Research strategy for
e-Science in Fluid Mechanics

Background and Motivation

The "e-science in fluid mechanics" research area has a different character compared to other research areas in FLOW. It is not focused on a single discipline of fluid mechanics but its activities span over all other research areas in FLOW. It also acts as a link to the Swedish e-Science Research Centre (SeRC) since it represents the FLOW community in that centre.

During the last 30 years, the field has experienced a change by the introduction of the computer: Numerical simulations of initially laminar, but also turbulent flows have dramatically increased our knowledge. Turbulence models of various complexity and accuracy have been developed over the years, with profound impact into the daily engineering workflow. The simulation of fluid flows usually requires a large amount of degrees of freedom. For instance, when considering turbulent flow, the range of excited scales is very wide, ranging from integral scales (of the size of the considered domain, such as an airplane wing or even a typical atmospheric eddy) down to small viscous scales on the order of a few micrometers. Thus, CFD applications have always been among the best customers of computer centres. Nowadays, DNS using up to order 10 billion grid points are feasible, and a few million grid points are considered to be small simulations.

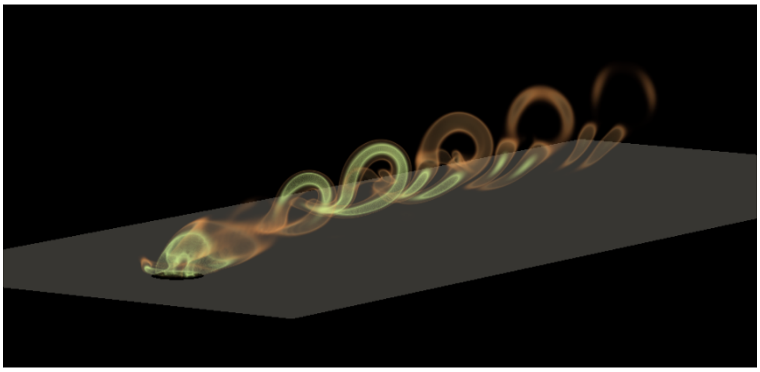

Fig 1: Visualisation of the vortical structures in a jet in crossflow, showing the appearance of hairpin vortices downstream of the nozzle. Volume rendering of the λ_2 field.
For complete animation see http://arxiv.org/abs/1010.3766.

However, the growing capability of computer systems also causes an increasing dependency of researchers on the employed simulation methodology, as the whole process chain of tools is getting more and more complex; up to the point that a complete oversight of the process is impractical for an individual scientist. Issues such as pre-processing (grid generation, initial data), simulation runs (high-performance computing on parallel systems) and post-processing (data storage, mining and visualisation), have become specialised areas of expertise, which are hardly managed by a single researcher. Rather, the processes leading up to performing a successful simulation of a problem at hand have to be considered aspects of e-Science, involving knowledge of a broad range of areas including physics, numerical analysis, computer science, and software skills. It is the aim of this research area to improve the e-Science capabilities for researchers within FLOW.

Research environment

Within FLOW, research in computational fluid dynamics is performed in groups at *KTH Mechanics*, *KTH Numerical Analysis*, *KTH Aeronautical and Vehicle Engineering*. However, within the Swedish e-Science Research Centre (SeRC), also related departments with similar research interest are included, namely *NORDITA, Stockholm University (Bert Bolin Centre)* and *LiU Management & Engineering/Mathematics*. These groups are very diverse in terms of the applied computational methods and the physical problems addressed. Also, their involvement in the areas of e-Science is different: Some groups focus on code development and the related software-engineering aspects, whereas other groups mainly apply commercial codes and direct their research activities towards a deeper understanding of complex physical phenomena. The strength of the present research area directly lies in the variety of backgrounds of the members, uniquely combining strong expertise in areas such as large-scale computations, advanced numerical methods, modelling of complex flows and innovative visualisation. Members act as main developers in many of the below software projects (e.g. Simson, FEMLEGO), or as active contributors to international software projects (FEniCS, Nek5000). The wider SeRC community can also act as a meeting place for developers, sharing ideas and techniques for software development and maintenance, and support a common platform including a forum and documentation for the software packages.

Due to the close collaboration between the departments within FLOW and SeRC, in the following the research goals and strategy for the combined activity is listed; including partners from Linköping University, Stockholm University and NORDITA. The activities of the SeRC FLOW Community are coordinated at KTH Mechanics. To further emphasise the close collaboration between PDC, NSC, SeRC and SNIC, an application expert with focus on CFD applications is also associated to the FLOW research area.

