit
```

```
Activities Visual Studio Code oct 17 10:30
demo.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
demo.py 1 X
home > jrbravo > Downloads > WorkshopExamples-20231017T082604Z-001 > WorkshopExamples > demo.py > ...
72
73
74 def GetRomManagerParametersExample1():
75     """
76     This function allows to easily modify all the parameters for the ROM simulation.
77     The returned KratosParameter object is seamlessly used inside the RomManager.
78     """
79
80     general_rom_manager_parameters = KratosMultiphysics.Parameters("""{
81         "rom_stages_to_train" : ["ROM", "HROM"], // ["ROM", "HROM"]
82         "rom_stages_to_test" : [], // ["ROM", "HROM"]
83         "parallelism" : null, // null, TODO: add "compps"
84         "projection_strategy": "galerkin", // "lspg", "galerkin", "petrov_galerkin"
85         "assembling_strategy": "elemental", // "global", "elemental"
86         "save_gid_output": false, // false, true #if true, it must exists previously in the ProjectParameters.json
87         "save_vtk_output": true, // false, true #if true, it must exists previously in the ProjectParameters.json
88         "output_name": "id", // "id", "mu"
89         "ROM":{
90             "svd_truncation_tolerance": 1e-2,
91             "model_part_name": "FluidModelPart", // This changes depending on the simulation: Structure, FluidModelPart, ThermalPart #TODO: Identify it automatically
92             "nodal_unknowns": ["VELOCITY_X", "VELOCITY_Y", "PRESSURE"], // Main unknowns. Snapshots are taken from these
93             "rom_basis_output_format": "numpy",
94             "rom_basis_output_name": "RomParameters",
95             "rom_basis_output_folder": "rom_data",
96             "snapshots_control_type": "step", // "step", "time"
97             "snapshots_interval": 1,
98             "galerkin_rom_bns_settings": {
99                 "monotonicity_preserving": false
100             },
101             "lspg_rom_bns_settings": {
102                 "train_petrov_galerkin": false,
103                 "basis_strategy": "residuals", // 'residuals', 'jacobian'
104                 "include_phi": false,
105                 "svd_truncation_tolerance": 1e-6,
106                 "solving_technique": "normal equations", // 'normal equations', 'qr_decomposition'
107                 "monotonicity_preserving": false
108             }
109         },
110         "HROM":{
111             "element_selection_type": "empirical_cubature",
112             "element_selection_svd_truncation_tolerance": 1e-4,
113             "create_hrom_visualization_model_part" : true,
114             "echo_level" : 0
115         }
116     }""")
117
118     return general_rom_manager_parameters
119
```



```

