Technical Report

Perspectives of High End Computing

A Joint Workshop of the
Munich Computational Sciences Centre and
KONWIHR
Garching, Dec. 7, 2005

The Munich Computational Sciences Centre is a cooperation of the Munich Universities LMU and TUM, the Bavarian Academy of Sciences and Humanities (BAdW), the Max-Planck-Society and its Computing Centre Garching (RZG), and Leibniz-Rechenzentrum (LRZ).

KONWIHR is the Competence Network for Technical and Scientific High Performance Computing in Bavaria.
Preface

In spring 2006 the new national supercomputing system at Leibniz Computing Centre (LRZ) will be installed. It will replace the current high-end system at LRZ, the Hitachi SR8000-F1.

In preparation for user operation on the new system, LRZ organized a workshop to identify potential applications and users of the new system in collaboration with the Computing Centre Garching (RZG) of the Max-Planck-Society, and KONWIHR, the Competence Network for Technical and Scientific High Performance Computing in Bavaria.

The workshop provided the opportunity to discuss and explore the potential of the new system and of the applications which are intended to run on it. It brought together researchers and computing centre staff. The goal of the workshop was to share understanding and experiences, to foster research communities, to learn from each other and to envision future directions in high performance computing. The workshop was intended as a forum for project presentations and a first step in the process of allocating resources to projects.

The time allotted for each presentation was approximately 20 minutes plus five minutes for discussion. The Workshop topics included:

- Planned user applications and their requirements
- Experiences with the migration system and current status of HLRB2
- Configuration and resource management of the new system
- New application areas
- Potential collaborations between research groups
- Requirements for support, software, tools and libraries
- Discussion with computing centre staff about resource allocation and modes of operation

The workshop showed again the manifold complex and challenging problems that can only be solved with high-end systems. The resource requirements – especially the computing times – for many proposed projects are huge. For the most ambitious ones the time requirements range up to one million CPU hours. For the most advanced codes single processor and cache optimization seems to be understood, and the focus on the algorithmic side shifts to issues which arise from the usage of many hundreds of processors.

Traditionally, computational fluid dynamics and physics have been main consumers of high performance computing systems; but presently, other disciplines like chemistry and biosciences are also pushing the limits of problem sizes. The need for incorporating more and more physics, to compute quantitatively more accurate results, and use large model domains is extremely demanding.

It became obvious, that there will be definitively enough scientific requests to fully load the capacities of the new high end system at LRZ from the very beginning. Thus, it will be a difficult task for the reviewers and the steering committee of the Höchstleistungsrechner in Bayern to properly and fairly balance the assignment of allocations and resources to the proposed projects.

Munich, February 2006

Matthias Brehm
## Contents

1. Parallel Astrophysical Codes on SGI Altix Systems – M. Wetzstein (Universitäts-Sternwarte LMU) .................................................................1

2. Simulating the formation of structure in the Universe – Volker Springel (Max-Planck-Institut for Astrophysics) .............................................................7

3. Modeling turbulent thermonuclear combustion – Prof. Dr. Wolfgang Hillebrandt, Friedrich Röpke (MPI für Astrophysik) ..................................................21

4. Multi-dimensional simulations of core collapse supernovae – Ewald Müller, H-Thomas Janka (Max Planck Institut für Astrophysik) .............................................28

5. The FEARLESS Cosmic Turbulence Project – Prof. Dr. Jens Niemeyer (Uni Würtzburg).35

6. Simulations of Black Holes in Numerical General Relativity – Prof. Dr. Bruegmann (Universität Jena) .........................................................................................45

7. Simulation of Lattice QCD at Physical Quark Masses – Prof. Gerrit Schierholz (DESY)....54

8. Lattice QCD with chirally improved quarks (for the Bern-Graz-Regensburg collaboration) – Prof. C. Gattringer (Universität Graz) .......................................................62

9. Many-body dynamics in quantum optical systems – Dr. Andreas Buchleitner (MPI für Physik komplexer Systeme) .............................................................................67

10. Simulation of Ultrafast Chemical Reactions – Dr. Irmgard Frank (Institut für physikalische Chemie, LMU).................................................................................75

11. Reconstructing a Tree of Life from DNA Sequence Data by High Performance Computing – Dr. Harald Meier (TU München) ...........................................................................85


