KTH ROYAL INSTITUTE
OF TECHNOLOGY

FEniCS HPC: An automated predictive high-performance framework for multiphysics simulations

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FEniCS-HPC

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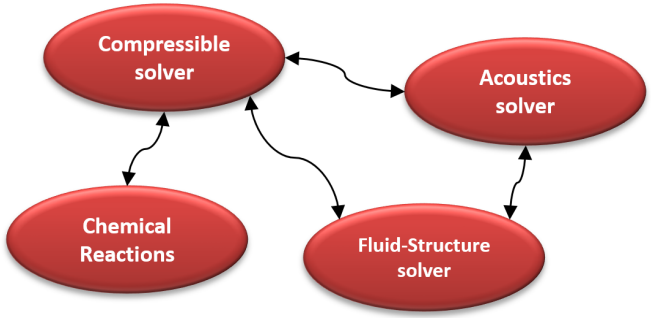
Challenges for Industrial Applications

Mesh generation for complex geometries

- High resolution
- Unstructured meshes
- Optimal element placement
- Memory footprint

Multiphysics problems

- Coupling of different simulation frameworks
- Different representation (Euler/Lagrange)
- Different data structures
- Difficult to achieve good performance



Automated scientific computing

The FEniCS project

- Seeks to automate the scientific software process
- High level language input of equation and discretization method

$$\Delta u = f \quad \text{in}\,\Omega$$

$$\int_\Omega \Delta u\, v\, dx = \int_\Omega f\, v\, dx$$

$$\int_\Omega \nabla u \nabla v\, dx = \int_\Omega f\, v\, dx + \int_\Gamma \frac{\partial u}{\partial \nu}\, v\, ds$$

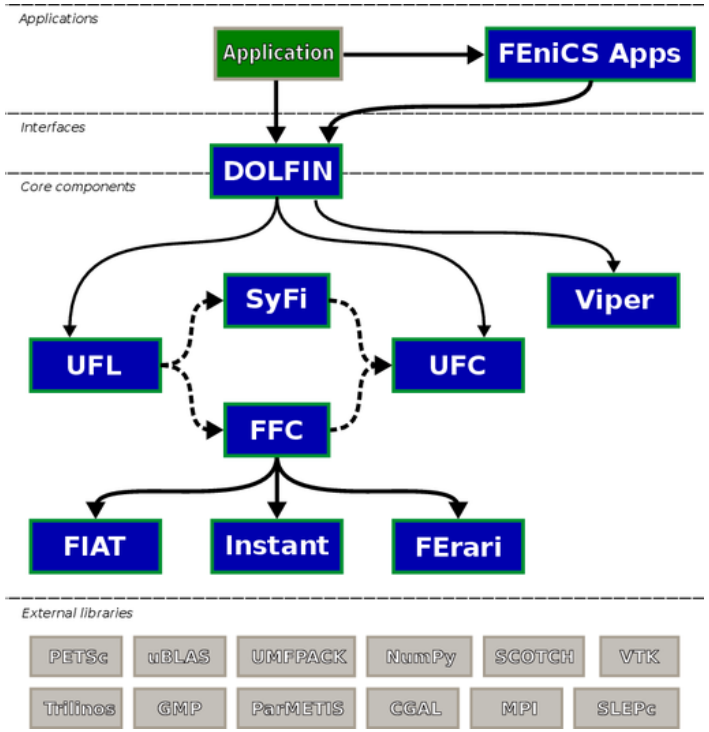
```
element = FiniteElement("Lagrange","triangle",1)

v = TestFunction(element)
u = TrialFunction(element)
f = Function(element)
g = Function(element)

a = dot(grad(v), grad(u))*dx
L = v*f*dx + v*g*ds
```

- Low-level (C++) generated by the FEniCS compiler

Automated scientific computing



DOLFIN Dynamic Object-oriented Library for FINite element computation

FFC FEniCS Form Compiler

FIAT FInite element Automatic Tabulator

UFL Unified Form Language

Automated scientific computing

Poisson's equation

$$
\begin{aligned}
-\nabla^2 u &= f, \quad \text{in}\,\Omega \\
u &= 0, \quad \text{on}\,\Gamma_D \quad \{(0,y)\cup(1,y)\subset\partial\Omega\} \\
\nabla u\cdot n &= g, \quad \text{on}\,\Gamma_N \quad \{(x,0)\cup(x,1)\subset\partial\Omega\}
\end{aligned}
$$

Find $u \in V$ such that

$$a(u,v) = L(v) \quad \forall v \in V,$$

where,

$$
\begin{aligned}
a(u,v) &= \int_\Omega \nabla u\,\nabla v\,dx \\
L(v) &= \int_\Omega f\,v\,dx + \int_{\Gamma_N} \frac{\partial u}{\partial \nu}\,v\,ds
\end{aligned}
$$

Automated scientific computing

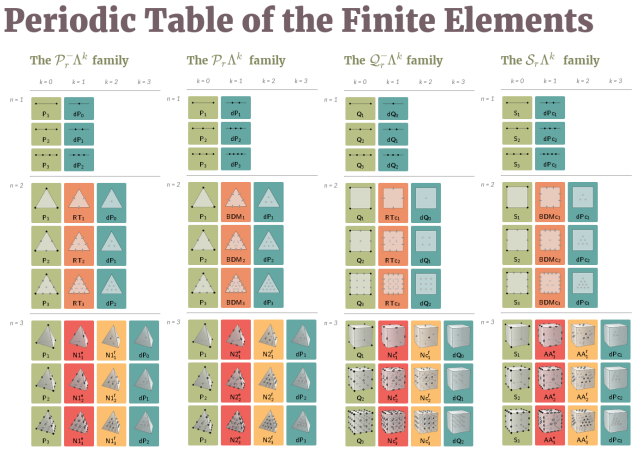
Unified Form Language

UFL provides a language for expressing $a(u, v)$ and $L(v)$ (tree like)

```
V = FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)
f = Expression("10*exp(-(pow(x[0] - 0.5, 2) + pow(x[1] - 0.5, 2)) / 0.02)")
g = Expression("sin(5*x[0])")
a = inner(grad(u), grad(v))*dx
L = f*v*dx + g*v*ds
```

- Easy to define large and complex equations
- No need to change a large amount of code when changing an equation or element type
- UFL implements several different kinds of elements, easy to change

```
V = FunctionSpace(mesh, "Lagrange", 2)
V = FunctionSpace(mesh, "Lagrange", 4)
```



- https://femtable.org

Automated scientific computing

FInite element Automatic Tabulator

Generates the finite element space to evaluate on the reference cell and possibly the mapping

FEniCS Form Compiler

- Loops on the tree and inserts the FIAT contribution
- Spits out code using snippets (provided by consumers)

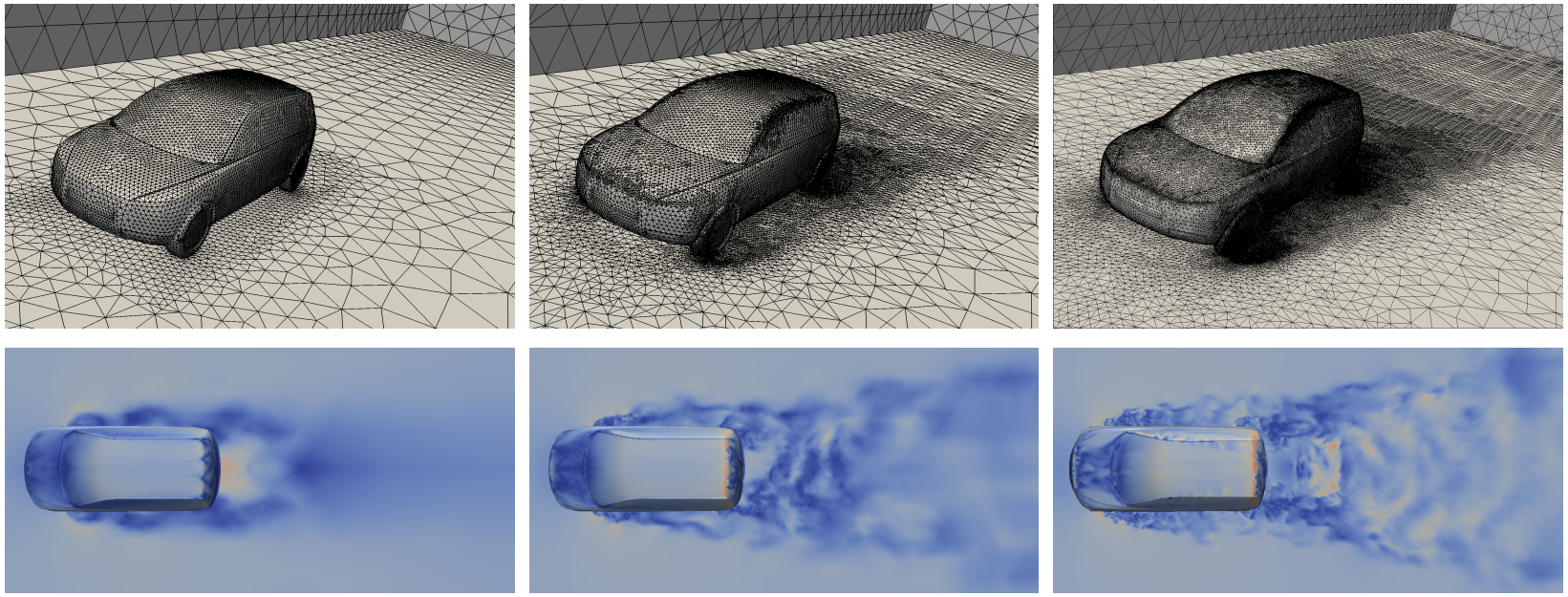
FEniCS Code Generation

- Everything is implemented as python modules
- Great for “std” FEniCS (JIT of equations, solvers in python)
- Not so great for certain arch. BG/L, K computer...
- Code generation only concerns evaluation of element integrals
- Parallelization of discretization and linear solvers left to consumers