Activities Visual Studio Code oct 17 10:30 demo.py - Visual Studio Code
File Edit Selection View Go Run Terminal Help
demo.py 1 x
home > jbravo > Downloads > WorkshopExamples-20231017T082604Z-001 > WorkshopExamples > demo.py > ...
177 def Example1():
178     mu_train = [[1]] #[param1, param2, ..., param_p] #list of lists containing values of the parameters to use in POD
179
180     general_rom_manager_parameters = GetRomManagerParametersExample1()
181     project_parameters_name = "ProjectParameters.json"
182
183     rom_manager = RomManager(project_parameters_name,general_rom_manager_parameters,CustomizeSimulation,UpdateProjectParameters,UpdateMaterialParametersFile)
184
185     """if no list "mu" is passed, the case already contained in the ProjectParametes and CustomSimulation is launched (useful for example for a single time dependent sim
186     rom_manager.Fit(mu_train)
187     rom_manager.RunHRROM(mu_train)
188     rom_manager.PrintErrors()
189
190
191
192
193
194 def Example2():
195     mu_train = [[4],[6]]#train parameters
196     mu_test = [[5],[7]] #test parameters
197
198     general_rom_manager_parameters = GetRomManagerParametersExample2()
199     project_parameters_name = "ProjectParameters.json"
200
201     rom_manager = RomManager(project_parameters_name,general_rom_manager_parameters,CustomizeSimulation,UpdateProjectParameters,UpdateMaterialParametersFile)
202
203     """if no list "mu" is passed, the case already contained in the ProjectParametes and CustomSimulation is launched (useful for example for a single time dependent sim
204     rom_manager.Fit(mu_train)
205     rom_manager.Test(mu_test)
206     rom_manager.PrintErrors()
207
208
209
210
211 if __name__ == "__main__":
212     #Example1()
213     Example2()
214
215
216
Ln 44, Col 63 Spaces: 4 UTF-8 LF Python 3.8.10 64-bit

```

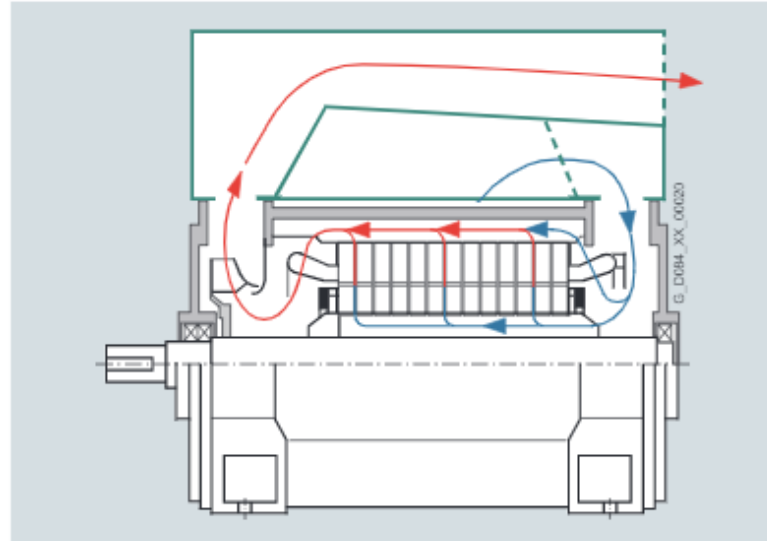


# EFLWS4HPC USE CASE





Simotics H compact PLUS



Schematic airflow

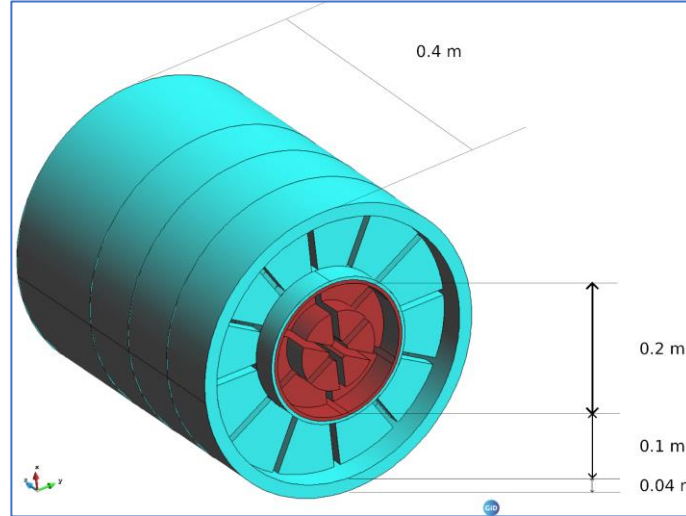




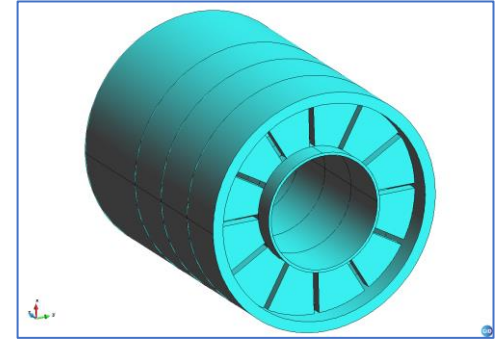
# Model Definition



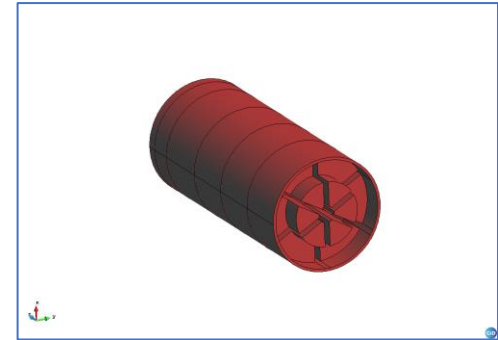
Simotics H compact PLUS



10 million elements

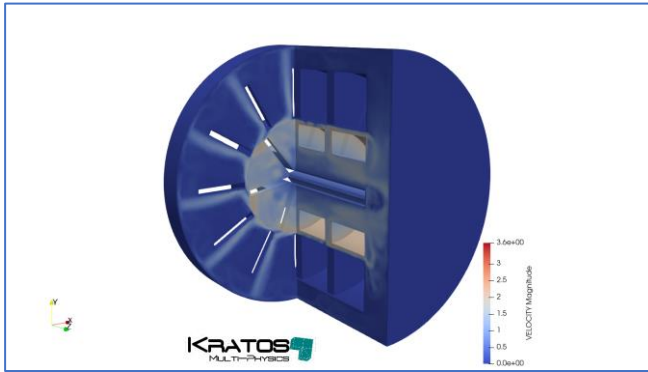


Stator

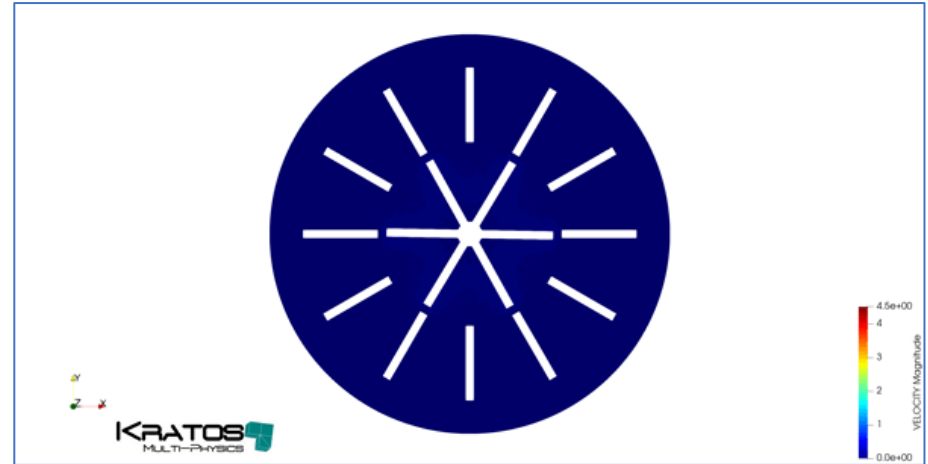
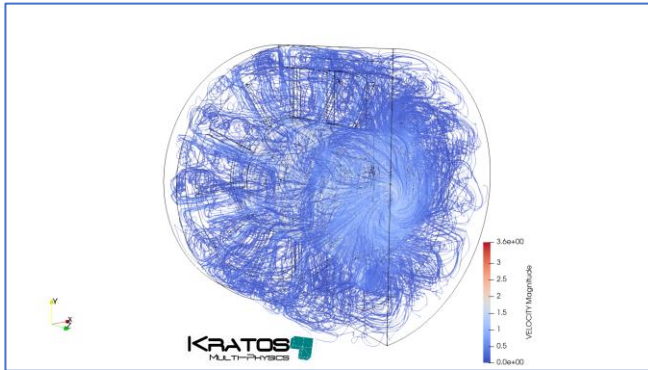


Rotor

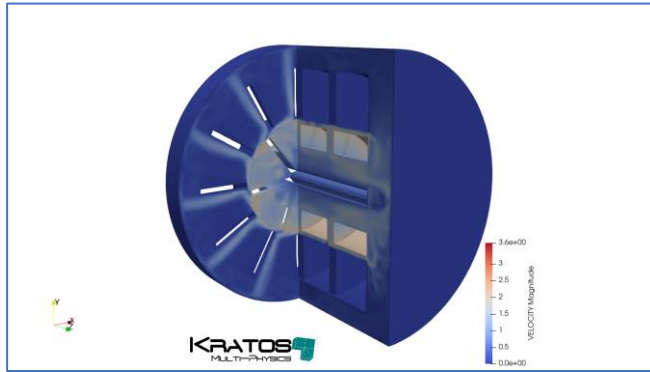
# Convection Using Navier-Stokes



Snapshot of Velocity Contour Field with Sliding Mesh (t=4 sec).



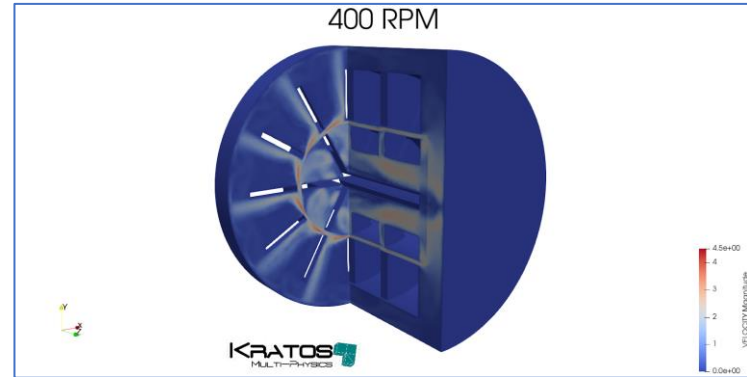
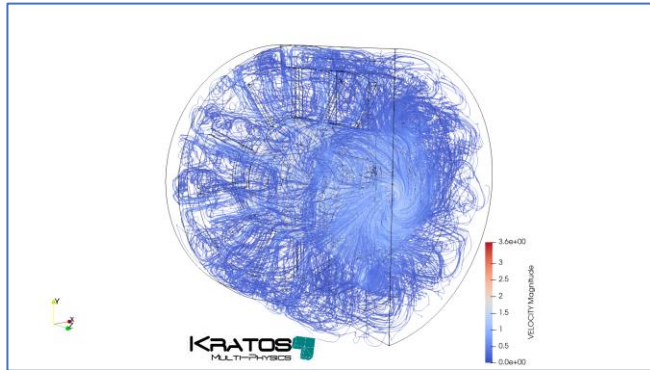
# Convection Using Navier-Stokes



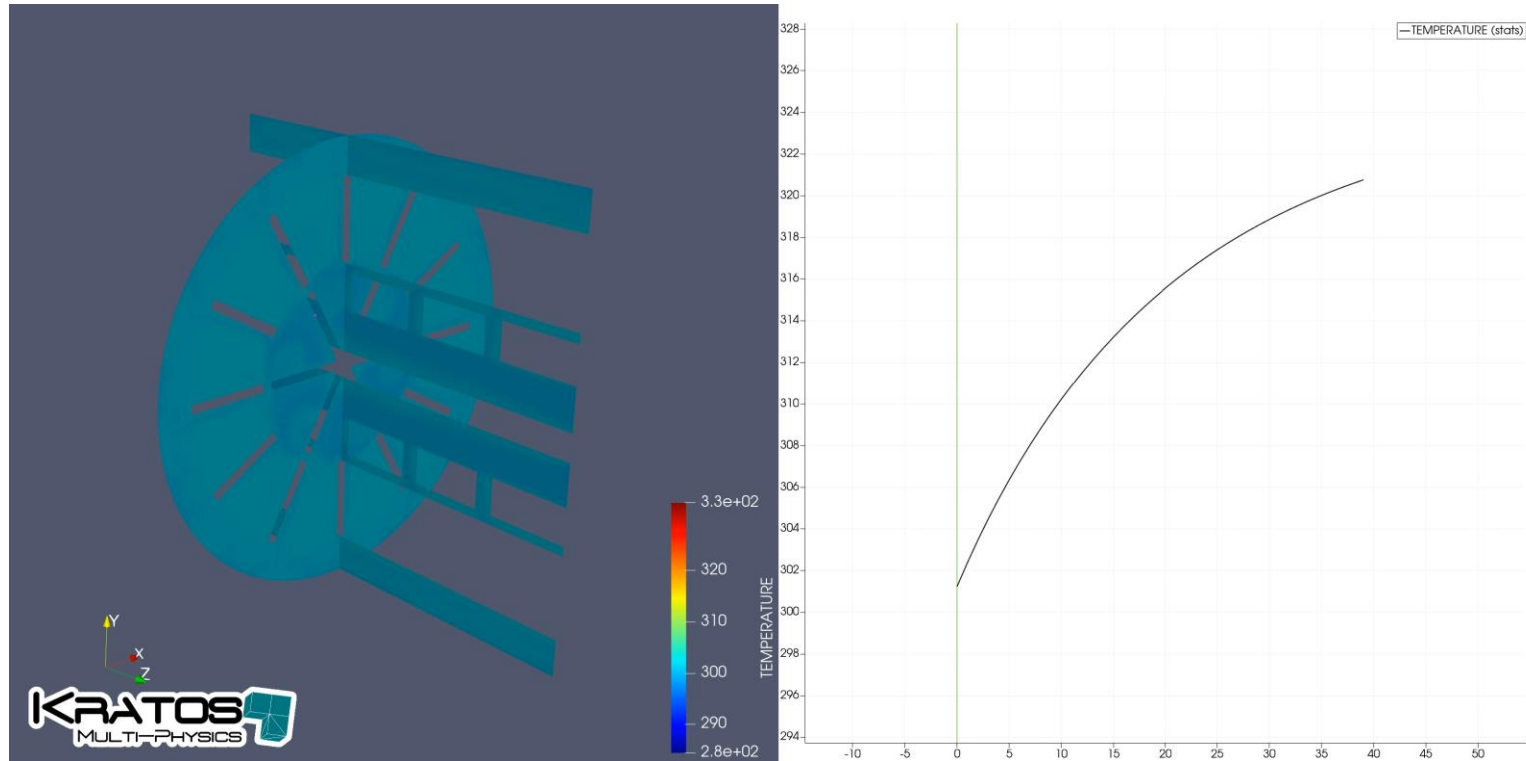
Snapshot of Velocity Contour Field with Sliding Mesh (t=4 sec).



Relative Temporal Average Velocity for Various RPMs (Mesh Velocity Subtracted).

