Parallel Finite Element Computations of Three-Dimensional Benchmark Problems*

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Abstract

This paper presents the numerical results of two benchmark problems for the three dimensional Navier-Stokes equations. The first benchmark problem prescribes the flow around a cylinder and the second a flow through a T-shaped mixing reactor with chemical species. The numerical schemes for solving the three dimensional Navier-Stokes equations and the species equations using the parallel adaptive finite element framework *padfem2* are illustrated. Furthermore, some efficiency results and the comparison of the numerical computations with existing reference values are shown.

Keywords: finite element methods, Navier-Stokes equations, species equations, parallel algorithms, *padfem2*

1 Introduction

In this paper numerical solutions of two different benchmark problems for the incompressible three dimensional Navier-Stokes equations are presented. The benchmark problems are defined within the German Science Foundation high priority programs "Flow Simulation on High Performance Computers" and "Analysis, Modeling and Calculation of Mixing Processes with and without Chemical Reaction". The first benchmark problem is a flow around a cylinder and the second the mixing of chemical species in a T-shaped micro-mixer. In both cases the inflow velocity fields are given and ensue a Reynolds number of $Re = 20$ for the flow around a cylinder and $Re = 186$ for the mixing problem. In case of the cylinder problem the lift coefficient, the drag coefficient and the pressure difference are calculated. The second benchmark problem comprised additionally a transport problem for the species. For this, we compute in advance a stationary solution of the Navier-Stokes system. Afterwards, with the known velocity field the instationary transport of the species is computed. Here, the pressure decay along the mixing channel, the mixing quality and the variation of the species are of interest. The mean values for the species distribution are computed on different cut planes of the T-shaped mixing channel. The numerical simulation has been carried out with our parallel adaptive finite element framework padfem^2. The method of characteristics based on a pressure correction splitting scheme ([Cho68, Pro97, Pir89]) is

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used for solving the three dimensional Navier-Stokes equations. The solving method employs a stable finite element approach (mini-element) ([GR96]). The paper is organized as follows: In the next section both benchmark problems are presented. In section 3 the numerical schemes for solving the three dimensional Navier-Stokes equations and the species equations are illustrated. Then the numerical results of both benchmark problems and the comparison with existing reference values follows. Furthermore, some parallel runtime results using the padfem^2-framework are shown. In the last section we give a short conclusion and a remark on further work.

1.1 The Benchmark Problems

The flow for both benchmark problems is governed by the Navier-Stokes equations,where $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$ describes the velocity, $p = p(t, \mathbf{x})$ the pressure, t the time and $\mathbf{x}$ the spatial variables. The kinematic viscosity ν is expressed by the dynamic viscosity μ and the density ρ by $\nu = \frac{\mu}{\rho}$. Using the incompressibility condition and the assumption that the density is constant, the Navier-Stokes equations reads:

$$\frac{\partial}{\partial t}\mathbf{u} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \nu\Delta\mathbf{u} - \frac{1}{\rho}\nabla p, \quad \text{div } \mathbf{u} = 0 \quad \text{in } \Omega \tag{1}$$

with boundary conditions

$$\begin{aligned} \mathbf{u} &= \mathbf{u}_0^{\mathrm{Cyl}}(\mathbf{x}) \text{ on } \Gamma_{\mathrm{in}} \\ -p\mathbf{I} + \nu\nabla\mathbf{u} &= 0 \text{ on } \Gamma_{\mathrm{out}} \\ \mathbf{u} &= 0 \text{ on } \Gamma/(\Gamma_{\mathrm{in}} \cup \Gamma_{\mathrm{out}}) \end{aligned}$$

for the Cylinder-Problem

$$\begin{aligned} \mathbf{u} &= u_0^{\mathrm{Mix}}(x) \text{ on } \Gamma_{\mathrm{in}}^{1,2} \\ -p\mathbf{I} + \nu\nabla\mathbf{u} &= 0 \text{ on } \Gamma_{\mathrm{out}} \\ \mathbf{u} &= 0 \text{ on } \Gamma/(\Gamma_{\mathrm{in}}^{1,2} \cup \Gamma_{\mathrm{out}}) \end{aligned}$$

for the Mixing-Benchmark.