FEniCS-HPC

- Code generation: FIAT (FErari) FFC UFC UFL
- DOLFIN-HPC
  - HPC branch of FEniCS's FEM framework DOLFIN
  - Portable: MIPS, PowerPC, SPARC, ia64, x86, ...
  - Hybrid parallelization (MPI + X)
  - Fully distributed mesh
  - Parallel I/O (MPI I/O)
  - Parallel adaptive mesh refinement
  - Predictive (multi constrained) dynamic load balancer
  - Insitu processing (libsim/VisIt)
  - External libraries for linear algebra (e.g. PETSc)
- Unicorn
  - A posteriori error estimation based on adjoint problems
  - Parameter-free turbulence modeling
  - Fluid-structure interaction
  - ALE moving meshes

Adaptive error control



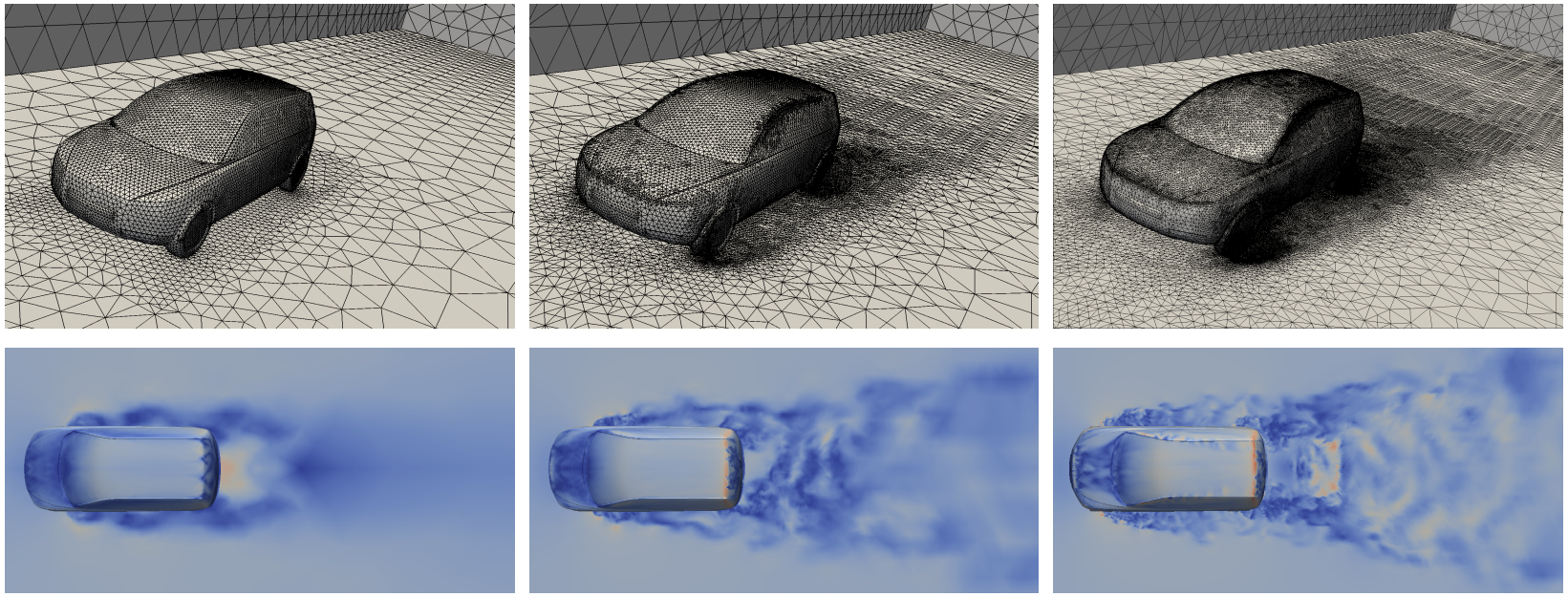
A posteriori error estimate

$$|M(\hat{u}) - M(\hat{U})| \leq \sum_{n=1}^{N} \Big[\int_{I_n} \sum_{K \in \mathcal{T}_n} |R_1(\hat{U})|_K \cdot \omega_1 \, dt + \int_{I_n} \sum_{K \in \mathcal{T}_n} |R_2(U)|_K \, \omega_2 \, dt \Big]$$

$$R_1(\hat{U}) = \dot{U} + (U \cdot \nabla) U + \nabla P - \nu \Delta U - f$$

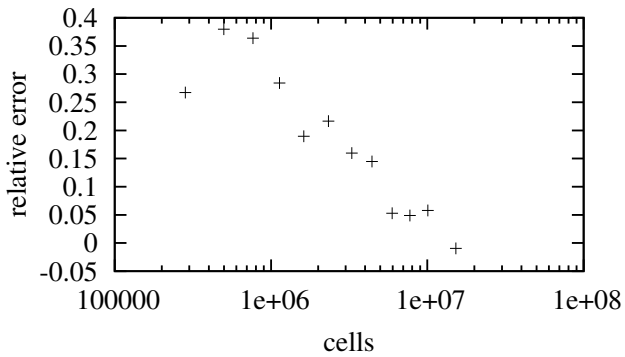
$$R_2(U) = \nabla \cdot U$$

Adaptive error control



Adaptive algorithm

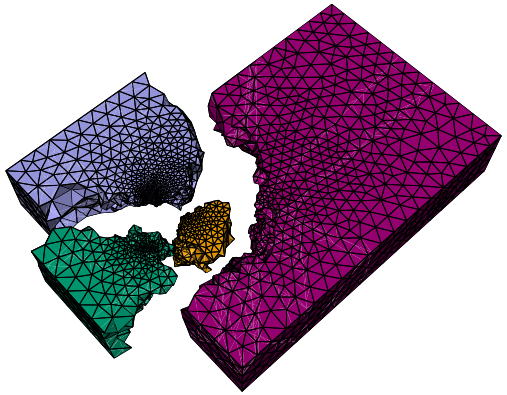
1 Solve the flow problem
2 Compute *a posteriori* errors $\mathbf{e}_K$
3 If $\mathbf{e}_K$ is less than a given tolerance, stop
4 Refine elements K where $\mathbf{e}_K$ is large, restart



Parallelization

Element based decomposition

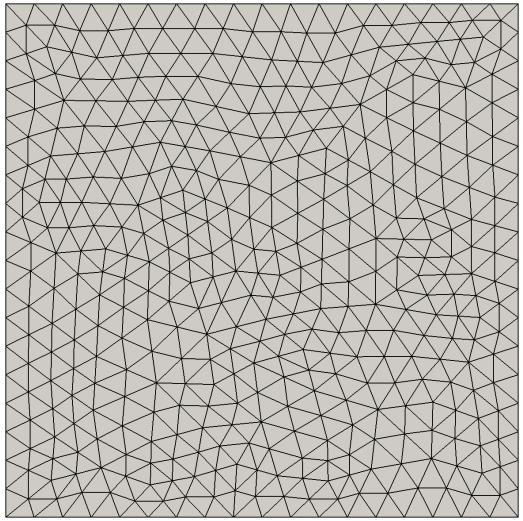
- Dual graph based partitioning
- Overlap represented as ghosted entities
- Low data dependency during FE assembly
- Fully distributed mesh
  - Single input file
  - All pre/post proc. steps performed in parallel
  - Entire problem nor mesh rep. on a single core

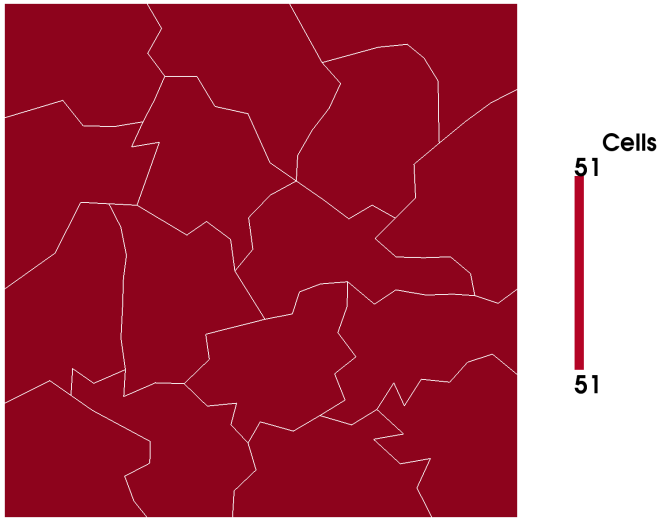


Parallel Mesh Refinement

Recursive Rivara Longest Edge Bisection

- Two phase process, local refinement and propagation
- PEs can change state between “active” and “idle”
- Non-centralized termination detection algorithm