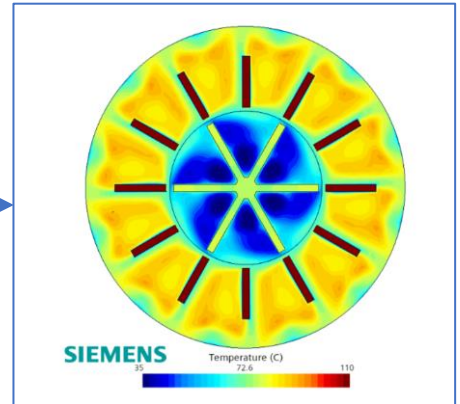
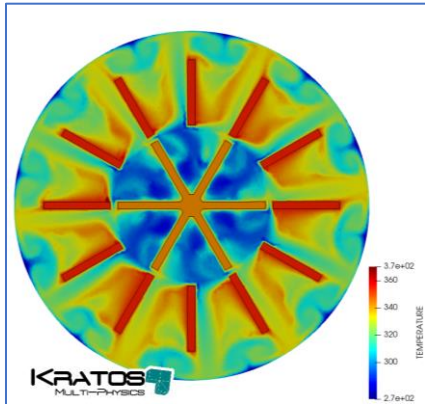
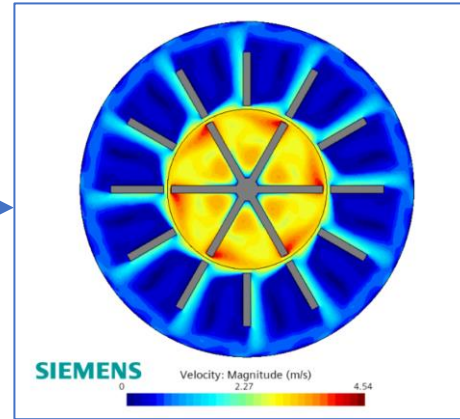
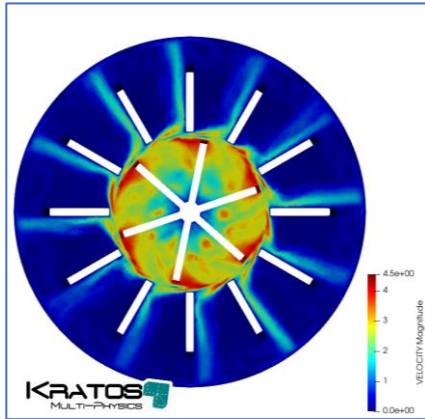


# Thermal solution

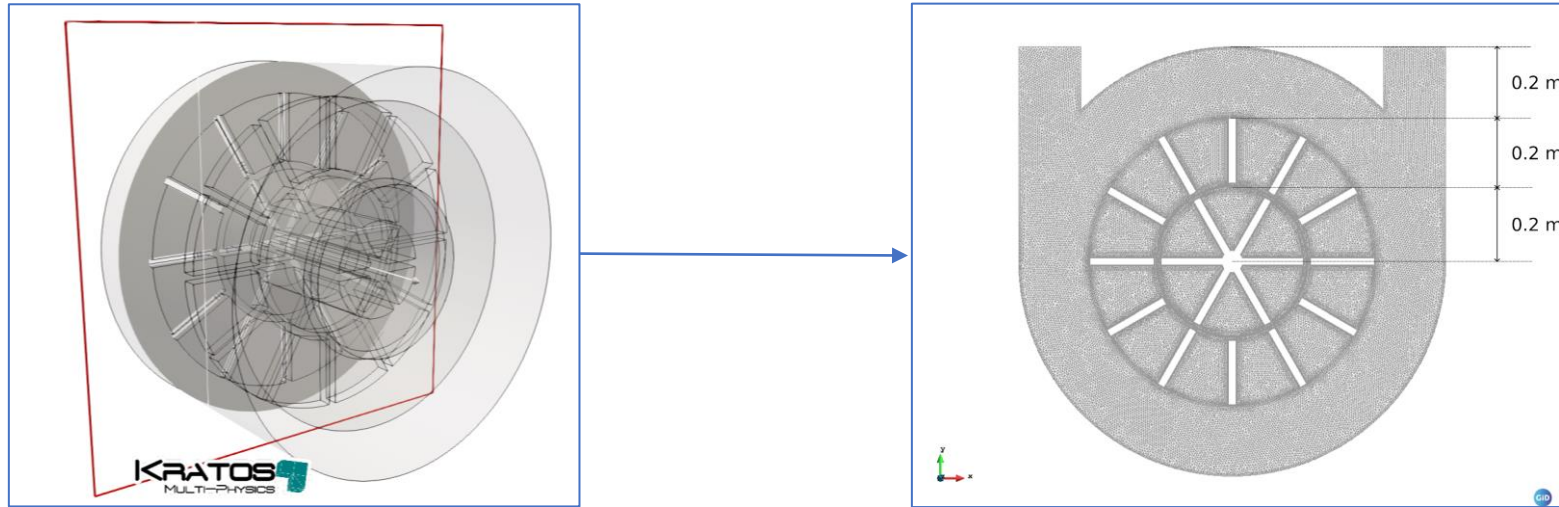


Solution of thermal case.

# Validation

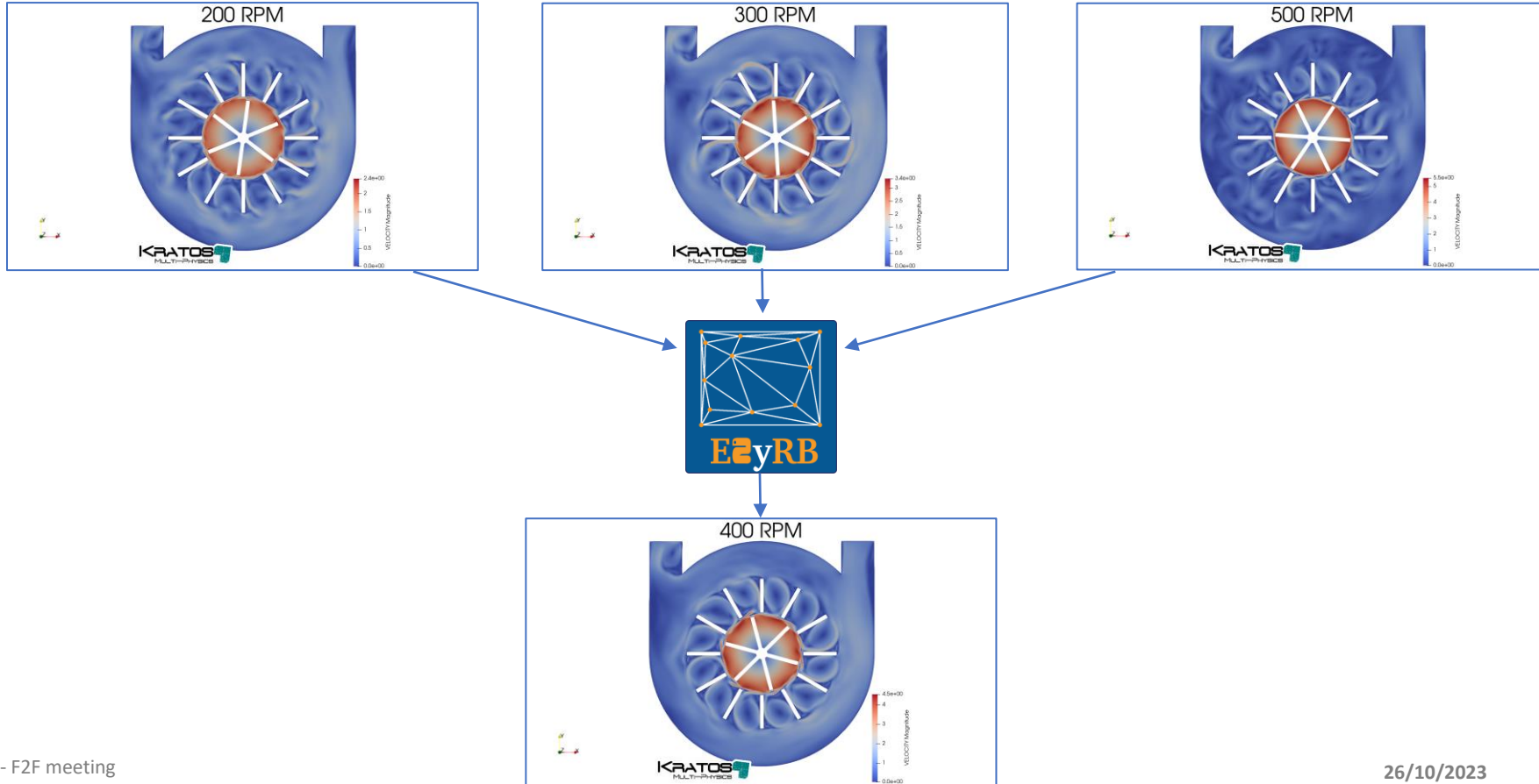


# 2D Demo Case

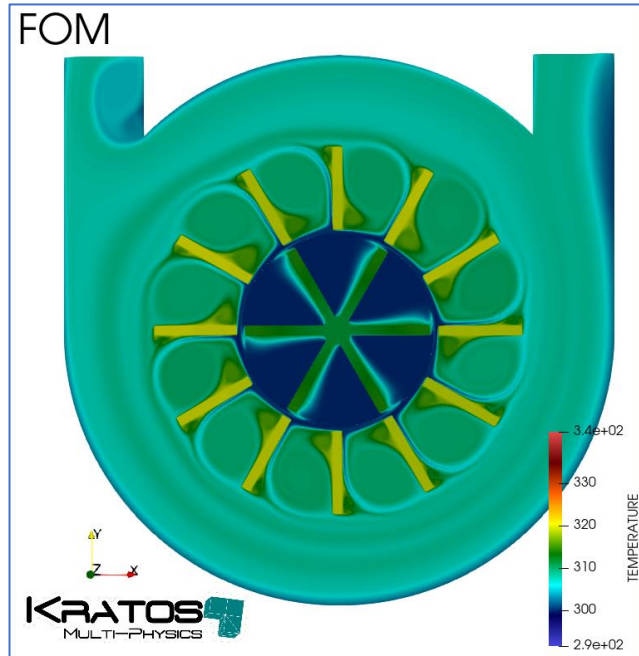


3D cut plane used for building 2D simplification.

