Parallel workflows for computational science and engineering: FEniCS

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DOLFIN
- Hybrid parallelization
- MPI+OpenMP
- MPI+PGAS
- Parallel I/O (MPI I/O)

Unicorn
- Adaptive continuum mechanics solver
- Deforming/moving mesh algorithms
Dependencies

• autotools
• DOLFIN
  – PETSc
  – ParMETIS
  – UFC
  – MPI
  – FFC
• Unicorn
  – BLAS
  – Cray’s libsci (FORTRAN blas)
Distributed mesh
Distributed mesh

- Each core has a separate mesh
- Glued together using `MeshDistributedData`
- Shared entities are shared or ghost
- Mapping from local to global indices
- Mapping from global to local indices
- Iterators for shared and ghosted entities
Mesh algorithms

- Recursive longest edge bisection
  - Local serial refinement on each PE (concurrently)
  - Global propagation
  - Fully distributed termination criterion

- Dynamic load balancing
  - Scratch and remap (based on PLUM)
  - A priori work load estimation (serial LEPP)

- Mesh smoothing
  - Linear elastic analogy (PDE solve)
Functions and linear algebra

Functions
• Defined by a mesh and a vector of dofs
• dofmap tabulated for each cell

Linear algebra
• Row-wise data distributions
• Non-local data accessed through ghost points
• PETSc, Janpack
Binary file format

Mesh
Mesh mesh("mesh.bin");
File m_out("mesh_out.bin");
m_out << mesh;

Functions
Function u;
File file("primal.bin");
file << u;

The flat binary files can be converted to Paraview or Visit
High Re turbulent flow

- High Reynolds number turbulent flow, shocks, boundary layers, complex geometry, fluid-structure interaction
- Full computational resolution in DNS impossible
- State of the art: RANS, or LES for moderate Re
- Ad hoc mesh design: non-optimal and expensive
G2 Adaptive FEM Implicit LES

- Approximate turbulence as weak solutions by FEM with residual based stabilization (General Galerkin (G2)/Adaptive DNS/LES)
  - No RANS/LES averaging/filtering
  - No explicit turbulence/subgrid model (parameter free model)
  - Turbulent dissipation only from numerical stabilization (cf. Implicit LES, MILES [Fureby/Grinstein AIAA 99], VMM-LES [Bazilevs et.al. CMAME 07, Guasch/Codina 07])
- Error control with respect to output functionals of weak solutions (e.g. forces, mean values, etc.): $|M(u)-M(U)|$
- Automatic mesh design: by (parallel) adaptive algorithms based on a posteriori error control of $|M(u)-M(U)|$
- Modeling the effect of turbulent boundary layers by a cheap wall shear stress model (cf. [Schumann JCP 75])

[Hoffman SISC 05, JFM 06, CM 06, IJNMF 08, Hoffman/Johnson CMAME 06, Springer 07]
G2 Adaptive FEM Implicit LES

- [G2/GLS] For \((v,q)\) in \(W_h\): find \((U,P)\) in \(V_h\) such that

\[
(U_t + U \cdot \nabla U, v) + (\nu \nabla U, \nabla v) - (P, \nabla \cdot v) + (q, \nabla \cdot U) \\
+ (\delta R(U,P), R(v,q)) = (f,v)
\]

- Slip (no penetration) velocity: \(u \cdot n = 0\) (strong BC)
- Wall shear stress: \(\tau = n^T \sigma t = \beta(u \cdot t)\) (weak BC: \(\beta\) friction coeff.)

- Least squares stabilization of a residual: \(R(U,P)\), with \(\delta \sim h\)
- No explicit (physics based) subgrid model of unresolved scales
- Dissipation: \(-dK/dt = |\beta^{1/2}u \cdot t|^2 + |\nu^{1/2}\nabla U|^2 + |\delta^{1/2}R(U,P)|^2\)

[Hoffman SISC 05, JFM 06, CM 06, IJNMF 08, Hoffman/Johnson CMAME 06, Springer 07]
G2 Adaptive FEM Implicit LES

- A posteriori error estimate: \(|M(u) - M(U)| \leq \sum K E_K\) (cells K)
- Error indicator \(E_K = S_K \times h_K |R_K|\) (\(S_K\) stability weight, \(R_K\) residual)
- Output sensitivity of \(M(\cdot)\) by adjoint equation: stability weight \(S_K\)
- Adjoint equation: \(- \partial \phi / \partial t - (u \cdot \nabla) \phi + \nabla U^T \phi + \nabla \theta = \psi, \quad \nabla \cdot \phi = 0\)
G2 - Adaptive FEM for turbulence

Adjoint solution show sensitivity with respect to drag

[Geometry by Volvo Cars]

[N.Jansson/J.Hoffman/M.Nazarov Supercomputing SC11]
Optimal scaling – adaptive CFD/FSI

Full adaptive cycle: primal problem, dual, error estimation and mesh refinement

[Cray XE6 Lindgren at PDC/KTH ]

[N.Jansson/J.Hoffman/M.Nazarov Supercomputing SC11]
G2 validation: basic benchmarks

- NACA 0012 Re = 10^6 [Jansson/Jansson/JH, 2012]
- Cube Re = ”∞” [JH/Jansson/Vilela, CMAME 2011]
- Circular cylinder Re = 3900 [JH, IJNMF 2009]
- Sphere Re = 10000 [JH, JFM 2006]
- Square cylinder Re=22000 [JH, SISC 2005]
- Surface mounted cube Re = 40000 [JH, SISC 2005]
Workshop on Benchmark problems for Airframe Noise Computations (BANC-I)

Landing gear test case
Re = $10^6$, boundary layers tripped

Experimental results [Boeing/Nasa]
$C_x = 1.60$
$SPL_{max} = 149 \text{ dB}$

Computation: G2/free slip bc ($\beta=0$)
Turbulent BL left unresolved!
$C_x = 1.62$
$SPL_{max} = 152 \text{ dB}$

[Vilela De Abreu/Jansson/Hoffman BANC-I 2010, AIAA 2011]
Surface flow separation patterns
No boundary layer - inviscid separation
Experiment vs Simulation
oil film visualization

Side view of front and rear wheels.