The computational domains for both benchmark problems, see Figure 1, are denoted by

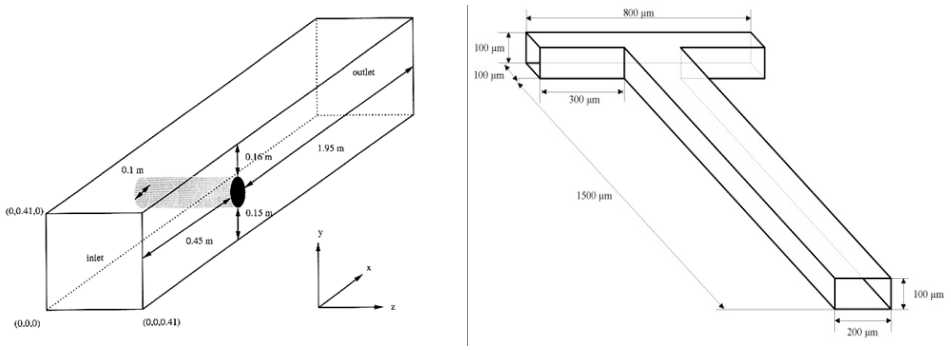

Figure 1: Geometry of the benchmark problems

Ω and the boundary by Γ. The height and depth of the cylinder benchmark problem is

H=0.41m and the L=2.5m, respectively. The diameter of the cylinder is D=0.1m, the kinematic viscosity of the fluid $\nu = 10^{-3}m^2/s$ and the density is given by $\rho = 1kg/m^3$.
The inflow velocity field for the cylinder benchmark problem is defined as follows $u_0^{\mathrm{Cyl}}(x,y,z) = 16Uyz(H-y)(H-z)/H^4$, with $U = 0.45m/s$ and mean velocity $\overline{U} = 0.2m/s$. The inflow channels of the mixing reactor have the dimension of $100\mu m \times 100\mu m$, where the outflow dimension is prescribed by $200\mu m \times 100\mu m$. Both inlets have a length of $300\mu m$, so that the whole top length is given by $800\mu m$. The mixing channel length is defined by $1500\mu m$ without the inflow channel broadness. The density of the fluid is set to $\rho = 998.2kg/m^3$, the dynamical viscosity to $\mu = 0.001003kg/ms$ and the diffusion coefficient in the species equation to $D = 1$. The inflow profile for both inlets are prescribed by $u_0^{\mathrm{Mix}}(x,y,z) = \pm\frac{U}{0.2138}\sum_{k,l=0}^{4}\frac{sin((2k+1)\pi y/d)sin((2k+1)\pi z/d)}{(2k+1)(2l+1)((2k+1)^2+(2l+1)^2)}$, with $U = 1.4m/s$. The additional transport equation required for the chemical species c is described by the species equation $\partial_t c + (u\cdot\nabla)c = D\Delta c$ in Ω with boundary conditions $c_0(x) = 1$ on Γ_{in}^1, $c_0(x) = 0$ on $\Gamma/(\Gamma_{\mathrm{in}}^1 \cup \Gamma_{\mathrm{out}})$.

2 Numerical Approximation

Solving the Navier-Stokes equations various methods are developed in the last decades. In this paper we use a characteristic method based on Chorin's Projection Scheme. The characteristic method reformulates the convective term of the Navier-Stokes equations with the Lagrangian (material) derivative. $D_t\mathbf{u} = \frac{\partial}{\partial t}\mathbf{u}(t,\mathbf{u}) + (\mathbf{u}(t,\mathbf{u})\cdot\nabla)\mathbf{u}(t,\mathbf{u})$. Using the Lagrangian derivative and substitute $q = q(t,\mathbf{x}) = p(t,\mathbf{x})/\rho$ equations (1) reads

$$D_t\mathbf{u} = \nu\Delta\mathbf{u} - \nabla q, \quad \text{div } \mathbf{u} = 0. \tag{2}$$