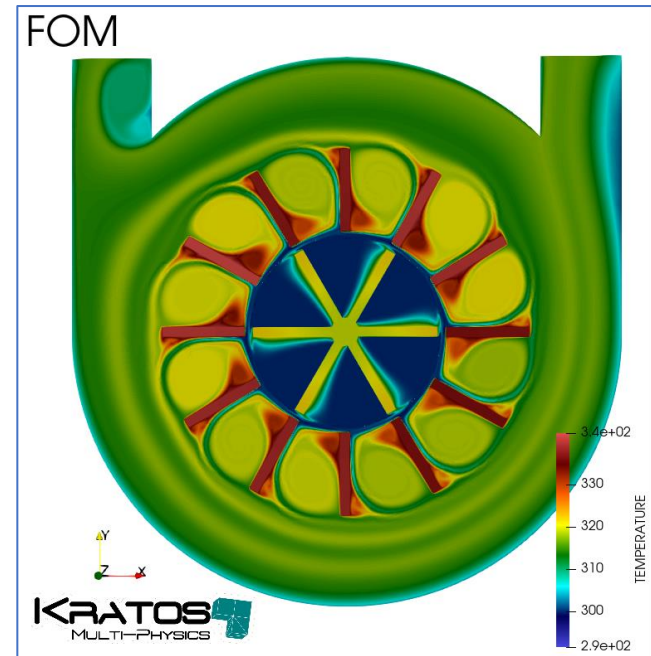
# Convection Interpolation using EZyRB



# Thermal solution



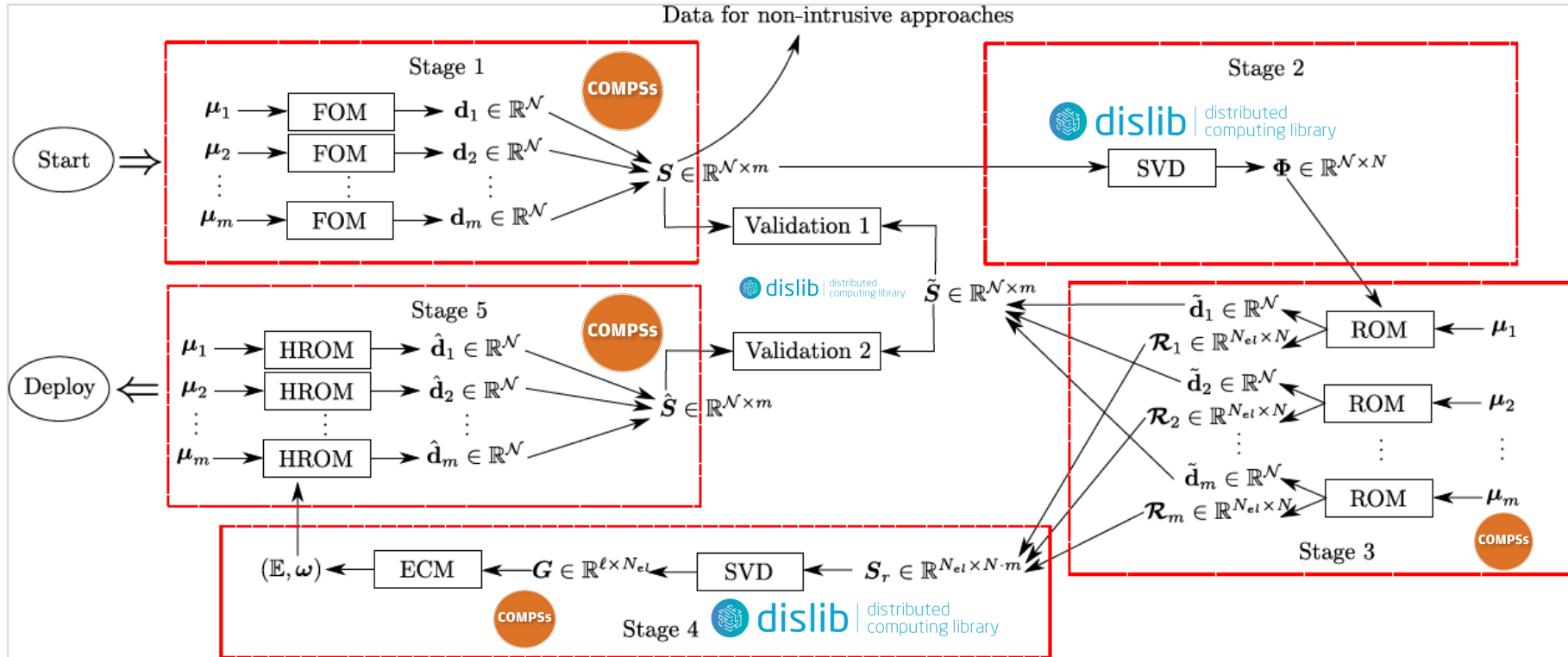
Temperature Field at 4200 secs for 200 RPM.



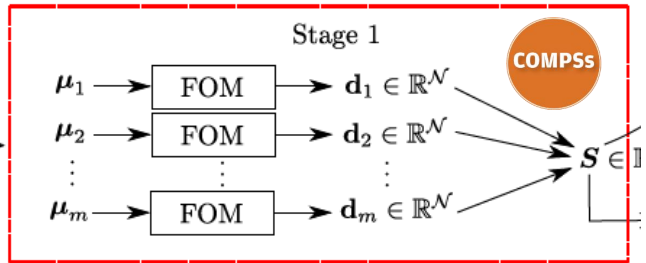
Temperature Field at 4200 secs for 400 RPM.