[Vilela De Abreu/Jansson/Hoffman BANC-I 2010, AIAA 2011]
Experiment vs Simulation

oil film visualization
BANC-II 2012
AFEM for aeroacoustics
[Initial mesh by ANSA, postprocessing by SAAZ]
Validation against experiments

[Vilela De Abreu/Jansson/Hoffman BANC-II 2012, AIAA conference 2012]
Lighthill source - mesh convergence

Result on initial mesh...

...after 2 refinements...

...after 4 refinements...

...after 6 refinements (final mesh).
Lambda 2
HiLiftPW-2 full aircraft aoa = 21°
Adjoint - drag of right halfplane
Mesh 700 k vertices

[Initial mesh by ANSA, postprocessing by SAAZ]
1.1 M vertices

[Initial mesh by ANSA, postprocessing by SAAZ]
1.6 M vertices

[Initial mesh by ANSA, postprocessing by SAAZ]
2.2 M vertices

[Initial mesh by ANSA, postprocessing by SAAZ]
3.1 M vertices

[Initial mesh by ANSA, postprocessing by SAAZ]
HiLiftPW-2 aoa=12
(Lambda 2 visualization in an box)
HiLiftPW-2 aoa=12
HiLiftPW-2 aoa=22.4
HiLiftPW-2 aoa=24
aoa = 12
Oilfilm visualization
Unified Continuum FSI (UC-FSI)

[Hoffman/Jansson/Stöckli M3AS, 2011]

\[ \rho \left( \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \sigma_{ij} + f_i, \]

\[ \frac{\partial u_j}{\partial x_j} = 0, \]

\[ \frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = 0. \]

\[ \sigma = \theta \sigma^f + (1 - \theta) \sigma^s \]

\[ \sigma_{ij} = \sigma_{ij}^D - p \delta_{ij} \]

\[ \sigma_{ij}^f = 2\mu f \epsilon(u)_{ij} \]

\[ \frac{\partial \sigma_{ij}^s}{\partial t} = 2\mu s \epsilon(u)_{ij} + \frac{\partial u_i}{\partial x_k} \sigma_{kj}^s + \sigma_{ik}^s \frac{\partial u_k}{\partial x_j} \]

- Mesh smoothing/local remeshing
- Validated for 2D benchmark [Turek]
FP7 Eunison - the human voice

Goal: unified simulation of the human voice
• FSI of flow through vocal folds
• UC-FSI continuum contact model
• Acoustic propagation in vocal tract
• Implementation in FEniCS

• Future and Emerging Technologies (FET)
• Partners: KTH, Erlangen (FAU), Grenoble (CNRS-GIPSA), Barcelona (CIMNE, La Salle)
Vocal folds replica – FAU Erlangen
FSI: Self-oscillation with contact

[C.Degirmenci/J.Jansson/JH, 2012]
FSI: Self-oscillation with contact

Unified Continuum Simulation of Self Oscillating Vocal Folds

Computational Technology Lab. CSC/NA

[C.Degirmenci/J.Jansson/JH]
FSI: Self-oscillation with contact

[C.Degirmenci/J.Jansson/JH]
Simulation in health care

- Individualized diagnosis
- Treatment planning
Patient specific LV heart model

- Left ventricle (LV) geometry from ultrasound data
- Blood flow ALE simulation in deforming domain
- Validation: ultrasound, MRI, pressure measurements
- Basic research, decision support for diagnosis and treatment
- KTH-STH, Karolinska U Hospital, Umeå U, Linköping U

Diastole

Systole

[Volume-Time curve]

[P.Vesterlund/U.Gustafson/M.G.Larson (Umeå University)]
Blood flow in LV
Embedding aortic heart valves

Mechanical bileaflet valves

Biological aortic valves

Work in progress
Interactive Visualization Demo

FEniCS-HPC tool chain

- FEniCS-HPC tool chain: FIAT FFC **DOLFIN(-HPC) Unicorn**
- Fully distributed unstructured mesh, parallel I/O with MPI
- Hybrid parallel model MPI-OpenMP/MPI-PGAS
- LA back-end: PETSc, **Janpack** (MPI+PGAS)
- A posteriori error estimation based on adjoint problems
- Parallel adaptive mesh refinement, ALE moving mesh
- Turbulent flow, fluid-structure interaction, contact models
- Today installed at supercomputing centers in Sweden (under way: Finland, Spain, ...)
- Central for a number of application projects: aerodynamics, aeroacoustics, geophysics and biomedicine
FEniCS-HPC tool chain

• Unicorn
• DOLFIN(-HPC)
• Janpack

• All projects available at fenicsproject.org/Launchpad (through Unicorn [https://launchpad.net/unicorn]) or at CTL Forge [http://dryad.csc.kth.se] (git/Redmine)