13. Direct Numerical Simulation (DNS) of zero pressure gradient turbulent boundary layer flow – Ph.D. George Khujadze (TU Darmstadt) ..........................................................110

14. Adaptive Hoehstleistungssimulationen zur Kurzzeitprognose von Ueberflutungserignissen - Prof. Manfred Krafczyk (TU Braunschweig) .................111

15. Large three-dimensional direct numerical simulations of convective turbulence – Dr. Wolf-Christian Müller (Max-Planck-Institut für Plasmaphysik) ..........129

16. Numerical aerodynamic research activities at the Lehrstuhl fuer Aerodynamik – Dr. Christian Stemmer (TU München) .........................................................................134
17 Challenges in computational Seismology: Earthquakes and the Structure of the Deep Interior – Michael Ewald (Geophysics Section, LMU)........................................................................ 151
Parallel Astrophysical Codes on SGI Altix Systems – M. Wetzstein (Universitäts-Sternwarte LMU)

M. Wetzstein  Universitäts-Sternwarte der LMU
F. Heitsch, P. Ciecielag, T. Naab, A. Burkert
Simulation Codes

- **Flash**
  - adaptive mesh refinement
  - hydro modules: PPM, Kurganov, MHD
  - nuclear burning, conductivity, cosmic expansion, etc.
- **Proteus**
  - fixed grid, finite volume scheme
  - gas-kinetic flux splitting based on Bhatnagar-Gross-Krook model
  - Navier-Stokes, MHD + resistivity, 2 fluids, tracer particles and fields
- **VINE**
  - particle based, N-body + Smoothed Particle Hydrodynamics (SPH)
  - tree for gravity + special purpose hardware GRAPE

Our Machine

- **SGI Altix Bx2**
  - 48 Intel Itanium2 cpus
  - 1.5 GHz, 4MB L3 cache
  - 64 GB memory
  - Disk space: 7 TB SAN via 2 Fibre Channel cards
- **MicroGRAPE for gravity calculation**
  - PCI cards with special purpose ASICs
Porting the Codes to Altix

- Very little effort necessary
- Several useful tools & scripts by SGI for performance analysis
- Optimization of several specific parameters
  - MPI: SGI environment variables
  - OpenMP: Intel compiler environment vars.
- Some problems with Intel Fortran compiler

FLASH - Performance on Altix

- Hydro: Sedov blast wave
- Hydro + Grav: dense cloud moving in low density environment
Proteus - Performance on Altix

Turbulent molecular cloud

VINE - Single CPU Performance

Gravity: 7 Mio particle DM halo
SPH smooth: 3.5 Mio particle molecular cloud
SPH evolved: same simulation, later evolutionary state (more clumpy)
**VINE – Parallel Scaling**

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**Special Purpose Hardware**

- GRAPE (Gravity Pipe), University of Tokyo
  MicroGRAPE: PCI card, 4 GRAPE-6 chips, equivalent speed 125 GFlops
- Modified software libraries for IA64 of SGI Altix
VINE with GRAPEs

- GRAPE designed for collisional N-body
- Gravity calculation on GRAPE scales linear for small particle numbers
- In combination with tree code, interaction lists are reasonably short, in linear regime of GRAPE

Linear scaling of gravity calculation

7 Mio particles:
force calculation on GRAPE 14 times faster than on 1 CPU on host

Summary

- Altix offers extremely competitive performance
- Porting codes easy, helpful tools for performance optimization
- Successfully ported 3 large codes
- Flash: modest parallel efficiency, due to intrinsic code structures, highly problem dependent
- Proteus: good efficiency
- VINE: very high efficiency
  large benefits of GRAPE usage
2 Simulating the formation of structure in the Universe – Volker Springel (Max-Planck-Institut for Astrophysics)

Simulating the Formation of Structure in the Universe

Volker Springel
Simon White

- The Universe as an initial conditions problem
- Tree and TreePM algorithms for gravitational force calculation
- Parallelization for distributed memory computers and code scalability
- Coping with large data sets
- Science possible on HLRB-2
Cosmology has arrived at a **standard paradigm** for structure formation in the universe

**BASIC TENETS OF THE CDM MODEL**

- There was a hot big bang
- Most of the matter is dark, non-baryonic, and weakly interacting
- The universe is spatially flat and vacuum-dominated at present
- Structure formation was seeded by inflation

---

The initial conditions of cosmological structure formation are now **almost unambiguously known**