# High-Performance Computing: Parallel Workflow



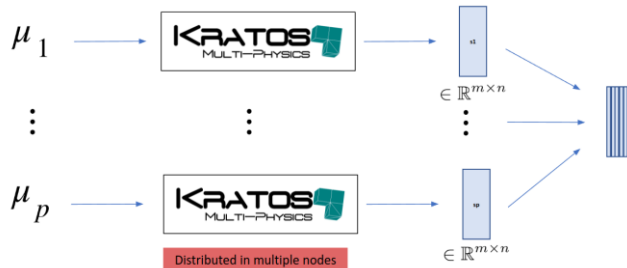
# High-Performance Computing: Decorator



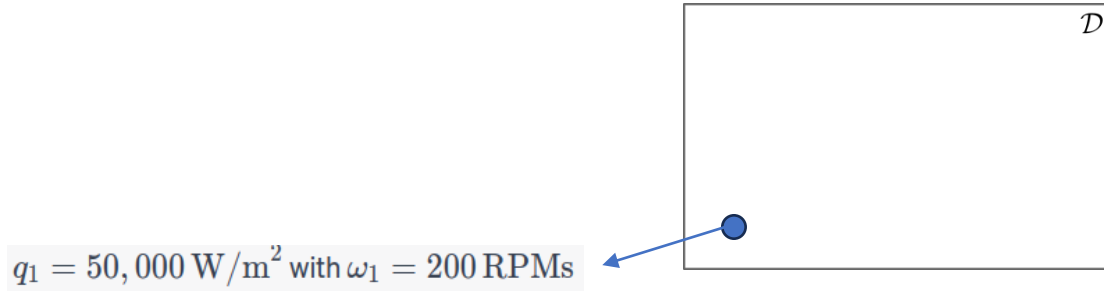
```
@constraint(computingUnits=argv[2])
```

```
@task(returns = 3)
```

```
def ExecuteInstance_Task(pickled_parameters,Cases,instance, path):  
    # overwrite the old parameters serializer with the unpickled one  
    serialized_parameters = pickle.loads(pickled_parameters)  
    current_parameters = KratosMultiphysics.Parameters()  
    serialized_parameters.Load("ParametersSerialization",current_parameters)  
    del(serialized_parameters)  
    # get sample  
    sample = GetValueFromListList(Cases,instance) # take one of them  
    simulation = TrainROM(current_parameters,sample,path)  
    simulation.Run()  
    snapshots = simulation.GetSnapshotsMatrices()  
    control_point_matrix = simulation.GetSolutionsAtControlPoint()  
    return snapshots[0], snapshots[1], control_point_matrix
```

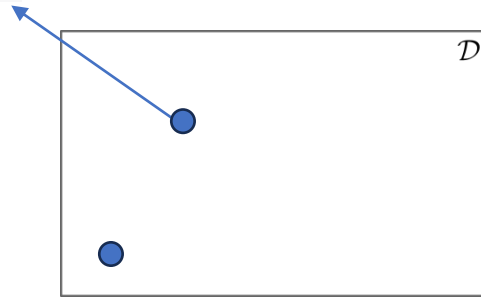


# Convection-Diffusion Parameters



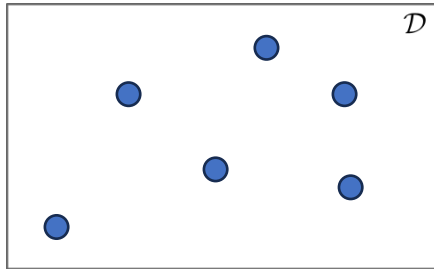
# Convection-Diffusion Parameters

$q_2 = 62,500 \text{ W/m}^2$  with  $\omega_2 = 250 \text{ RPMs}$



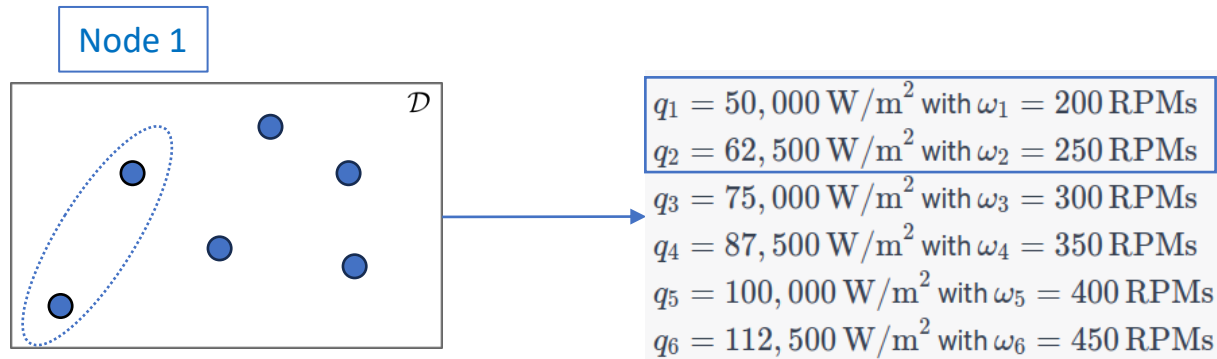
$q_1 = 50,000 \text{ W/m}^2$  with  $\omega_1 = 200 \text{ RPMs}$

# Convection-Diffusion Parameters

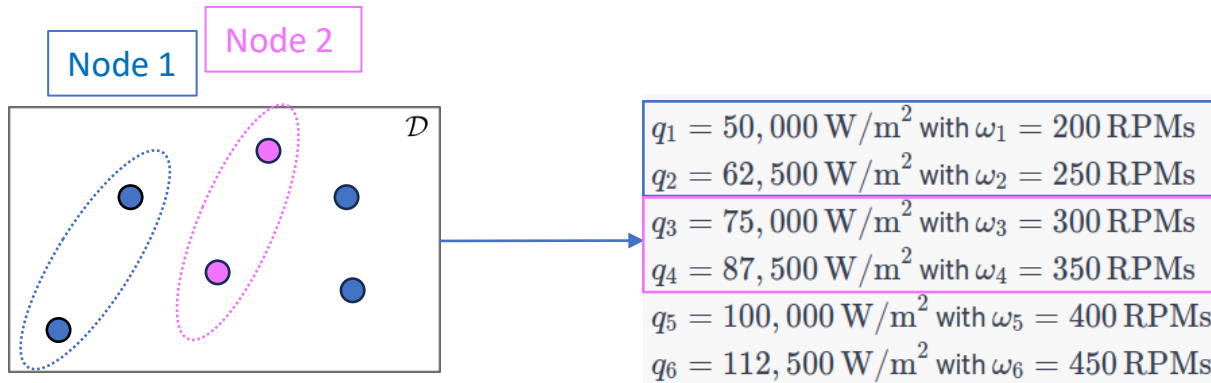


- $q_1 = 50,000 \text{ W/m}^2$  with  $\omega_1 = 200 \text{ RPMs}$
- $q_2 = 62,500 \text{ W/m}^2$  with  $\omega_2 = 250 \text{ RPMs}$
- $q_3 = 75,000 \text{ W/m}^2$  with  $\omega_3 = 300 \text{ RPMs}$