Members (including members of SeRC outside FLOW, but with interest in fluid mechanics):

- *Professors* (Full/Associate): Gustav Amberg, Axel Brandenburg, Luca Brandt, Gunilla Efraimsson, Laszlo Fuchs, Ardeshir Hanifi, Dan Henningson, Johan Hoffman, Arne Johansson, Matts Karlsson, Erik Lindborg, Jan Nordström, Philipp Schlatter, Gunilla Svensson, Anna-Karin Tornberg, Stefan Wallin.
- *Assistant Professors, Researchers, Postdocs*: Jenny Brandefelt, Katarina Gustavsson, Lisa Prahl, Geert Brethouwer, Mattias Chevalier, Minh Do-Quang, Miloš Ilak, Gaetano Sardina, Ciarán O'Reilly.

Research topics: The large number of active researchers and involved departments within the present FLOW research area and associated SeRC members, directly leads to a wide scope of the performed research, ranging from nano-fluidics applications to large-scale simulations of turbulence in the earth's atmosphere. A wide range of different numerical methods is employed, including small homemade test codes, larger in-house software suites, and commercial codes. In the following, two classifications are listed, based on physical problem and numerical approach:

Physical aspects: Turbulence and Modelling, Climate and Geophysical Flows, Transition and Control, Complex and Biological Flows, Aeroacoustics.
Numerical aspects: Large-Scale Simulations, Parallelisation / Optimisation / Adaptivity, Method Development, Visualisation, Applied CFD.

During the last years, computational work has increasingly become more difficult and more specialized, leading to an increased gap between the three fields *Application Area*, *Computational Tools* and *Core Expertise*. To this end, the efforts of the FLOW e-Science research area will be focused on closing the gap, in order to deliver the best results. It is only when combining these three aspects in the best possible way that optimal results can be obtained.

Project	Student/ Postdoc	Senior Researcher	Project Duration	Sponsor / Department
Turbulence and Modeling				
Wall-bounded turbulence: Re-visit using numerical experiments		Schlatter	2011-2012	VR / MEK
Simulations of turbulent boundary layers with passive scalars	Li	Schlatter, Henningson	2007-2011	KTH / MEK
Spectral-element simulations of turbulent separation	Malm	Henningson, Schlatter	2007-2011	FLOW / MEK
Lagrangian particles in turbulent wall flows	Sardina	Schlatter, Brandt	2008-2012	KTH / MEK
Rotating channel flow at high Reynolds number		Brethouwer, Schlatter, Johansson	2010-2011	KTH / MEK
Simulation and modelling of turbulent combustion	Pouransari	Johansson, Brethouwer	2009-	Cecost&Energimynd. / MEK
Development of subgrid models and application of large-eddy simulations	Rasam	Johansson, Brethouwer	2009-	VR / MEK
Method Development				
DNS of high-Reynolds number turbulent pipe flow	Lenaers	Johansson, Schlatter Brethouwer	2009-2013	FLOW / MEK, PDC
Parallel adaptive FEM	Jansson	Hoffman, Jansson	2008-	EXT / NA
Methods for Lagrangian particles in complex geometries	Noorani	Schlatter, Brandt, Karlsson	2011-	SeRC / MEK
Visualisation				
Tools for Visualisations with Simson	Ilak	Chevalier, Schlatter, Henningson	2010-	FLOW, PDC / MEK, PDC
Climate Modeling / Geophysical Flows				
Stratified wall-bounded flows	Deusebio	Lindborg, Schlatter, Brethouwer	2010-2014	FLOW / MEK
Simulations of quasi-geostrophic turbulence	Vallgren	Lindborg	2007-2011	FLOW / MEK
Arctic Sea ice in warm climates	Berger	Johansson, Brandefelt	2010-2014	VR / MEK
Transition and Control				
Bifurcation and stability analysis of a jet in crossflow	Ilak	Bagheri, Schlatter, Henningson	2009-2011	FLOW / MEK
Edge states in shear flows		Duguet, Schlatter,	2010-2012	KTH / MEK