Furthermore, let $\mathcal{X} = \mathcal{X}(t;s,\mathbf{x})$ be the characteristic path of $\mathbf{u}$. $\mathcal{X}$ is the unique solution of the ordinary differential equation system

$$\frac{\partial}{\partial t}\mathcal{X}(t) = v(t,\mathcal{X}(t)), \quad \mathcal{X}(s;s,\mathbf{x}) = \mathbf{x} \tag{3}$$

satisfying $\mathcal{X}(t) = \mathcal{X}(t;s,\mathbf{x})$ and $\mathcal{X}^{-1} = \mathcal{X}(s;t,\mathbf{x})$. A usual backward implicit Euler discretization of $D_t\mathbf{u}$ leads with $s = t_{n+1}$ to $\left(\mathbf{u}(t_{n+1},\mathcal{X}(t_{n+1})) - \mathbf{u}(t_n,\mathcal{X}(t_n))\right)/\mathrm{dt} = \left(\mathbf{u}(t_{n+1},\mathbf{x}) - \mathbf{u}(t_n,\mathcal{X}(t_n;t_{n+1},\mathbf{x}))\right)/\mathrm{dt} = \left(\mathbf{u}^{n+1} - \mathbf{u}^n\circ\mathcal{X}^{-1}\right)/\mathrm{dt}$, where $\mathbf{u}^n \equiv \mathbf{u}(t_n,\mathbf{x})$ and $\mathrm{dt} = t_{n+1} - t_n$. The term $\mathbf{u}^n\circ\mathcal{X}^{-1} =: \hat{\mathbf{u}}$ demanded the solution of (3). Antagonize the numerical diffusion a higher order approximation of (3) is indispensable. This usually leads to higher order Runge Kutta Methods. Here, a Runge Kutta method of second order, also known as Heun's method: $\hat{\mathbf{x}} = \mathbf{x} - \delta t\mathbf{u}^n(\mathbf{x})$, $\mathcal{X}^{-1} = \mathbf{x} - \delta t\left(\mathbf{u}^n(\mathbf{x}) + \mathbf{u}^n(\hat{\mathbf{x}})\right)$ is used. With $\kappa = \mathrm{dt}\nu$ the time discrete Navier-Stokes equations are now given by the following generalized Stokes system

$$\mathbf{u}^{n+1} - \kappa\Delta\mathbf{u}^{n+1} = \hat{\mathbf{u}} - \mathrm{dt}\nabla q^{n+1}, \quad \text{div } \mathbf{u}^{n+1} = 0. \tag{4}$$

Let $\mathcal{T}_h$ be a decomposition of Ω into tetrahedra. In *padfem2* all tetrahedra are transformed to a standard tetrahedra. Therefore an easy implementation and integration of the resulting bi-linearform is guaranteed. Problem (4) is discretized with the

well known mini-finite-element approach, which fulfills the Babuska-Brezzi condition $\inf_{p_h \in M_h} \sup_{\mathbf{v} \in \hat{\mathbf{X}}} \frac{\langle p, \text{div } \mathbf{v} \rangle}{|v|_1 \|p\|_0} \geq \beta > 0$, where $M_h = P_1 \cap L^2_0(\Omega)$, $\hat{\mathbf{X}} = P_1 \oplus \mathbf{B}$, $\|p\|_0$ denotes the L^2-Norm and $|\mathbf{v}|_1$ the seminorm in H^1. In this case the linear velocity ansatz-function space $P_1 := \left\{ \mathbf{v} \in H^1(\Omega) : \mathbf{v}|_T \in \mathcal{P}^1 \right\}$ is enriched with bubble functions $b \in \mathbf{B} = \left\{ \Phi \in H^1 : \Phi(x) = \alpha_T \prod_{i=1}^4 \lambda_i \right\}$ on each tetrahedra, where $\lambda_1 = 1 - x - y - z, \lambda_2 = x, \lambda_3 = y, \lambda_4 = z$ are the standard ansatz-functions on the reference tetrahedra $T = \{(0,0,0),(1,0,0),(0,1,0),(0,0,1)\}$ with $\alpha_T = 256$ and $\mathcal{P}^1$ the set of linear polynomials. Moreover, numerical tests with the non stable P1/P1-ansatz are considered.