- $q_4 = 87,500 \text{ W/m}^2$  with  $\omega_4 = 350 \text{ RPMs}$
- $q_5 = 100,000 \text{ W/m}^2$  with  $\omega_5 = 400 \text{ RPMs}$
- $q_6 = 112,500 \text{ W/m}^2$  with  $\omega_6 = 450 \text{ RPMs}$

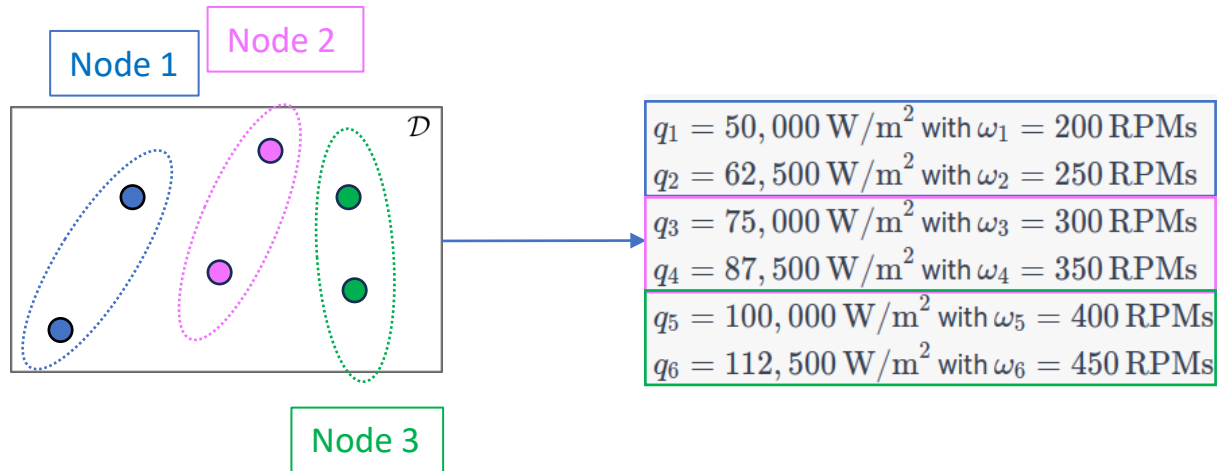
# Convection-Diffusion Parameters: Parallel Simulations



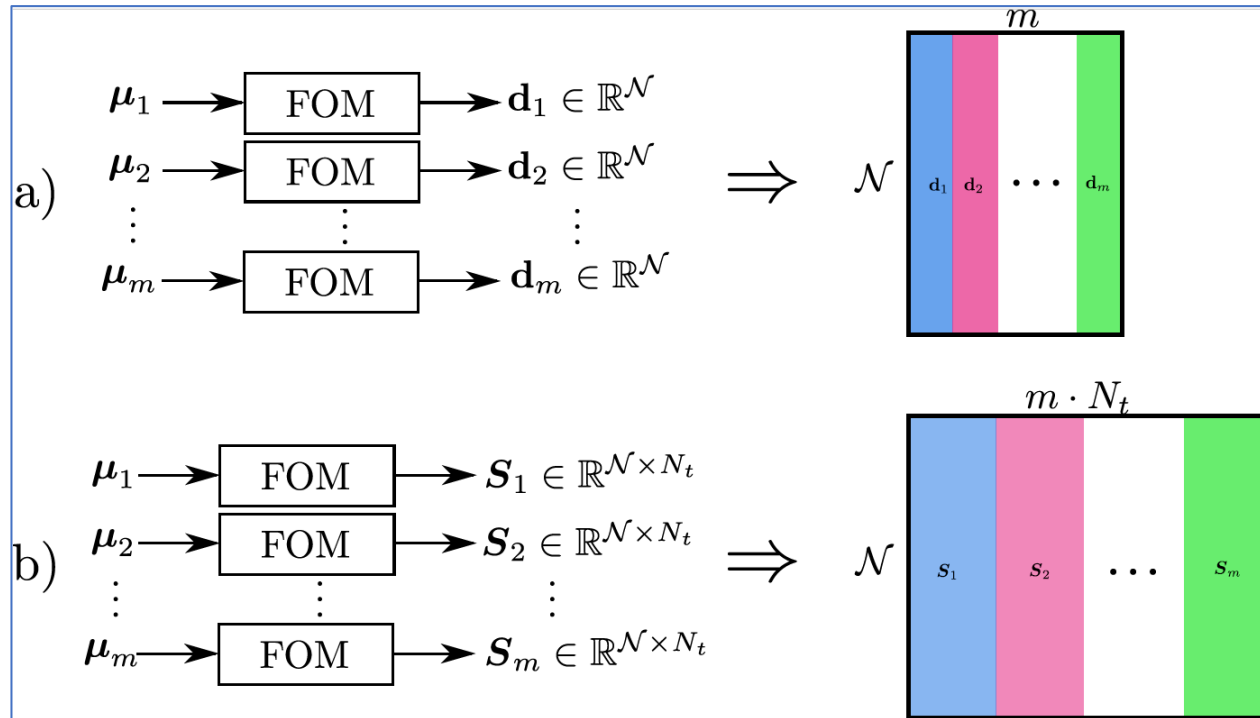
# Convection-Diffusion Parameters: Parallel Simulations



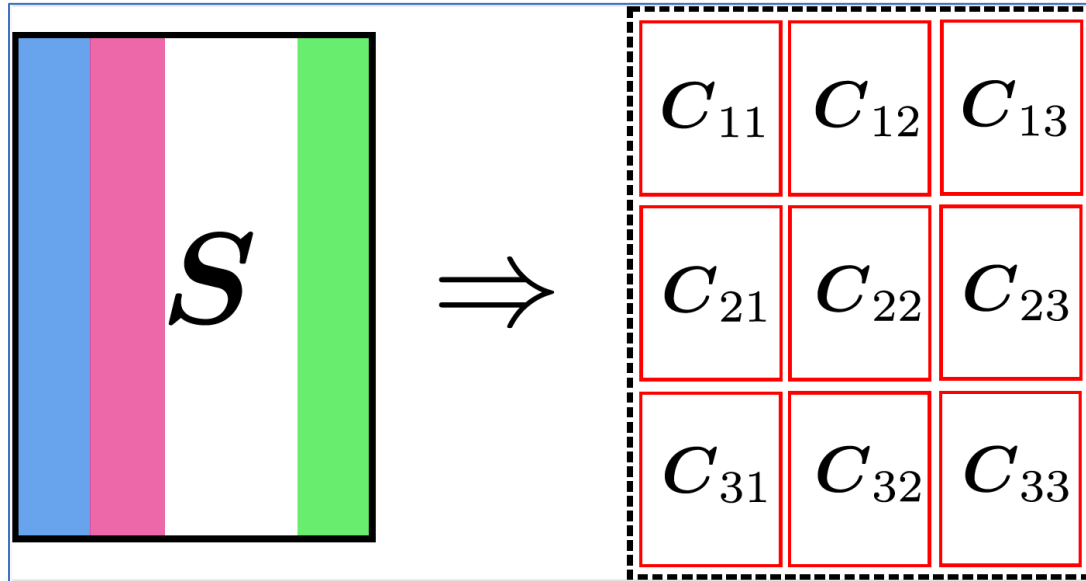
# Convection-Diffusion Parameters: Parallel Simulations



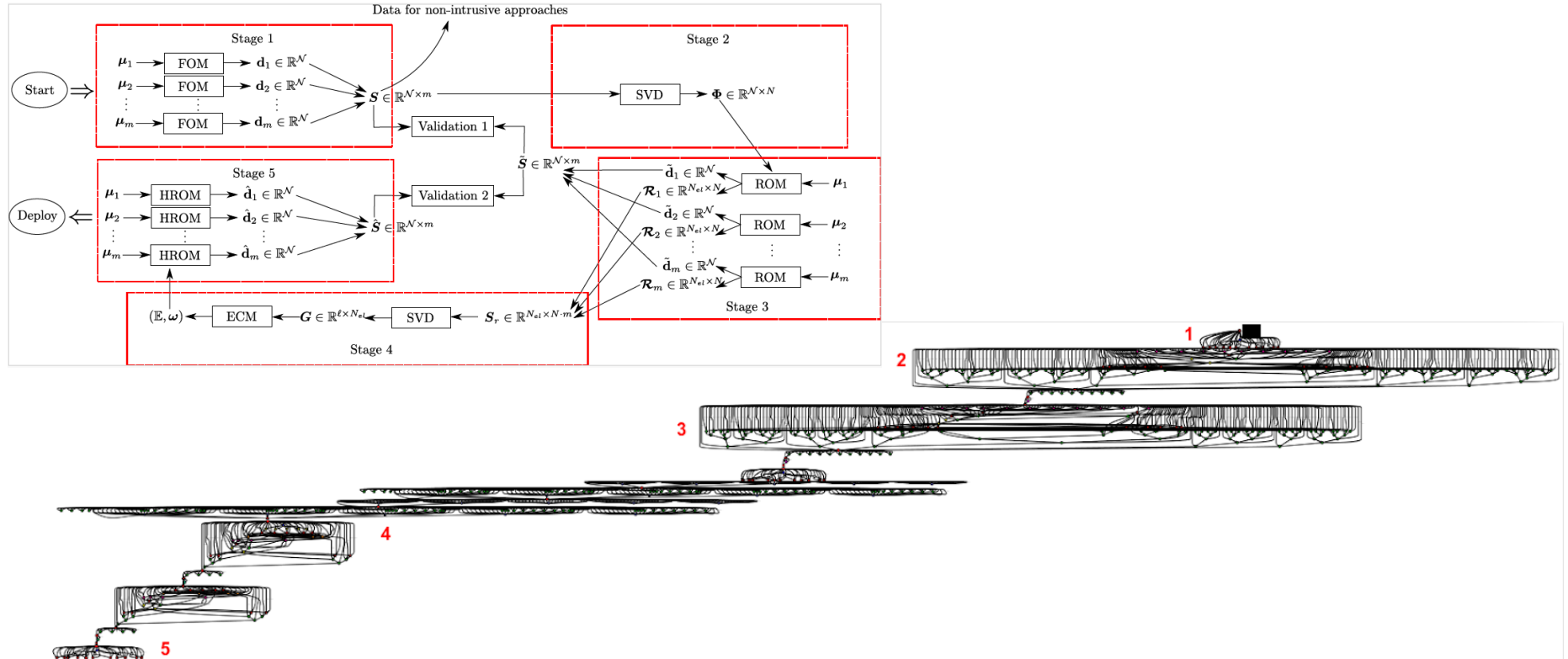




# High-Performance Computing: Parallel SVD (Tall and Skinny QR)

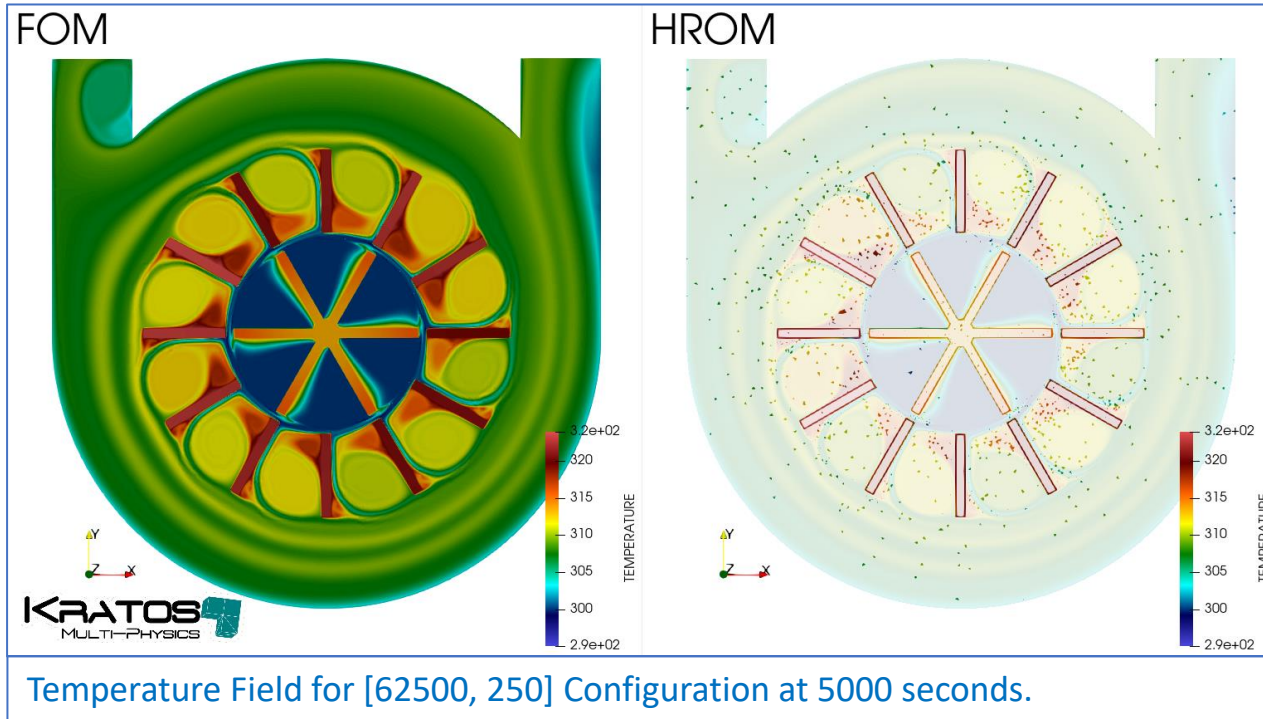


# High-Performance Computing: Graph

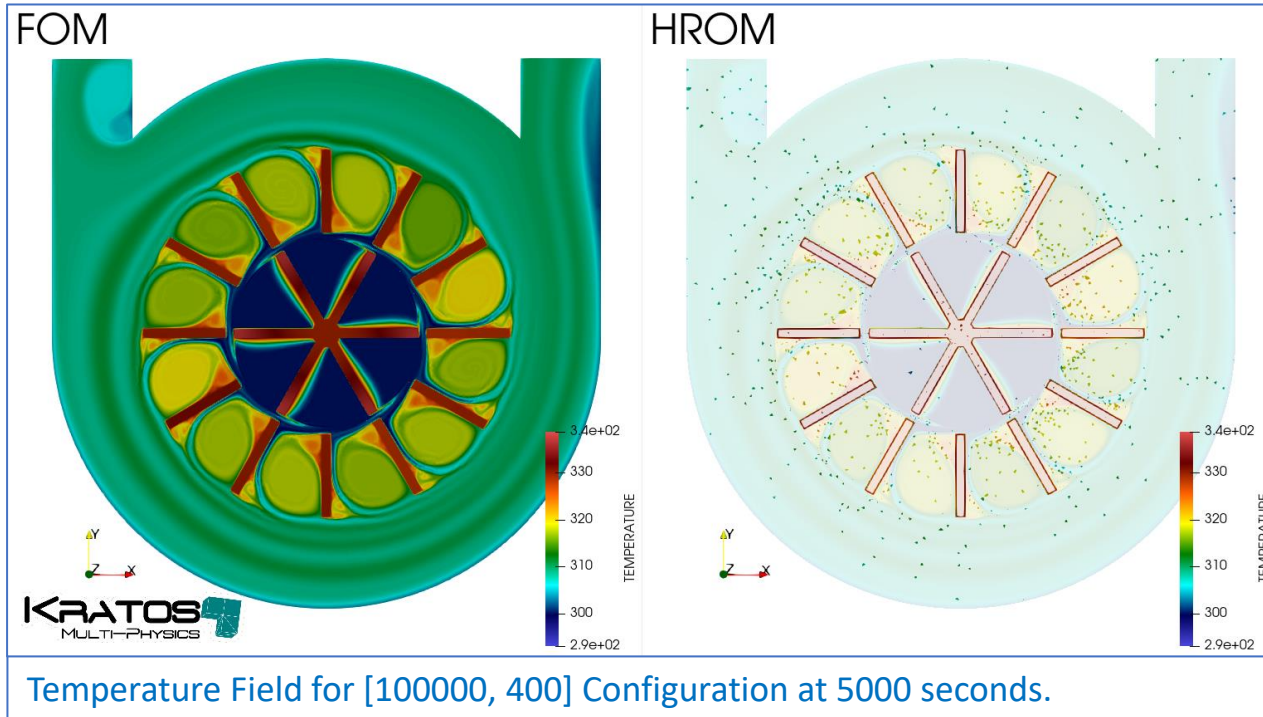


Graph of the Workflow execution using the Co-Simulation Example

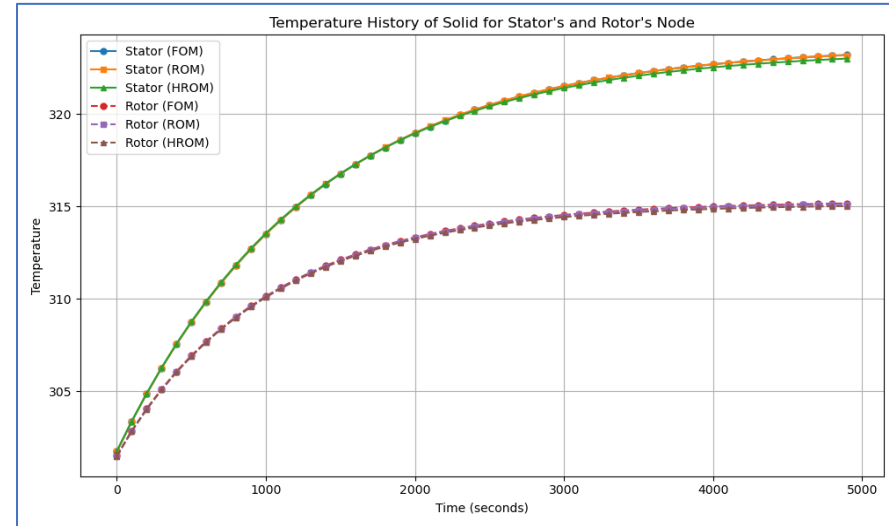
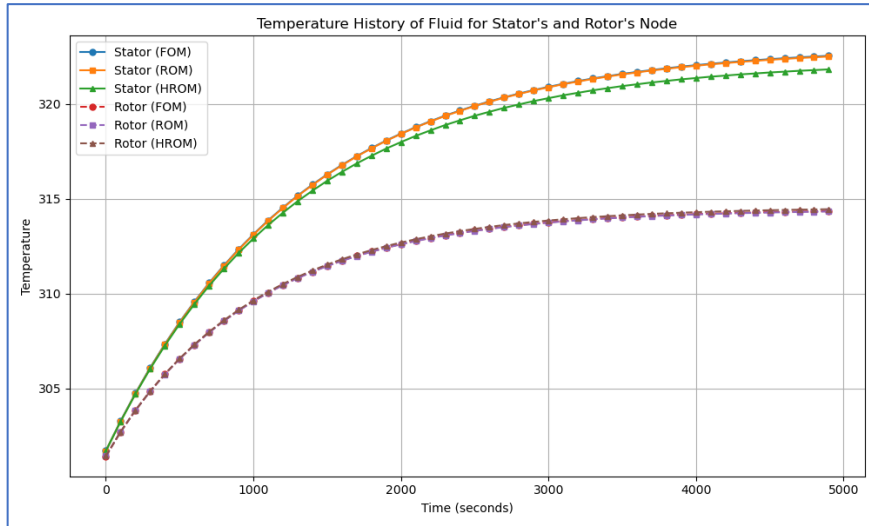
# High-Performance Computing: Demo Results



# High-Performance Computing: Demo Results



# High-Performance Computing: Demo Results



Fluid and Solid Control Point Response for [62500, 250] Configuration at 5000 seconds.

# High-Performance Computing: Speed-ups

Model	Construction (Solid)	Solving + Projection (Solid)	Total (Solid)	Construction (Fluid)	Solving + Projection (Fluid)	Total (Fluid)
ROM	0.72	22.25	3.05	0.84	62.69	6.41
HROM	1.13	24.19	4.56	2.01	59.96	13.52
HHROM	1.54	38.52	6.37	5.57	260.80	40.39

Speed-ups for Configuration 1 (RPM of 250 and heat flux of 62500 W/m<sup>3</sup>)

Model	Construction (Solid)	Solving + Projection (Solid)	Total (Solid)	Construction (Fluid)	Solving + Projection (Fluid)	Total (Fluid)