**THE MICROWAVE SKY**

*WMAP Science Team (2003)*
In principle, simulations of the CDM cosmology should be able to reproduce the variety in shapes and sizes of observed galaxies.

\[ \Omega_m = 1 \text{ flat space-time} \]

\[ \Omega_\Lambda = 0.73 \text{ Cosmological Constant "Dark Energy"} \]

\[ \Omega_0 = 0.27 \text{ Matter} \]
Dynamics of Structure Formation

Gravity
- general relativity, but
  - Newtonian approximation in expanding space usually sufficient

↓

dark matter is collisionless

↓

Monte-Carlo integration as an N-body system

↓

3N coupled, non-linear differential equations of second order

Hydrodynamics
- shock waves
- radiation processes
- star formation
- supernovae
- black holes, etc.

Problems:
- N is very large
- All equations are coupled to each other

Two conflicting requirements complicate the study of hierarchical structure formation

DYNAMIC RANGE PROBLEM FACED BY COSMOLOGICAL SIMULATIONS

Want small particle mass
to resolve internal structure of halos

Need large N
where N is the particle number

Want large volume to obtain representative sample of universe

Problems due to a small box size:
- Fundamental mode goes non-linear soon after the first halos form. Simulation cannot be meaningfully continued beyond this point.
- No rare objects (the first halo, rich galaxy clusters, etc.)

At any given time, halos exist on a large range of mass-scales!
**Cosmological N-body simulations have grown rapidly in size over the last three decades**

* "N" AS A FUNCTION OF TIME *

- Computers double their speed every 18 months (Moore's law)
- N-body simulations have doubled their size every 16-17 months
- Recently, growth has accelerated further. The Millennium Run should have become possible in 2010 – we have done it in 2004!

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The first article on the Millennium Simulation has been a cover story in *Nature*

**COMPUTATIONAL PHYSICS APPEALS TO A GENERAL SCIENCE AUDIENCE**

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**E V O L U T I O N O F T H E U N I V E R S E**

Supercomputer simulation of the growth of 20 million galaxies
The simulation was run on the *Regatta* supercomputer of the RZG

**REQUIRED RESOURCES**

1 TByte RAM needed

16 x 32-way Regatta Node
64 GByte RAM
512 CPU total

**CPU time consumed**

350,000 processor hours

- 28 days on 812 CPUs/16 nodes
- 38 years in serial
- ~6% of annual time on total Regatta system
- sustained average code performance (hardware counts) 400 MFlop/s
  - 5 x 10^17 floating point ops
- 11000 (adaptive) timesteps

**The Universe has structure on all scales...**

need large $L/\epsilon$, and spatial adaptivity
Gravity is the driving force for structure formation in the Universe

Hierarchical Tree Algorithms

The $N^2$-scaling of direct summation puts serious limitations on $N$...

But we want $N \sim 10^6$-$10^{10}$ for collisionless dynamics of dark matter!

Idea: Group distant particles together, and use their multipole expansion.
- Only $\log(N)$ force terms per particle.

---

The TreePM technique combines the advantages of PM-method and Tree-algorithm

The Tree-PM Force Split

Periodic peculiar potential

$$\nabla^2 \phi(x) = 4\pi G [\rho(x) - \bar{\rho}] = 4\pi G \sum_{i} \sum_{j} \frac{m_i}{|x - x_j - n L| - \frac{1}{L^3}}$$

Idea: Compute the long-range force with the PM algorithm, and only a local short-range force with the tree.

Let's split the potential in Fourier space into a long-range and a short-range part:

$$\phi_{k}^{\text{long}} = \phi_k \exp(-k^2 r_s^2)$$
$$\phi_{k}^{\text{short}} = \phi_k \left[1 - \exp(-k^2 r_s^2)\right]$$

Solve with PM-method
- CIC mass assignment
- FFT
- multiply with kernel
- FFT backwards
- Compute force with 4-point finite difference operator
- Interpolate forces to particle positions

Solve in real space with TRFF

Advantages of this algorithm include:
- Accurate and fast long-range force
- No force anisotropy
- Speed is insensitive to clustering (as for tree algorithm)
- No Ewald correction necessary for periodic boundary conditions
The cosmological code GADGET-2 is a versatile and portable code