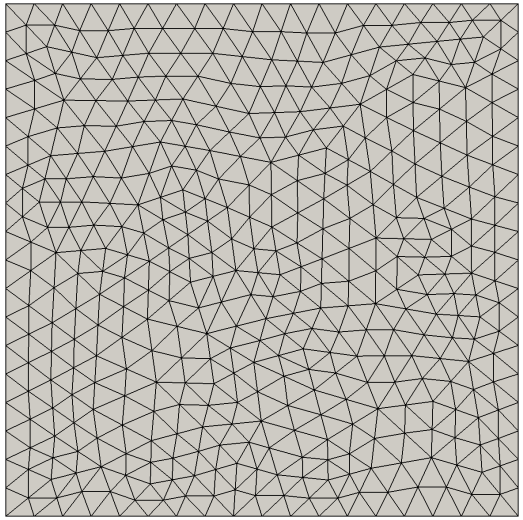


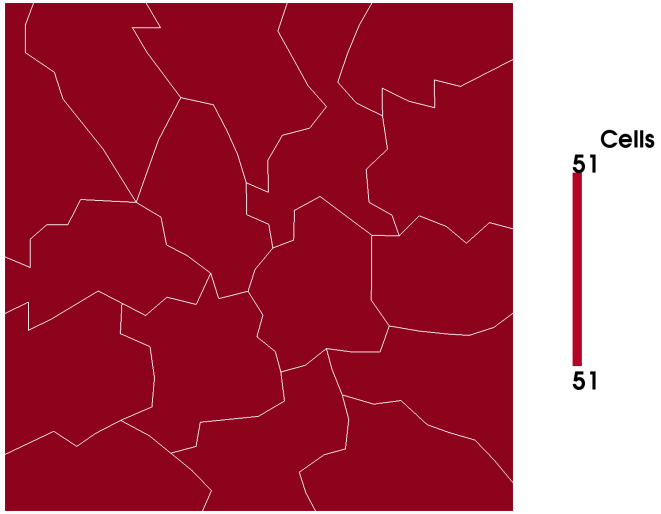


Parallel Mesh Refinement

Predictive Dynamic Load Balancer

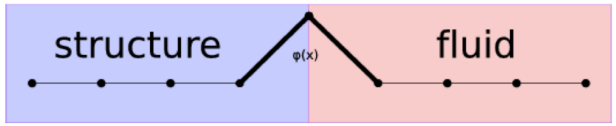
- Scratch and remap approach
- Weighted dual graph (predicted future workload)
- Longest-edge propagation paths to unroll recursion



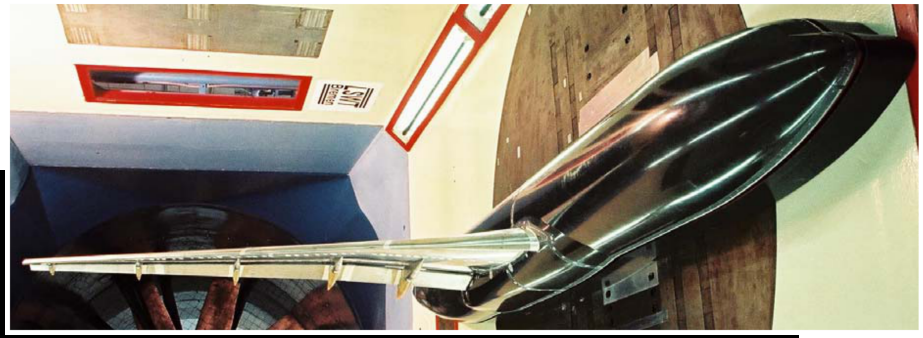


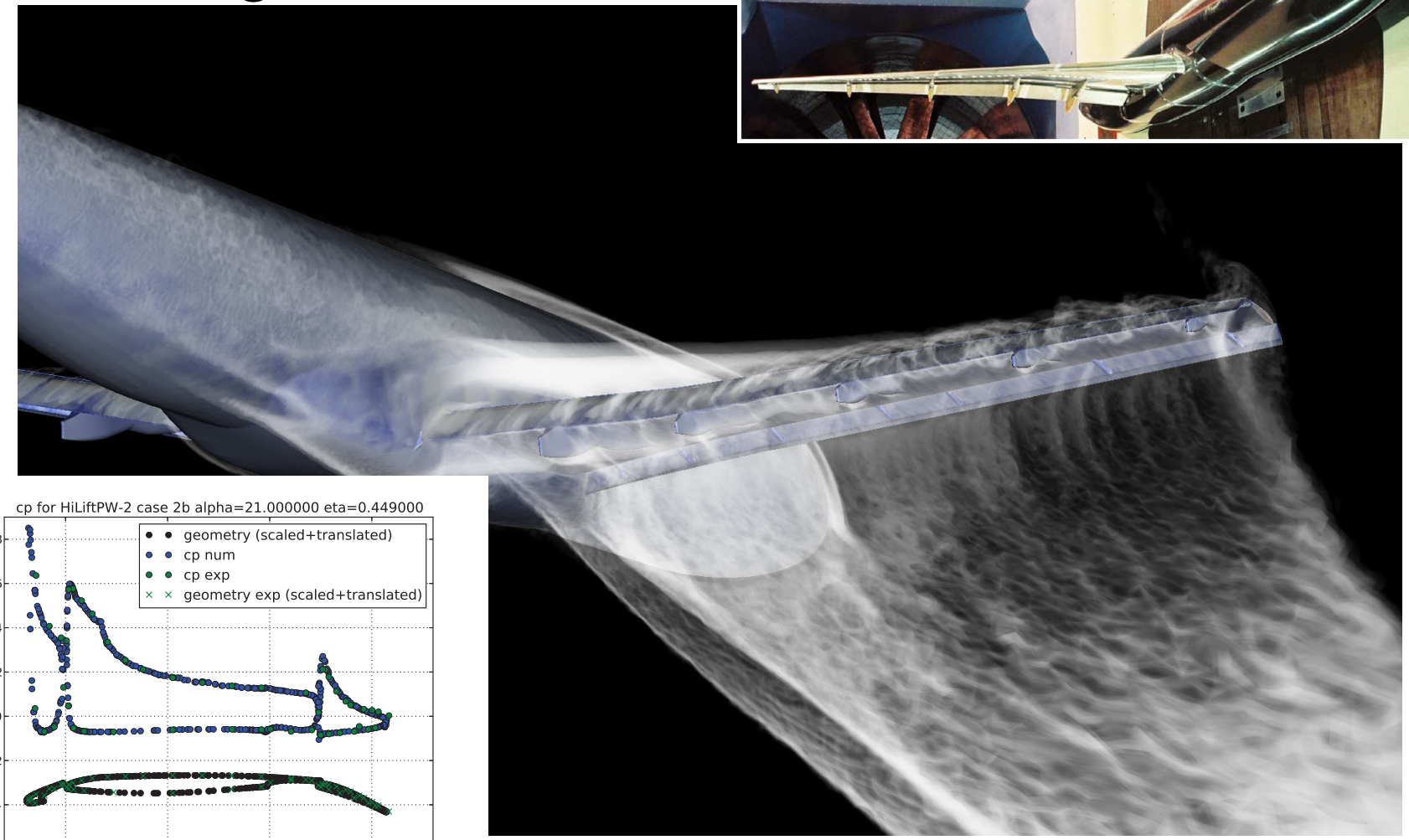
Fluid Structure Interaction

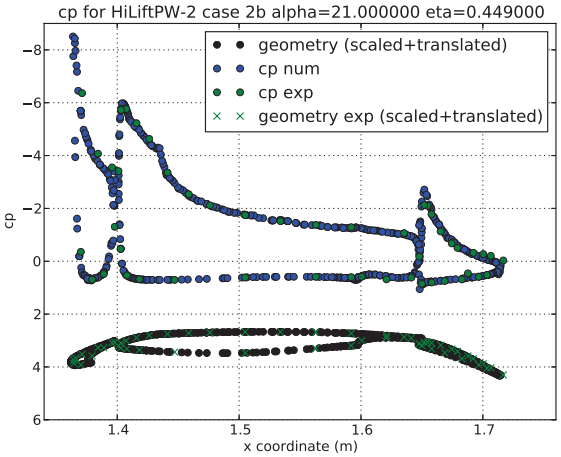
- Phase function $\varphi(x)$ marking fluid/solid
- Ekional equations for contact modeling
- Everything implemented in the form files



High Lift Prediction

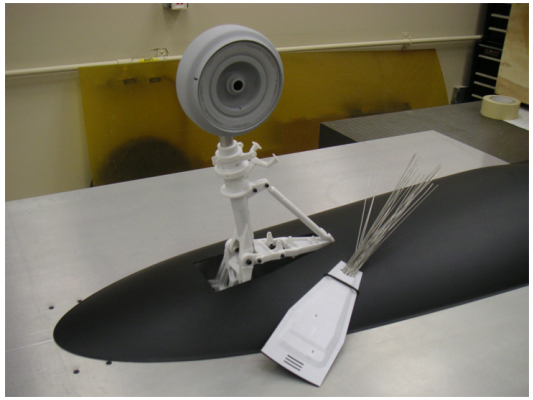






Aeroacoustic sources for a landing gear

A benchmark problem in connection with the 18th AIAA/CEAS Aeroacoustics Conference.