Algorithm 1 Chorin based projection scheme

1: With $\mathbf{v}^n$ known compute $\hat{\mathbf{v}} = \mathbf{v}^n(\mathcal{X}(t))$.
2: Compute $\overline{\mathbf{v}}$ from the elliptic boundary value $(\mathrm{I} - \kappa\Delta)\overline{\mathbf{v}} = \hat{\mathbf{v}} - \nabla q^n$ in Ω with boundary condition from (1) and $q = 0$ on Γ_{out}.
3: Solve Poisson-equation for the pressure correction $\pi = q^{n+1} - q^n$

$$-\Delta\pi = -\text{div } \overline{\mathbf{v}}/\text{dt} \text{ in } \Omega \ , \ \partial_{\mathbf{n}}\pi = 0 \text{ on } \partial\Omega.$$

4: With π known compute $\mathbf{v}^{n+1} = \overline{\mathbf{v}} - \text{dt}\nabla\pi, \quad q^{n+1} = q^n + \nabla\pi$.

The Poisson equation for π in step three is obtained by requiring the velocity $\mathbf{v}^{n+1}$ to be divergence free. The species equation was also solved with the characteristic approach.

3 Numerical Results

The numerical simulation has been carried out with our parallel adaptive finite element framework *padfem2*, see ([BKM03]). First we discuss the cylinder benchmark results. The reference values from ([Joh02, BR05]) for the pressure difference and the drag and lift coefficients are presented in Table 1. The computation of the drag coefficient c_d and lift coefficient c_l depends on the drag an lift force given by the following boundary integrals, $F_d = \int_{CS} \rho\nu \frac{\partial u_{\tau_1}}{\partial_n} n_y - p n_x \, dA$, $F_l = \int_{CS} \rho\nu \frac{\partial u_{\tau_1}}{\partial_n} n_x + p n_y \, dA$. The coefficients c_d and c_l are then defined by $c_d = \frac{2F_d}{\rho \overline{U}^2 DH}$ $c_l = \frac{2F_l}{\rho \overline{U}^2 DH}$. For the computation of the boundary integrals over the cylinder surface CS, a volume based approach is used, see ([Joh02]). The reference interval for the pressure difference $P_D = P_F - P_B$ computed at the points $P_F = (0.45, 0.2, 0.205)$ and $P_B = (0.55, 0.2, 0.205)$ is given by $P_D \in [0.165, 0.175]$.

Meshsize	c_d	c_l	P_D
Reference	6.1853267	$9.400983e-3$	$1.708754e-1$
40768	6.557287	$1.192181e-3$	$1.683390e-1$
623513	6.337317	$1.262727e-3$	$1.719964e-1$
4988104	6.440238	$2.240121e-2$	$1.688929e-1$

Table 1: Reference and Meanvalues

The reference values for the drag and lift coefficient are presented in Table 1. Figure 2 shows the error to the reference values computed by John. Next we consider the results