**PRIMARY FEATURES**

- New symplectic integration method
- Higher speed of the tree algorithm
- Less memory consumption for tree and particle storage (~100% saving)
- Code may be run optionally as a TreePM hybrid code
- SPH neighbour search faster
- Conservative SPH formulation
- Fully consistent dynamic tree updates
- Additional types of runs possible (e.g. 2D, hydrodynamics-only, long periodic boxes)
- Efficient and clean formation of star particles
- More physics
- More output options, including HDF5
- Still fully standard C & standard MPI. The FFTW and GSL libraries are needed.
- Reduced communication overhead, better scalability, arbitrary number of cpus
- Built in parallel group finder

---

Physics in GADGET-2 for simulations of galaxy formation

- Radiative cooling, UV background (homogeneous)
- Subresolution multiphase model for the ISM: Star formation and feedback
- Phenomenological model for galactic winds
- Detailed chemical enrichment
- Thermal conduction
- Magneto-hydrodynamics
- Non-thermal relativistic component (cosmic rays)
- Growth of supermassive black holes and AGN feedback
- Bubble heating and feedback by AGN
- Shock detection
- Long-range scalar interactions in the dark sector (multiple charges implemented)
- Time variable viscosity
- Navier stokes equation and physical viscosity
- On-the-fly generation of gas particles (stellar winds & SPH refinement)
For fixed timesteps and large cosmological boxes, the scalability of GADGET-2 is very good

RESULTS FOR A "STRONG SCALING" TEST (FIXED PROBLEM SIZE)

256³ particles in a 50 h⁻¹ Mpc box

The tree-algorithm of Gadget-2 has been optimized for providing better memory locality

REDUCTION OF CACHE MISSES AND DOMAIN DECOMPOSITION

Idea: Order the particles along a space-filling curve

Hilbert's curve: A fractal that fills the square
The space-filling Hilbert curve can be readily generalized to 3D
THE PEANO-HILBERT CURVE

A space-filling Peano-Hilbert curve is used in GADGET-2 for a novel
domain-decomposition concept
HIERARCHICAL TREE ALGORITHMS

Domain are obtained by exiting the
Peano-Hilbert curve into segments
The simulation produced a multi-TByte data set

**Data size**
- One simulation timeslice: 360 GByte
- we have stored 64 outputs
- Raw data volume: 23 TByte

**Structure of snapshot files**
- The particles are stored in the sequence of a 23^12 Peano-Hilbert grid that covers the volume. On average, 800 particles per grid-cell.
- Each output is split into 8^3 = 512 files which roughly map to subcubes in the simulation volume.
- Each file has ~20 million particles, 600 MB.

- A hash-table is produced for each file of a snapshot. Each entry gives the offset to the first particle in the corresponding cell of the 23^12 grid, relative to the beginning of the file.
  - Size of table: 512 x 128 KB = 64 MB
  - Allows random access to particle data of subvolumes.

**FoF group catalogues**
- Are computed on the fly
- Group catalogues: length of each group and offset into particle list
- Long list of particle keys (64 bit) that make up each group

**The distribution of dark matter on large scales**

**Dark Matter Density, color-coded by density and velocity dispersion**

125 Mpc/h
The millennium simulation tracks the formation of 20 million galaxies in a representative piece of the Universe

DARK MATTER AND GALAXY DISTRIBUTION IN A CLUSTER OF GALAXIES

---

**PROJECT 1**

**GIMIC – Galaxy-Intergalactic Medium Interaction Calculation**

*A proposal by the Virgo Consortium*

*Science: Explain the metal enrichment of the Universe*

- Carry out 1 large, ultra-high resolution simulation to study Lyman-alpha forest in different environments, and its relation to galaxy formation.
- **1 billion dark matter** and **1 billion gas particles** of 1/64 the mass resolution of Millennium embedded in a high-resolution region, gravitational softening 1.25 kpc/h, **mass resolution in gas 2.0x10^6 Msun/h**, in dark matter 1.4x10^7 Msun/h.
- total memory requirement: 450 GB, could be run on 256 CPU power4 partition in 500,000 cpu-hours to a target redshift of z=1.6
- 25 times slices of ~100 GB each should be stored, ~2.5 – 3.0 TB data volume.
PROJECT 2

**Ultra-highly resolved dark matter halos ("Millennium")**

Julio Navarro, Simon White, Volker Springel, Carlos Frank, Adrian Jenkins

- Carry out ultra-high resolution simulation of individual Milky Way halo with 1-2 billion dark matter particles (~20-100 improvement over all published work)
- Mass resolution ~10^3 Msun
- Memory requirement: 500 GB, ~2,000,000 million cpu-hours on power4