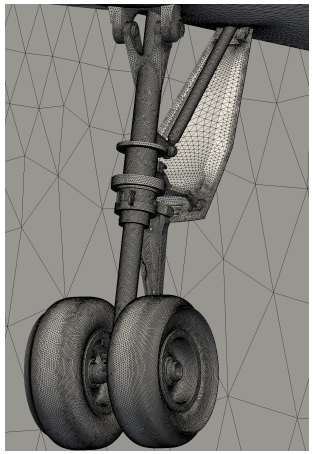


- Gulfstream G550 nose landing gear
- Initial coarse mesh 3.6M elements
- Final mesh 23.8M elements
- Ref. target: Lighthill's source term

Computational resources

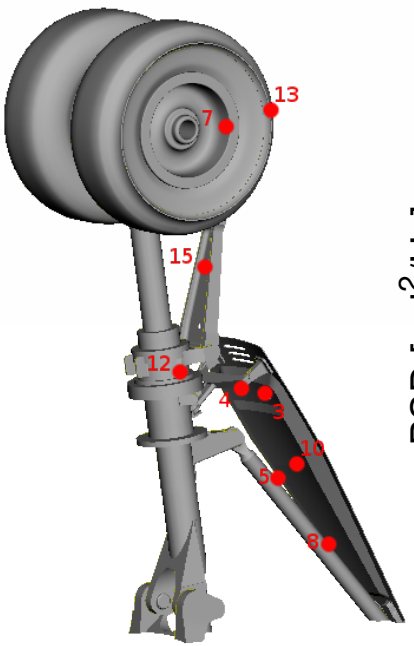
Computed on Lindgren a Cray XE6

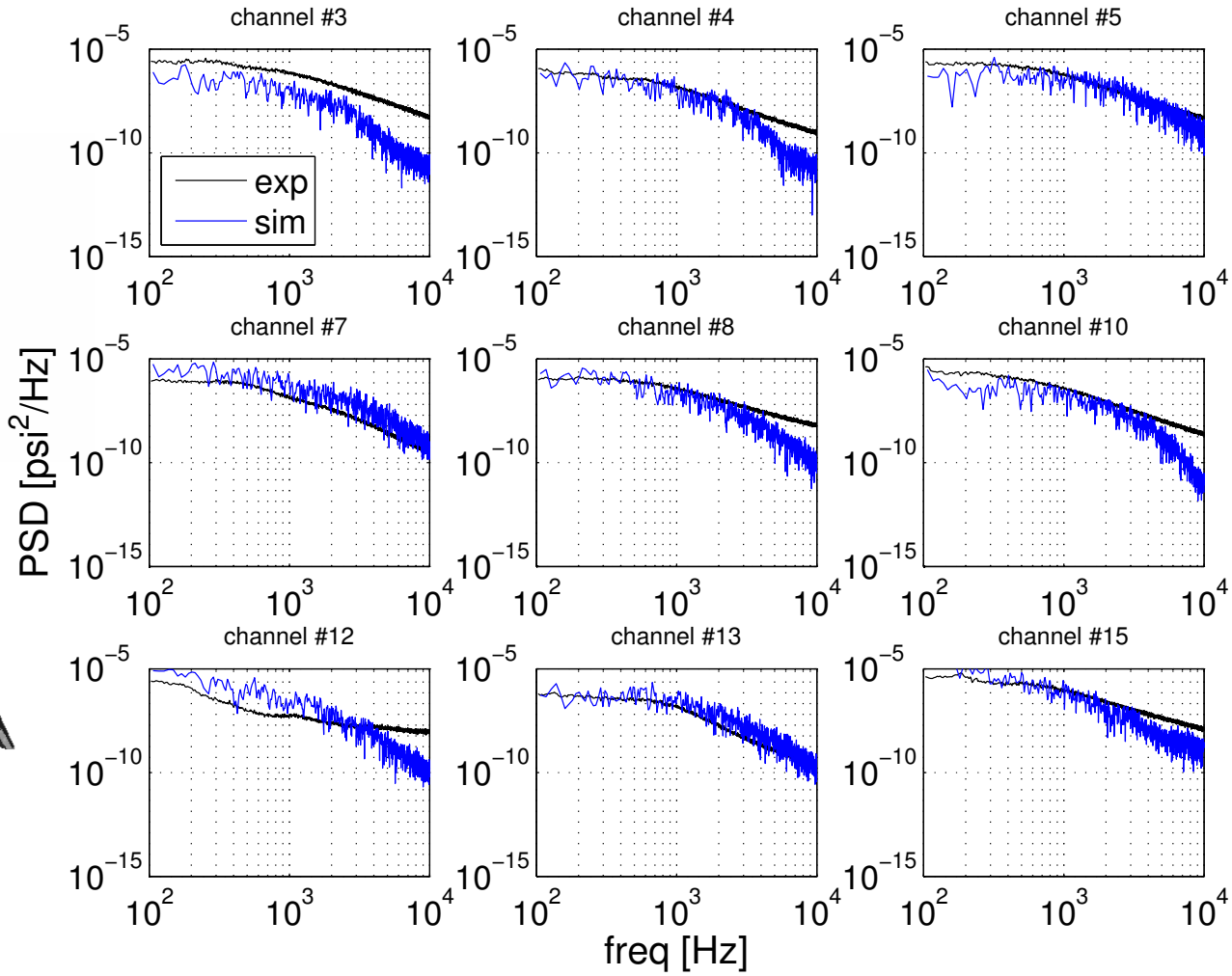
- 900k core hours for the adaptive process (various #PEs)
- 600k core hours for the final run (2304 PEs)
- 1.5M core hours in total (NASA used approx. 1.7M)
- 1.4TB of raw simulation data (final run)



Aeroacoustic sources for a landing gear

Near Field, dynamic pressure





Adaptive FEM for noise

Incompressible Navier-Stokes + Lighthill's wave eq.

$$\dot{u} + (u \cdot \nabla)u + \nabla p - \nu \nabla \cdot \epsilon(u) = f \tag{1}$$

$$\nabla \cdot u = 0$$

$$\ddot{\rho} - c_0^2 \Delta \rho = \nabla \cdot (\nabla \cdot T). \tag{2}$$

Adaptive algorithm

1. For mesh $\mathcal{T}_n$: compute Navier-Stokes and adjoint.
2. For mesh $\mathcal{T}_n$: compute Lighthill's equation and adjoint.
3. Mark ca. 10% of the elements with highest "error indicator" for refinement for each equation.
4. Generate the refined mesh $\mathcal{T}_{n+1}$, and goto 1.

Adaptive FEM for noise

What advantages?

- Fully automated, solution-based mesh generation.
- Final mesh has “optimal” size, avoids “over refinement”.
- No need for a “mesh study”.
- No need to choose porous or solid surfaces for integration.
- Less I/O operations.
- No pre-processing of acoustic sources.

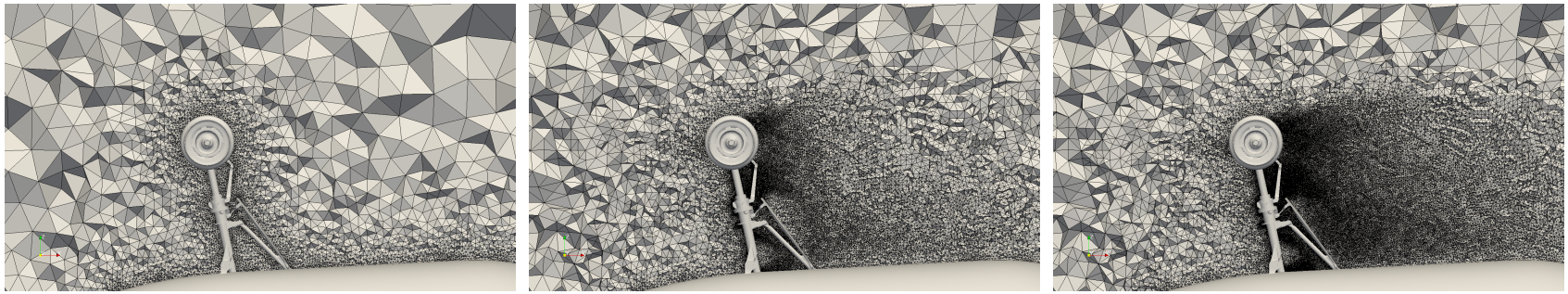


Figure: Initial mesh, and mesh after 4 and 6 adaptive refinements.