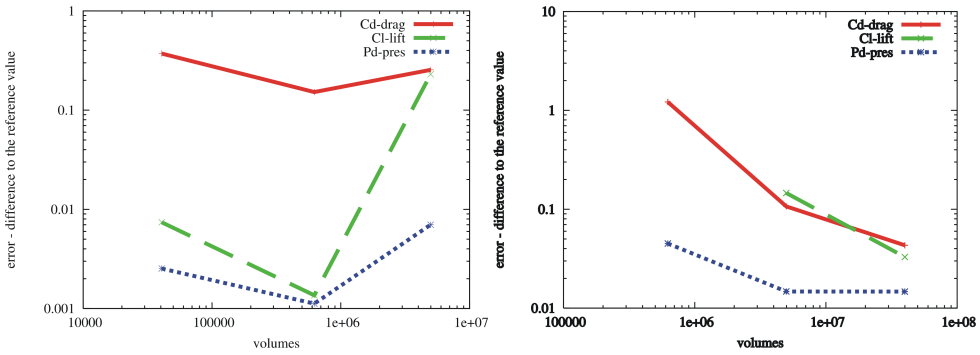

Figure 2: Error to reference values

of the mixing benchmark problem, see also ([War03]). Figure 3 (left picture) presents different mean values. The black and grey dotted curves show the minimum and maximum distribution of the species along the mixing channel and the solid one the mixing quality. The mixing quality is computed by the formula $MG = 1 - (\langle (c - \langle c \rangle)^2 \rangle) / (\langle c \rangle \langle c_{max} - c \rangle)$. In Figure 3 (right picture) one can see the pressure mean values along the mixing chan-

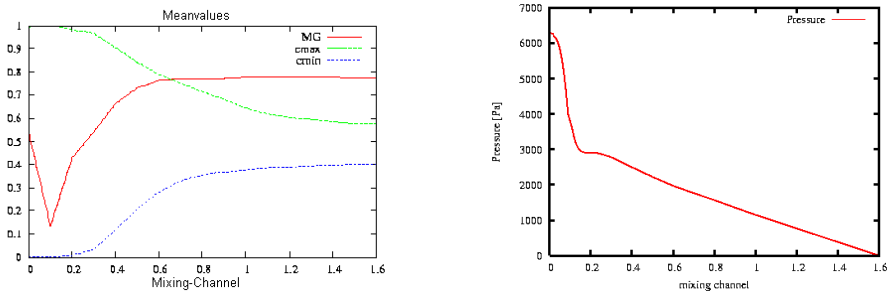

Figure 3: Meanvalues and species distribution

nel. A comparison and computation of reference values of this benchmark results is still in progress. All computations were performed on a 200 Compute-Node Cluster-System with a high speed Infiniband-Network. Each node consists a Dual INTEL Xeon 3.2 GHZ EM64T main board with 4 GB main memory. The peak performance of the system is 2.6 TFlops and allows a memory usage up to 896 GB. In the following some characteristic simulation data using 32 nodes is presented. This includes parallel mesh loading, halo constructing and the computation time of Algorithm 1. In the parallel case *padfem2* uses an overlapping technique for the partitioning, e.g. each partition knows the first neighbor elements from its neighbor partition. This overlapping region is called halo. Table 1 shows the data overhead for the halo constructing given in percent depending on the original sequential mesh. Table 2 presents the time in seconds needed for solving a Navier-Stokes time step. The mesh

dimensions for this computation are M1=857758, M2=5901445, M3=43519497 volumes.

Type	M1	M2	M3
N	56	27	14
E	45	22	11
F	40	19	10
V	37	18	9

Table 2: Halo-Overhead

Mesh	Load	Refine	Halo	RES-(X,Y,Z)	PRES	TP
M1	2.232	-	0.282	0.311	0.814	0.061
M2	2.345	0.968	0.280	1.224	8.985	0.832
M3	0.259	14.568	4.724	9.121	246.373	3.062

Table 3: Simulation time

A standard conjugate gradient solver was used for solving the linear systems of equations and as expected, the most expensive part is the solution of the pressure correction term.

4 Summary

In this paper we demonstrate two benchmark problems solved with the parallel adaptive finite element tool *padfem2*. The computed results were compared to reference values and exhibit an accuracy in the interval $[10^{-3}, 10^{-1}]$. The future work is related to study other finite element approaches, for example the Tayler-Hood element, using preconditioned conjugate gradient solver and alternative Stokes solver.

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