**Science:**
Resolve the core structure of dark halos – this is a critical challenge for LCDM

PROJECT 3

**Galaxy collisions with supermassive black holes and quasar activity**

Volker Springel, Tiziana Di Matteo, Lars Hernquist

- Carry out ultra-high resolution simulations of galaxy mergers including Milky Way halo with black hole feedback, use of order 100 million gas and dark matter particles per galaxy
- Memory requirement: 100 GB, ~1,000,000 million cpu-hours on power4 per run

**Science:**
Understand the role of supermassive black holes for galaxy formation
Conclusions

- Direct numerical simulations have become an indispensable tool for studying non-linear structure formation in the $\Lambda$CDM concordance model.

- We have implemented new numerical methods which allow us to carry out unprecedentedly large, high-resolution cosmological N-body simulations. We achieve $N>10^{10}$, with a formal dynamic range of $10^9$ in 3D. The need to increase $N$ remains present.

- For cosmological simulations with homogeneously sampled initial conditions, scalability up to thousands of processors is reached with our distributed memory code.

- Computational challenges now primarily lie in improving the treatment of baryonic physics, such as star formation and accretion onto supermassive black holes, and in ultra-high dynamic range simulations of collisionless dynamics.

- Access to HLRB-2 would allow us to reach several important science goals.
Modeling turbulent thermonuclear combustion – Prof. Dr. Wolfgang Hillebrandt, Friedrich Röpke (MPI für Astrophysik)

Modeling Thermonuclear Combustion in Type Ia Supernovae in 3D

Wolfgang Hillebrandt & Friedrich Röpke
MPI für Astrophysik
Garching

In collaboration with ....
Jens Niemeyer,
Martin Reinecke,
Wolfram Schmidt,
Claudia Travaglio,
Sergei Blinnikov,
Elena Sorokina,

......
Motivation:

- The “accelerating Universe”
- The nature of the “Dark Energy”
The "standard model"

Explosion energy:

Fusion of
\[ C+C, \, C+O, \, O+O \]
\[ \Rightarrow \ "Fe" \]

Laminar burning velocity:
\[ U_L \sim 100 \, \text{km/s} \ll U_S \]

Too little is burned!

How to model thermonuclear flames?

- The "flames" cannot be resolved numerically.
- The amplitudes of turbulent velocity fluctuations in the length scale of the flame are determined on the integral scale.

\[ \frac{\partial G}{\partial t} = -D_f \, \nabla G \]
\[ D_f = v_0 + s_{\text{tur}} \, n; \, |\nabla G| = 1 \]
Effective burning velocities in SN Ia

The (up to know) biggest simulation:
- "4π"
- 1024^3 grid
- initial resolution near the center ≈ 800 m
- moving grid
- Local & dynamical sgs-model
- ~ 1000h on 512 proc. of the IBM Regatta at RZG!

Ropke et al. (2005)
Some (preliminary) results

- $E_{\text{kin}} = 8.1 \times 10^{50}$ erg
- Iron-group nuclei (mostly $^{56}\text{Ni}$): $0.61 \ M_{\odot}$
- Intermediate-mass nuclei: $0.43 \ M_{\odot}$
- Unburnt C+O: $0.37 \ M_{\odot}$ (less than $0.08 \ M_{\odot}$ at $v < 8000 \text{km/s}$ !)
- $V_{\text{max}} \approx 17.000 \text{ km/s}$

Röpke et al. (2005)

Note: The code scales to 4000 CPUs (and beyond ?) on an IBM Blue Gene!

A few results and predictions

(mostly based on models with low resolution)

1. Light curves

(Sorokina et al. 2004, 2005)

V-band LC's
2. “Metallicity” dependence of the LC’s

(Model “b30_3d”)

Weak metallicity dependence (in agreement with Timmes et al. 2003)

3. “Abundance tomography”

SN 2002bo ....... and a model
Future projects and challenges

- A new generation of “full-star” models:
  To predict light curves and spectra based on variations of physical parameters!

- Ignition conditions:
  Center/off-center? In one point? Multiple points?