Adjoint Solution I, flow

Cells marked, Navier-Stokes equations only

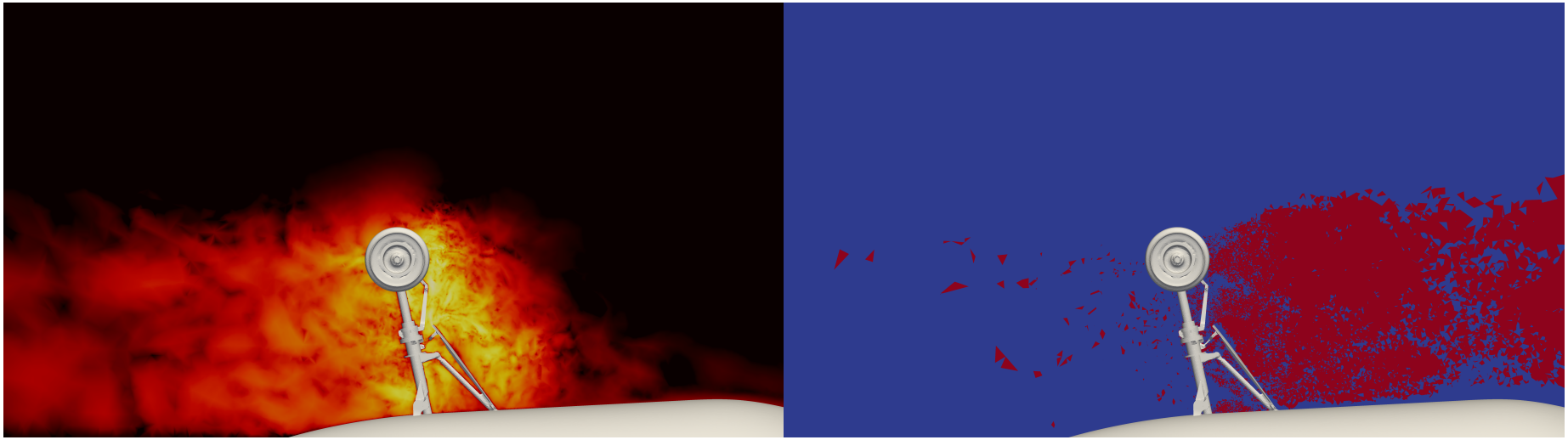


Figure: Snapshot of adjoint velocity (*left*), and cells marked for refinement (*right*).

Adjoint Solution II, flow + wave

Cells marked, Navier-Stokes + Lighthill

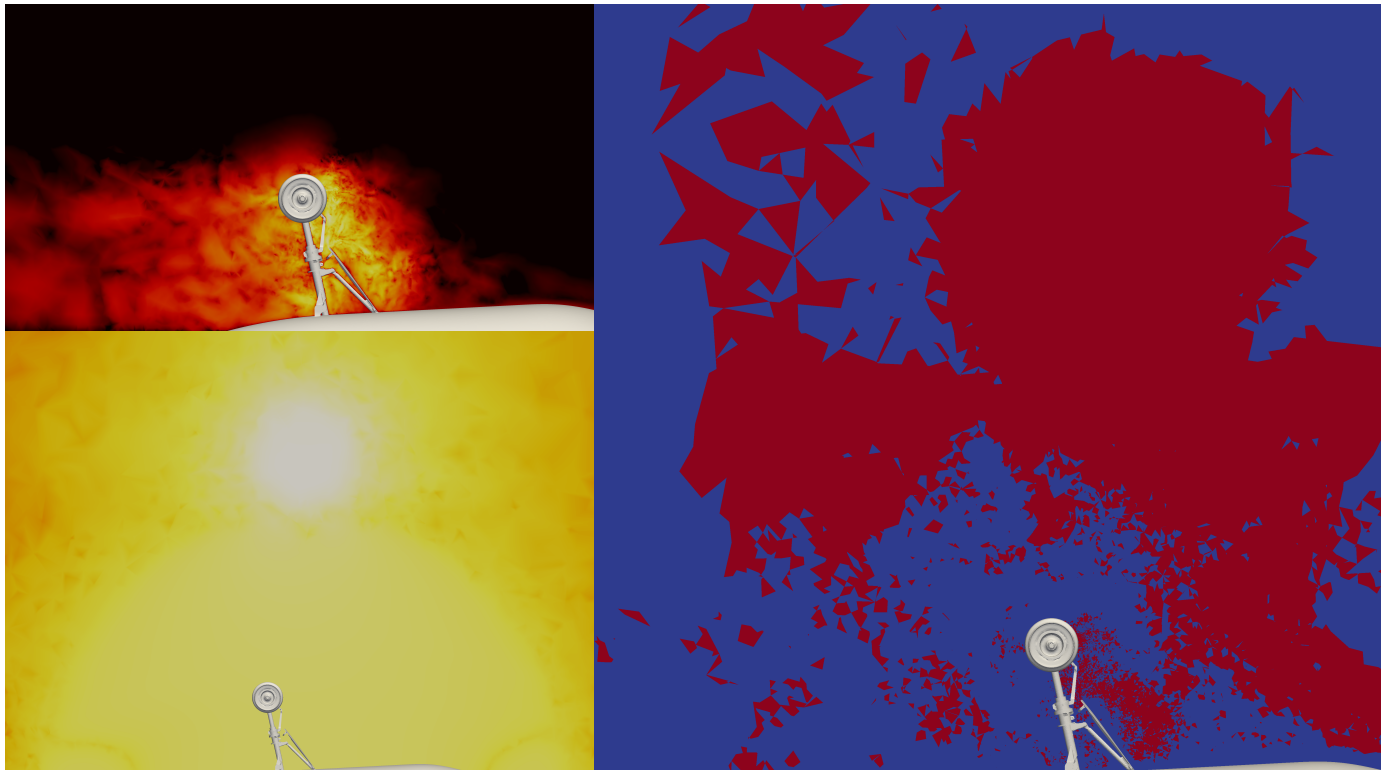


Figure: Snapshot of adjoint velocity (*upper left*), and adjoint density (*lower left*), and cells marked for refinement (*right*).

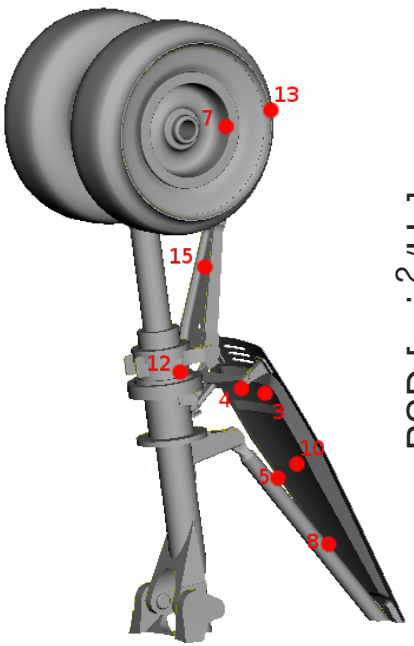
Aeroacoustic sources for a landing gear

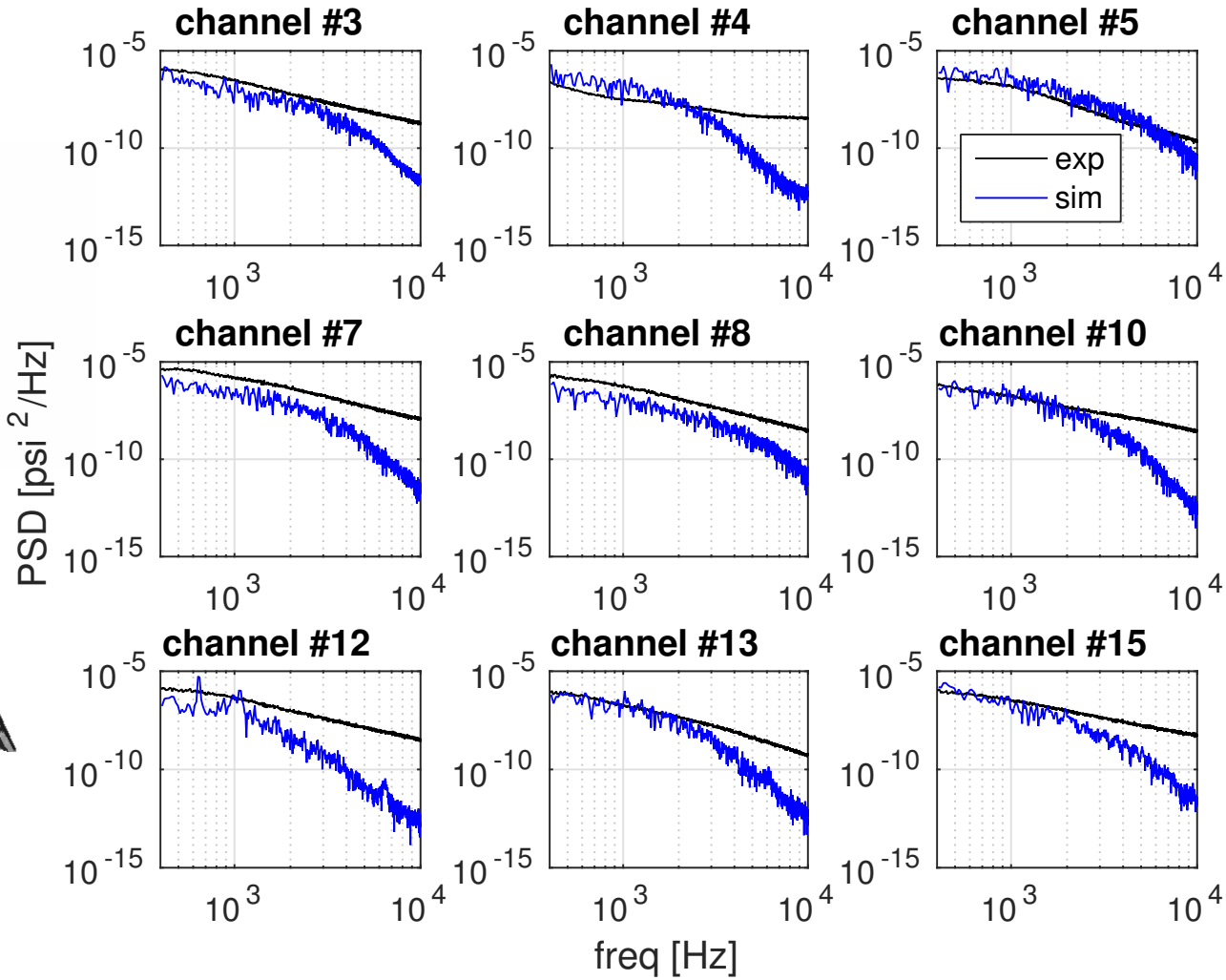
- New simulations for the 22th AIAA/CEAS Aeroacoustics Conference.
- UFAFF wind tunnel configuration
- Computed on Beskow a Cray XC40 system at PDC/KTH.
- Used resources:

	T_{sim}	T_{wall}	# *cores*	*core-hours*
start-up	0.24s	2 days	4,096	$\sim 200,000$
sampling	0.19s	1.5 days	4,096	$\sim 150,000$
adaptive ref	-	-	160-1,024	$\sim 100,000$

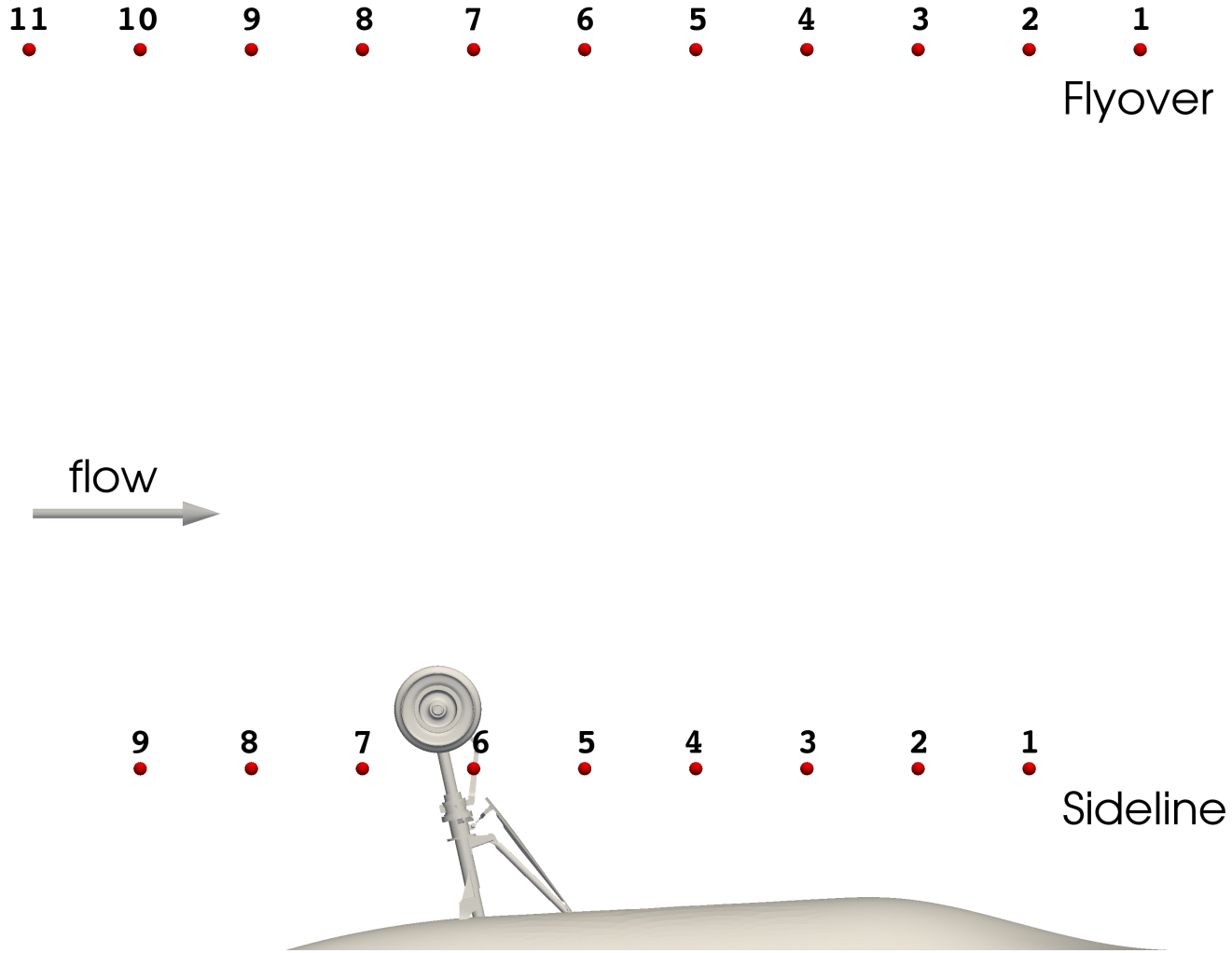
- Mesh sizes
  Coarsest mesh: 200K vertices (1M cells)
  Finest mesh: 12M vertices (66M cells)

Near Field, dynamic pressure





Far Field, sound pressure



Far Field, sound pressure

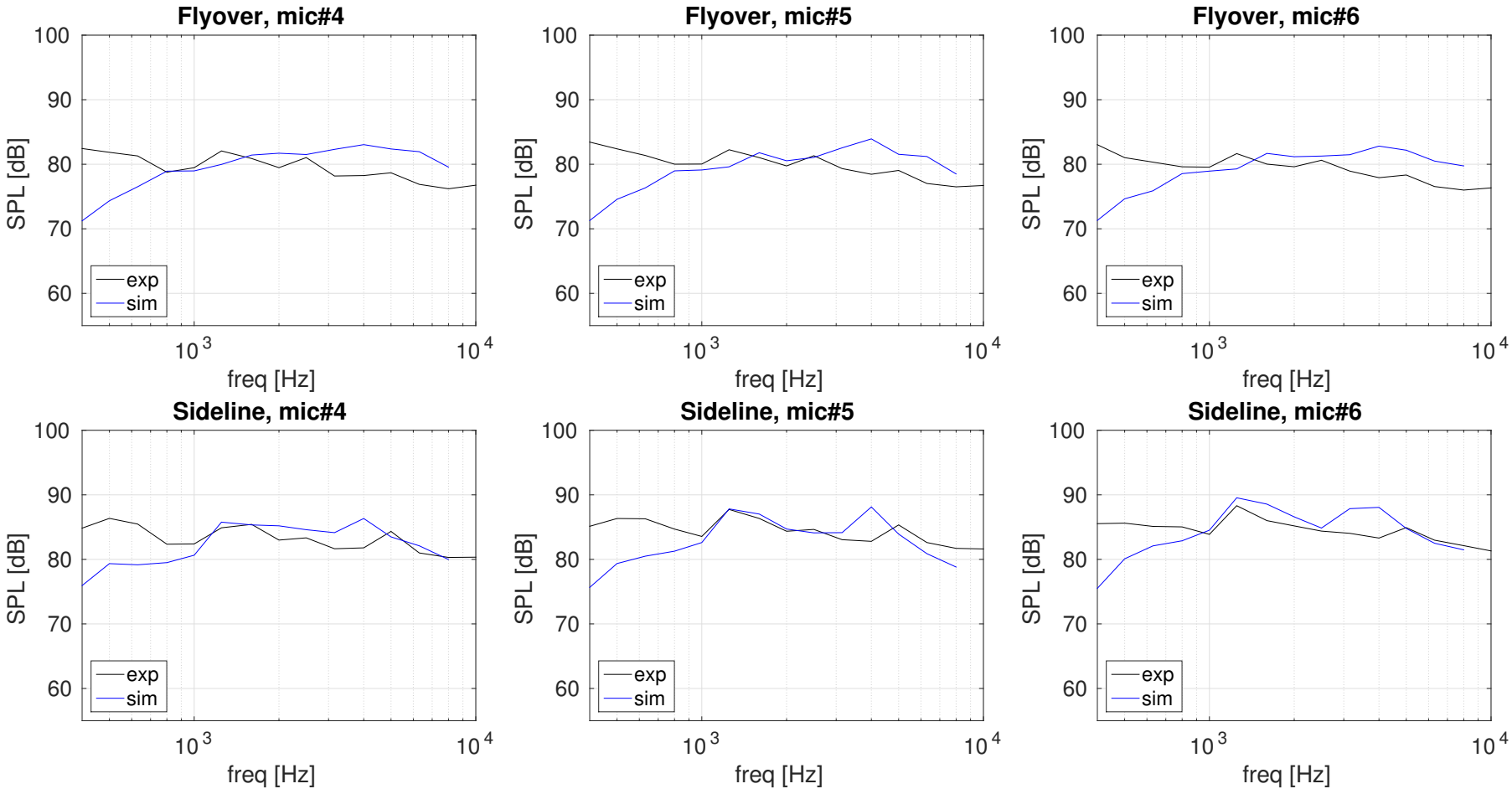
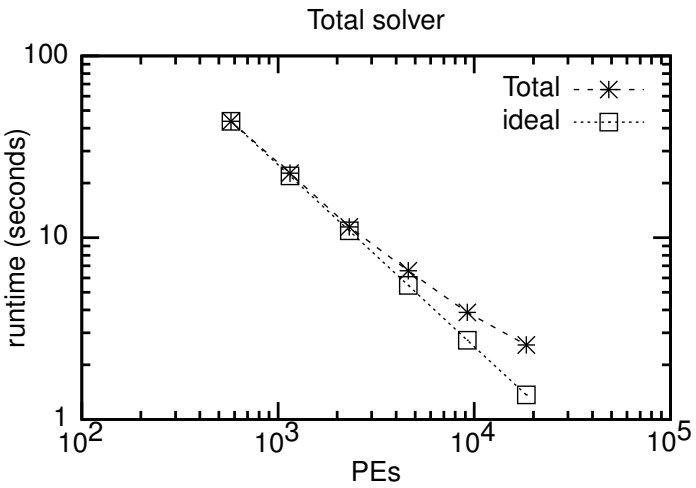


Figure: Far field Sound Pressure Level (SPL) for selected microphones.