ROM	0.71	21.74	3.03	0.86	64.42	6.61
HROM	1.15	24.56	4.72	2.10	62.13	14.10
HHROM	1.56	39.33	6.50	5.84	275.32	42.27

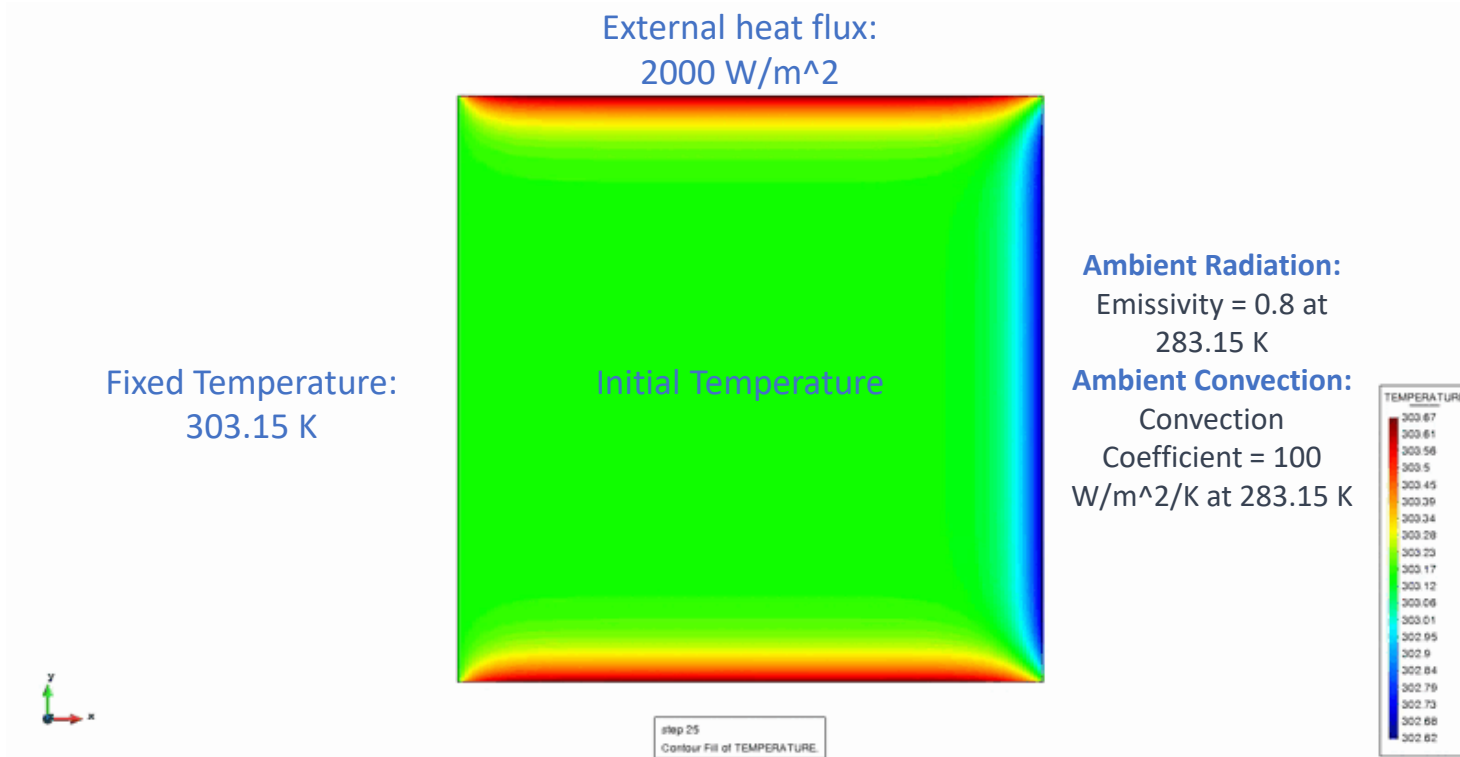
Speed-ups for Configuration 2 (RPM of 400 and heat flux of 100000 W/m<sup>3</sup>)



# HPCWAAS SMALL DEMO

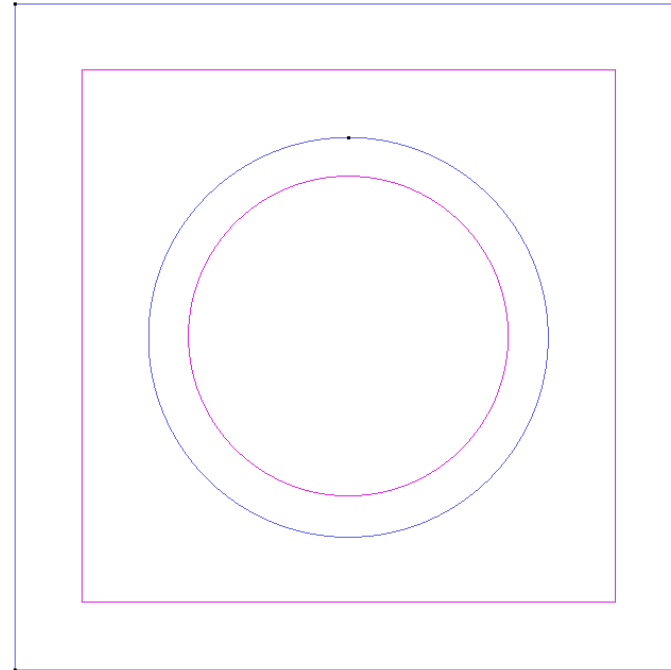


# HPCWaaS: Small Demo







# HPCWaaS: Coupling Different Domains

- Dimension: 2D
- Convection-diffusion
  - Analysis Type
  - Parts
    - group: Body
      - Material type: Convection-diffusion material
      - Material: Gold
      - Density: 19300.0 kg/m<sup>3</sup>
      - Thermal conductivity: 310 W/(m·K)
      - Specific heat: 125.6 J/(kg·K)
    - Time intervals
    - Initial Conditions
      - Temperature
        - group: Body//Initial
          - by function -> f(x,y,z,t): No
          - Value: 303.15 K
    - Conditions
      - External heat flux
        - group: Top\_Wall
        - group: Bottom\_Wall
      - Imposed temperature
        - group: Left\_Wall
      - Thermal face conditions
        - group: Right\_Wall
    - Solution
    - Results
    - Add SubModelPart
      - group: Interface\_outside
        - Write elements: False
        - Write conditions: True
    - Materials
    - Units








# HPCWaaS: Coupling Different Domains









Outer part:

Name
 ConvectionDiffusionMaterials_outside.json
 GUI_test_outside.mdpa
 MainKratos.py
 ProjectParameters_outside.json

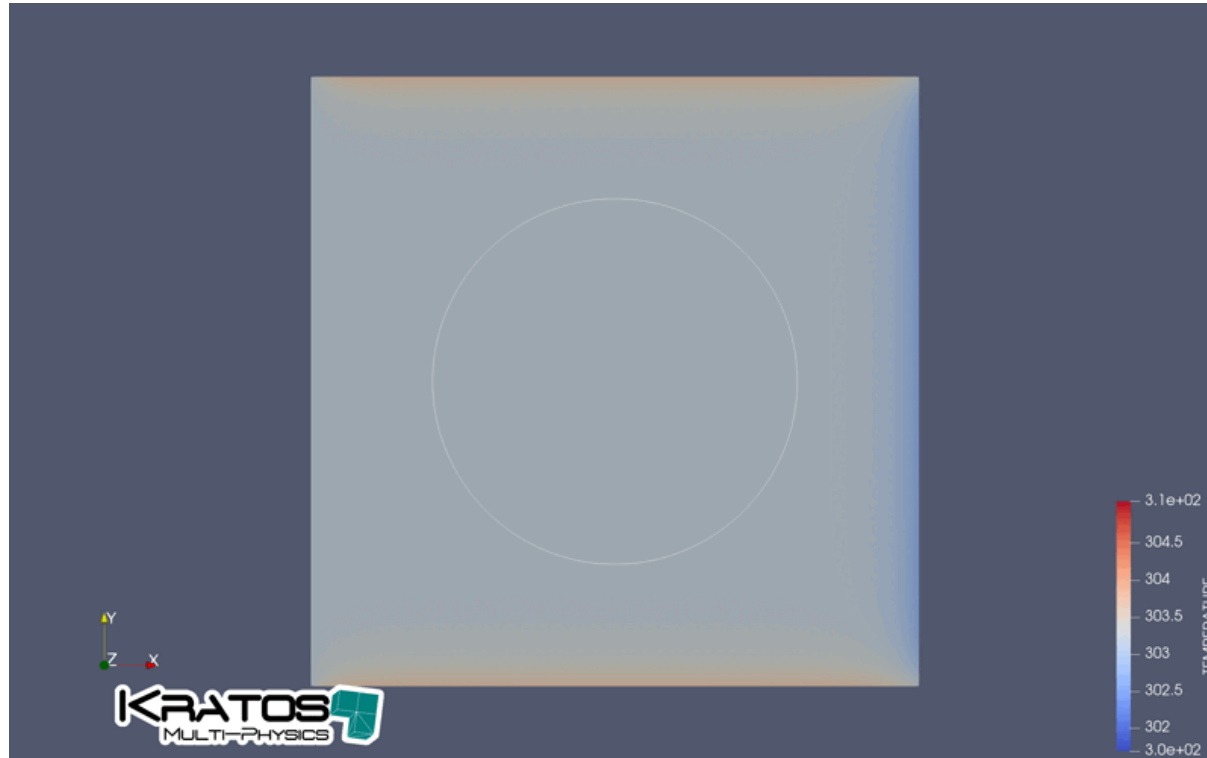
Central part:

Name
 ConvectionDiffusionMaterials_center.json
 GUI_test_center.mdpa
 MainKratos.py
 ProjectParameters_center.json



Name
 ConvectionDiffusionMaterials_center.json