- Combustion physics:
  Deflagration/detonation transition?
  “Active” turbulent combustion?
4 Multi-dimensional simulations of core collapse supernovae – Ewald Müller, H-Thomas Janka (Max Planck Institut für Astrophysik)

**Multi-dimensional simulations of core collapse supernovae**

Joint Workshop on "Perspectives of High End Computing", Garching, December 2005

Ewald Müller & H-Thomas Janka
Max-Planck Institut für Astrophysik

**Core collapse supernovae:** neutrino-driven delayed explosion (Wilson 82, Bethe & Wilson 85)

- Neutrinos stream freely through stellar envelope \( (\tau << 1) \)
- Neutrinos heat matter in semi-transparent post-shock region \( (\tau \sim 1) \)
- Neutrinos diffuse out of opaque proto-neutron star \( (\tau >> 1) \)

Illustration adapted from Mazzacappa (2003)
State-of-the-art 2D hydrodynamic simulations with

Boltzmann v-transport, realistic EOS, relativistic gravity, and realistic progenitors

2D HD + (1.5D + 2D) NuTrans: $3 \times 10^{17}$ ops/simu, i.e. $10^7$ s @ 30Gflops, or $10^6$ s @ 3Tflops

Snapshots from an axisymmetric
180° simulation of a non-rotating
11.2 $M_{\odot}$ progenitor
(Buras, Rampp & Janka 2003)  

$\rightarrow$ weak explosion (0.3 foe)!

The computational challenge:

a) **6D radiation + 3D hydrodynamics problem**
   multi-flavor, multi-d transport of neutrinos (fermions!)
   coupled to
   multi-d multi-fluid self-gravitating hydrodynamic flow
   most important SN explosion physics occurs in
   semi-transparent region $\rightarrow$ Boltzmann solver

b) **very different time and length scales**
   covering up to 10 orders of magnitude in time and space
   $\rightarrow$ implicit treatment of transport equations, symmetry
   assumptions, adaptive grids (AMR)
Approaches to numerical transport:

* trapping schemes

* flux-limited diffusion reduces dimensionality!

* variable Eddington factor technique:
  solve Boltzmann transport equation (BTE)
  & moments equations (ME)

* S-N solver: discretize BTE in all variables huge matrices!

* Monte Carlo method: reconstruct phase space very costly
  distribution (fermions!) by direct sampling for dynamics!

* Question: choice of reference frame (comoving, mixed, or
  fixed) and coordinates (Eulerian or Lagrangian)?

Specialities of neutrino transport in supernovae:

* diffusion or free streaming and stiff matter interactions limit
time step ---> implicit schemes advisable

* velocity fields & general relativistic effects

* energy (frequency) bin coupling

* interaction kernels nonlinear (stimulated absorption); transport
equation of integro-differential character

* neutrino-antineutrino coupling

* many time steps necessary ---> conservation form of lepton
  number, energy & momentum equations advantageous!

* coupling to hydrodynamics: different radial grids and temporal
  stepping ---> operator split techniques
The curse of the dimensions

- Boltzmann equation determines neutrino distribution function in phase space:
  \[ f(r, \theta, \phi, \Omega, \Phi, \epsilon, t) \]
- Integration over momentum space yields source terms for hydrodynamics:
  \[ Q(r, \theta, \phi, \epsilon, t), \dot{Y}_\nu(r, \theta, \phi, t) \]

Solution approach

- **3D hydro + 6D** direct discretization of Boltzmann Eq. (no serious attempt yet)
- **2D hydro + 5D** direct discretization of Boltzmann Eq. (planned by Holschneider at TU Munich)
- **2D hydro + ray-by-ray-plus** variable Eddington factor method (MPA)

Required resources

- \(\geq 1.10\) PFlops (sustained)
- \(\geq 10-100\) TFlops/Bytes
- \(\geq 1\) TFlops, \(\leq 1\) Byte

Selected neutrino radiation hydrodynamics milestones

in core collapse simulations

(Cardall et al., 2005, astro-ph/0510794)

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<td>A5 Crystal</td>
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<td>No</td>
<td>2.3</td>
<td>1 (3/4)</td>
<td>1 (3/4)</td>
<td></td>
</tr>
<tr>
<td>A5 Crystal</td>
<td>2004</td>
<td>No</td>
<td>2.3</td>
<td>1 (3/4)</td>
<td>1 (3/4)</td>
<td></td>
</tr>
<tr>
<td>Los Alamos</td>
<td>2004</td>
<td>Yes</td>
<td>2.3</td>
<td>1 (3/4)</td>
<td>1 (3/4)</td>
<td></td>
</tr>
<tr>
<td>Los Alamos</td>
<td>2004</td>
<td>Yes</td>
<td>2.3</td>
<td>1 (3/4)</td>
<td>1 (3/4)</td>
<td></td>
</tr>
</tbody>
</table>