Strong scaling (DLR F11)



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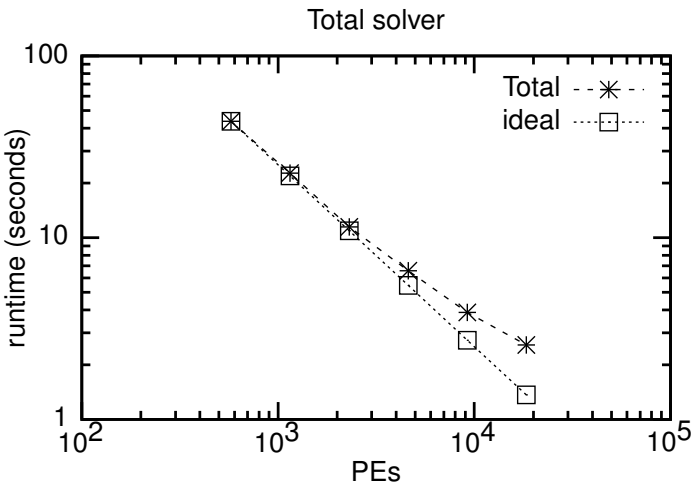

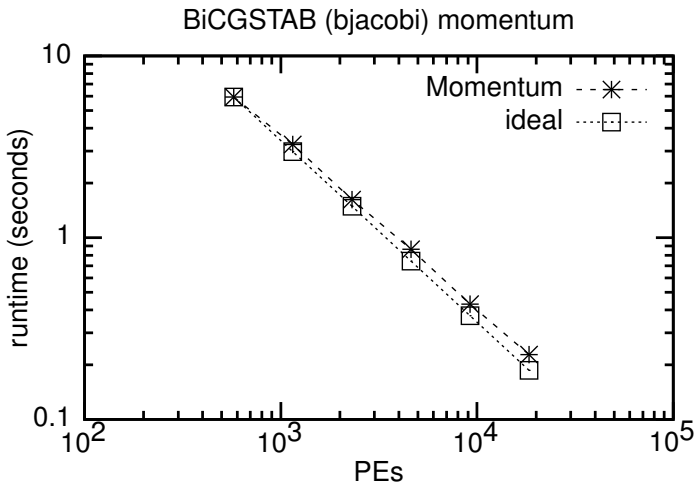

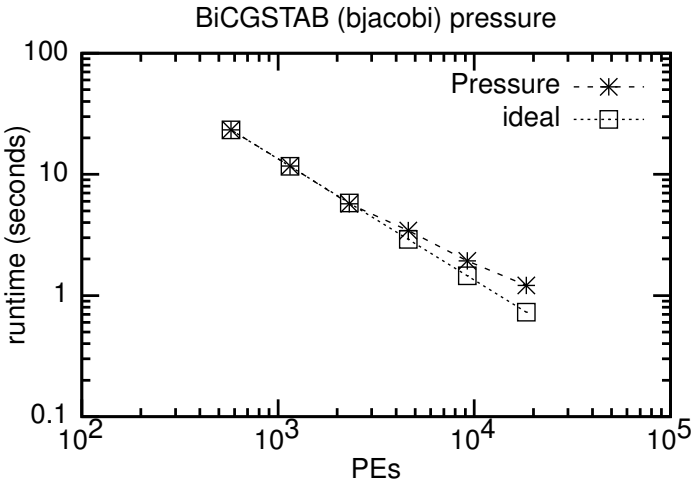

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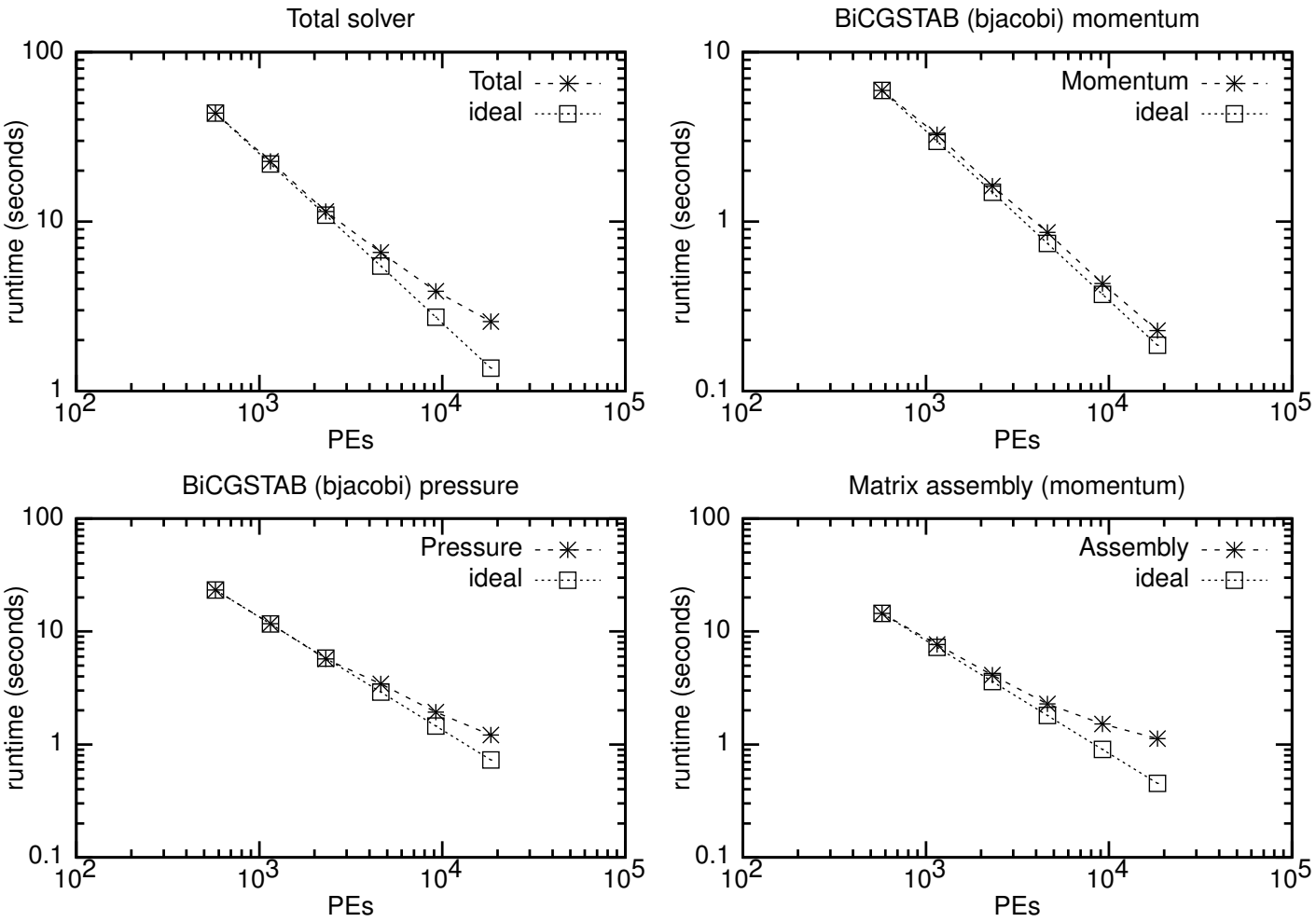
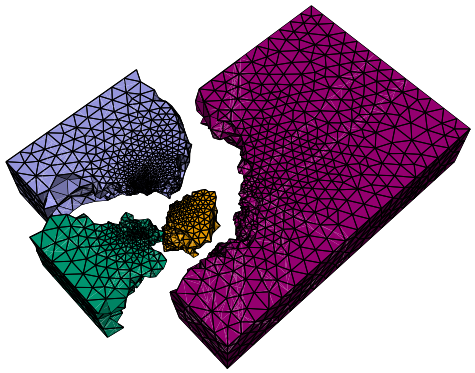


Large Scale Sparse Matrix Assembly

Compute and add element stiffness matrices A_{ij}^k to global matrix A

for $k \in \mathcal{T}$
  for $i = 1 \ldots n$
    for $j = 1 \ldots n$
      $A_{\mathcal{I}_{(i)},\mathcal{I}_{(j)}} += A_{ij}^k$



- Two phase assembly process
- Message matching is expensive on large #PEs
- One sided communication?
- PGAS languages?