 ConvectionDiffusionMaterials_outside.json
 GUI_test_center.mdpa
 GUI_test_outside.mdpa
 MainKratos.py
 ProjectParameters_center.json
 ProjectParameters_CoSimulation.json
 ProjectParameters_outside.json

# HPCWaaS: Coupling Different Domains



Coupled ROM: Temperature  
Contour Field

# Acknowledgements

The authors acknowledge financial support from the Spanish Ministry of Economy and Competitiveness, through the “Severo Ochoa Programme for Centres of Excellence in R&D” (CEX2018-000797-S)”. We acknowledge financial support from the Generalitat de Catalunya through the FLSDUR-2021 grant, which provided funding for the predoctoral training of Sebastian Ares de Parga Regalado. This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement Nos 955558 and 956104. The JU receives support from the European Union’s Horizon 2020 research and innovation programme and from Spain, Germany, France, Italy, Poland, Switzerland, and Norway. Spanish Ministry of Science and Innovation (MICINN) supports the project through the project PCI2021-121945. This publication is part of the R&D project PCI2021-121944, financed by MCIN/AEI/10.13039/501100011033 and by the “European Union NextGenerationEU/PRTR”.





# eFlows4HPC

Enabling dynamic and Intelligent workflows  
in the future EuroHPC ecosystem

[www.eFlows4HPC.eu](http://www.eFlows4HPC.eu)



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eFlows4HPC Project



This project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955558. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Spain, Germany, France, Italy, Poland, Switzerland, Norway.