		Henningson		
Adjoint-based linear and nonlinear optimisation in wall-bounded shear flow	Monokrousos	Brandt, Henningson	2007-2011	FLOW / MEK
Aeroacoustics				
Numerical simulation of generation of sound in separated internal flows	O'Reilly	Efraimsson, Åbom, Henningson	2009-	EXT / AVE
Numerical methods for fluid-structure interaction aero-acoustics	Vilela De Abreu	Hoffman, Åbom	2008-	EXT / NA
Complex Flows				
Simulation of free-boundary problems and phase change		Amberg, Do-Quang	2006-	VR / MEK
Numerical simulation of swimming micro-organisms in suspensions	Zhu	Brandt, Amberg	2009-	FLOW / MEK

MEK: KTH Mechanics, NOR: NORDITA, NA: KTH Numerical Analysis, AVE: KTH Aeronautical and Vehicle Engineering, LIU: LiU Management and Engineering, PDC: PDC Center for High Performance Computing, NSC: National Supercomputer Centre, LFC: Linné FLOW Centre (KTH), VR: Vetenskapsrådet, EXT: external

Strategic Goals

- To *develop efficient and accurate numerical methods* for simulation of complex flows such as high-Reynolds number transitional and turbulent flows, flow involving chemical reactions, geophysical flows and flows around wind turbines, and two-phase and biological flows.
- To use *high-performance computing* to enhance the understanding of different physical phenomena in complex flows and fluid-structure interaction.
- To use and develop advanced *tools for postprocessing* of simulation data, such as visualisation and long-term storage and access to data.
- To act as a *coordinator for FLOW e-Science research*, both internally and externally; including international HPC initiatives within FLOW research areas (PRACE etc.), and outside visibility of FLOW research.

Roadmap

Method development:
Categorize the employed numerical methods used within FLOW, leading to efficient use of the expertise by exchanging knowledge on available numerical methods. Specific projects include:

- To develop numerical algorithms based on mathematical formulations that include dissolution of the air in an air pocket into the liquid, or evaporation and condensation of the liquid vapour. This can be naturally included in diffuse interface models. This should then allow prediction of the size and appearance or disappearance of air/vapour pockets, depending on the ambient pressure, the properties of the liquid, dissolved gases, the electric field, etc.
- To investigate the possibility to predict sound that is generated and scattered by fluid-structure interaction via experiments and advanced FEM simulations, using so called unified continuum description for robust fluid-structure coupling and adaptive mesh refinement with error control.

High-performance computing:
Act as a coordinator for ongoing and future activities using large-scale computer resources. Sample projects include:

- To numerically study the tip-vortex breakdown generated by wind turbine rotor blades and the wind turbine wake interactions. These issues are of particular relevance when studying the setup of wind-turbine farms in which the mutual interaction between individual turbines strongly affects to the total energy production. Collaboration with J. Sørensen and S. Ivanell.
- First simulation of Lagrangian particles in complex geometries using Spectral Element Method. These studies would eventually allow for a better prediction of e.g. pollutant transport through blood veins. Collaboration with P. Fischer and C. Casciola.
- Extend Reynolds number range for turbulent boundary layers using large-scale DNS. Contribute to the fundamental discussion of near-wall regeneration cycle, appearance of coherent structures in the boundary layer. Such projects are directed towards a deeper understanding of the ubiquitous turbulence on solid walls, and eventually allow a reduction of drag.
- To study energy cascade processes in wall-bounded stratified turbulence by means of large-scale DNS. Develop suitable subgrid-scale models for the efficient simulation of atmospheric boundary-layer flows. Improved models for climate prediction are potential outcomes of these projects.

Postprocessing:
Provide and collect experience in using advanced methods for handling of large-scale simulation data. Act as general landing point for interested (internal/external) researchers. Specific aspects include:

- Develop and contribute to large-scale visualisation efforts.
- Provide and encourage a well-maintained and centralized database for storage of scientific data for open access by other researchers to build up a well-maintained data base for simulation data in Sweden.

Coordination:
Specific action items include:

- Coordination of applications to DEISA/PRACE within FLOW. A coordinated approach to such pan-European applications is crucial for successful and continuing participation.
- Initiate regular meeting within the research area to discuss current issues; organize tutorial relating to commonly used software, such as IDE, debuggers etc. in an effort to cross-fertilize efficient working environments. Share knowledge on core e-Science aspects such as visualization tools, optimization on new computer architectures etc.
- Initiate and define the collaboration with application experts and researchers from core areas. Collaboration with PDC and NSC
- Extend the available course curriculum in the area of e-Science and – together with the FLOW and KCSE graduate schools – suggest possible extensions/improvements.
- Act as contact point for commercial software distributers if requested by members.