Hybrid MPI+PGAS

Combining PGAS languages with legacy MPI codes

A path forward for MPI only codes

- Too costly to rewrite a large code base
- Rewrite latency sensitive kernels in PGAS

JANPACK

A sparse matrix library written in Unified Parallel C

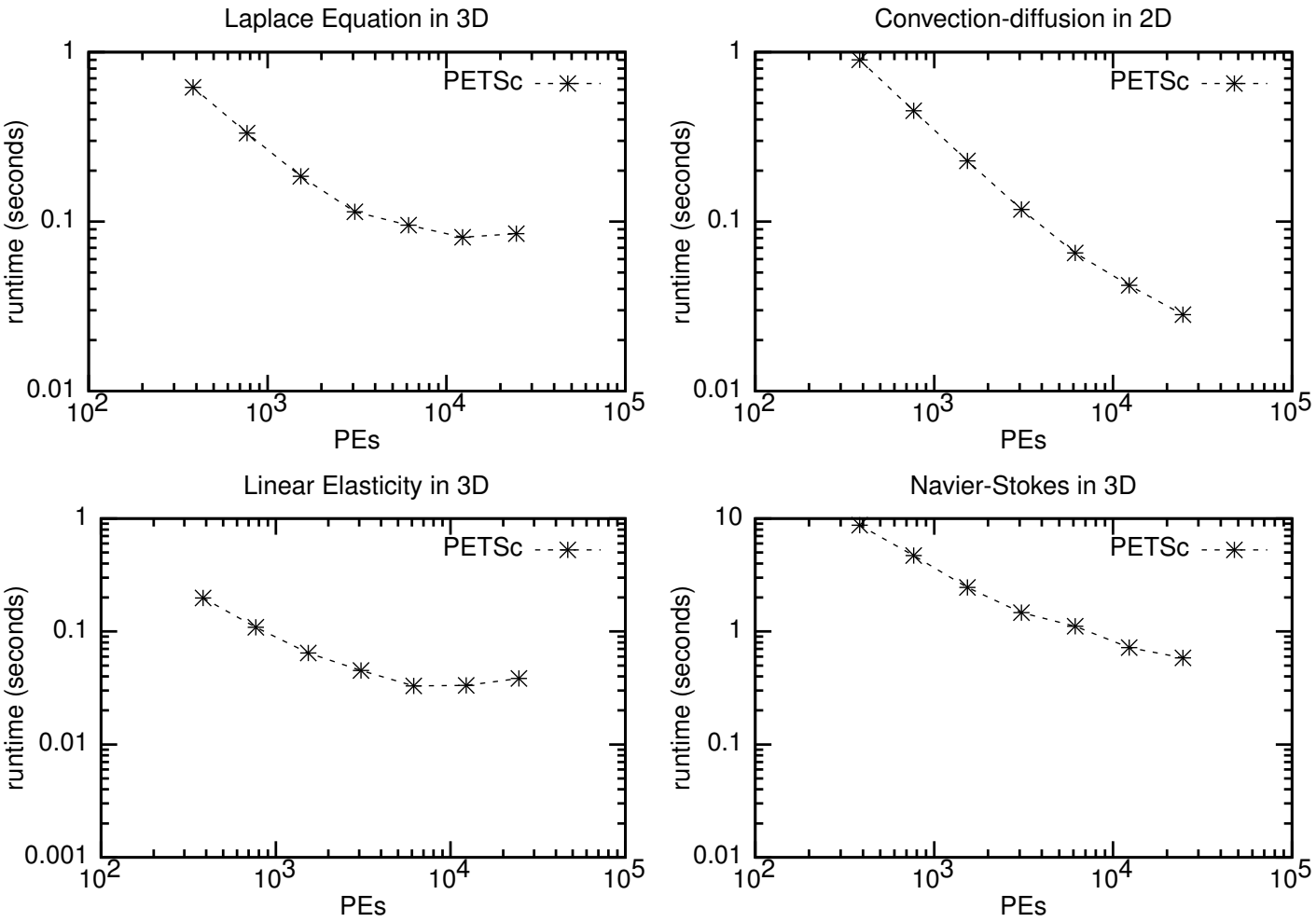
- General, but influenced by our FEM needs
  - Row based data distribution
  - CRS like representation
- Algebraic multigrid
- Krylov solvers (CG (std., pipe., async.), BiCGSTAB (std., ro.))
- Preconditioners (block Jacobi, D-ILU, ILU(0), AMG)

Large Scale Sparse Matrix Assembly

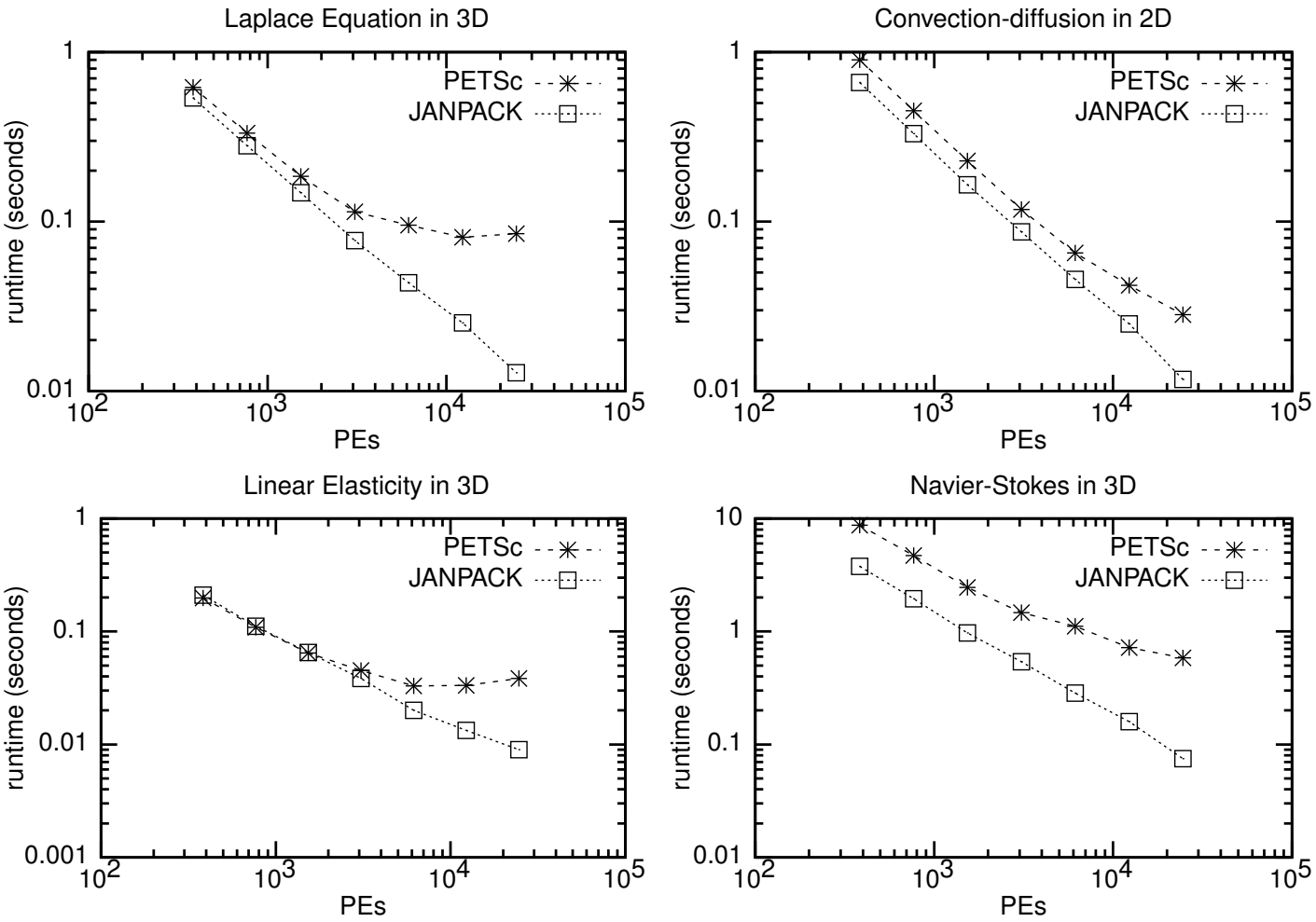
Benchmark suite

- Four different problems with various characteristics
  - 3D Laplace , 317M elements
  - 2D Convection-diffusion, 214 M elements
  - 3D Linear Elasticity, 14M elements
  - 3D Navier-Stokes (Momentum part), 645M elements
- Compute FEM integrals in DOLFIN
- Compare two different LA backends
  - PETSc (MPI)
  - JANPACK (UPC)
- Measure reassembly times
- Each reassembly was repeated 100 times
- Cray XC40 Hornet (HLRS)

Sparse matrix assembly



Sparse matrix assembly



Summary

FEniCS HPC – Automated scientific computing

- Easy expression of complex multiphysics problems
  - Code generation
- General and portable FEM kernel
- Automatic “optimal” mesh generation through adjoints
  - Adaptive algorithm with error control in output of interest
  - Adjoints equations from code generation