Total dimensions:

average of "fluid space dimensions" and "\(\nu\) space dimensions"
added to "\(\nu^2\) momentum space dimensions"
The MPA “Boltzmann“ Supernova Code

**VERTEX (1D), MuDBaTH (2D)**

**Hydrodynamics: PROMETHEUS**
* based on Riemann solver, 3rd order PPM
* time-explicit
* approx. general relativistic (GR) potential

**Neutrino transport: variable Eddington factor technique**
* moments equations for lepton number & neutrino energy
* closure by solution of Boltzmann equation
* fully time-implicit
* multi-frequency (energy-dependent)
* order v/c
* approx. GR (relativistic redshift & time dilation)
* state-of-the-art description of neutrino-matter interactions

**Neutrino transport in 2D**: multi-energy, “ray-by-ray” solution of Nν one-dimensional problems

---

**Implicit discretization**

- Discretize MEs with backward time differencing (e.g. Euler, Gear, etc.):
  \[ U^{n+1}_i = U^n_i - \Delta t \sum_j R_{ij} (U^{n+1}) \]
- Newton-Raphson:
  - Linearize the algebraic equations:
  - Solve the linear system for \( \delta U \)
  - Iterate to convergence

- Structure of Jacobian for moment eqs. in PROMETHEUS/VERTEX supernova code:

  **Dense Blocks**: Coupling in energy, due to source terms
  (collision term of Boltzmann eq.)

  **Diagonals**: Coupling in radius
Inversion of Block-Pentadiagonal Matrix

- Major computational kernel
- Three direct solvers implemented at present
  - **THOMAS**: Block-Thomas algorithm vectorized over energy (i.e. within the blocks, using LAPACK, BLAS)
  - **CYCLIC**: Block-Cyclic-Reduction vectorized over energy
  - **VCYCLIC**: Block-Cyclic-Reduction vectorized over radius (i.e. along the diagonals)
- THOMAS solver superior if number of energy bits $N_E \geq 20$
- For $N_E \leq 20$, VCYCLIC solver may be faster due to short vector length within blocks

2\times N_E + 1

Block length:

2\times N_E + 2 \quad \text{for calls within ME/BE iteration}

4\times N_E + 2 \quad \text{for final call}

---

**One cycle of the entire algorithm**

```plaintext
Do n = 1...Nsteps_hyd
  Do for all 0
    hydro_advect_r
  end
  eos
  poisson
  Do for all r
    hydro_advect_theta
  end
  eos
  poisson
  end
  Do for all r
    transp_advect_theta
  end
  Do for all 0
    transp_r
  end
```

- Coarse grain parallelism
- Vectorization
- Coarse grain + vectorization

"Hydro": Needs 0.5% of total serial time

Transport. Needs 99.5% of total serial time
### Preliminary benchmark results of MPA supernova neutrino radiation hydrodynamics code (SGI Altix 3100 Bx2, 1.6 GHz, 6MB L3-Cache)

<table>
<thead>
<tr>
<th>$N_{\text{CPU}}$</th>
<th>CPU time [s]</th>
<th>speed-up</th>
<th>efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>19266</td>
<td>1.63</td>
<td>0.82</td>
</tr>
<tr>
<td>8</td>
<td>4384</td>
<td>7.18</td>
<td>0.90</td>
</tr>
<tr>
<td>16</td>
<td>2361</td>
<td>13.3</td>
<td>0.83</td>
</tr>
<tr>
<td>32</td>
<td>927</td>
<td>34.0</td>
<td>1.06</td>
</tr>
<tr>
<td>64</td>
<td>530</td>
<td>59.4</td>
<td>0.93</td>
</tr>
<tr>
<td>128</td>
<td>353</td>
<td>89.1</td>
<td>0.70</td>
</tr>
<tr>
<td>256</td>
<td>366</td>
<td>86.0</td>
<td>0.34</td>
</tr>
</tbody>
</table>

Flow: $400 (r) \times 256 (\theta)$  Neutrinos: $234 (r) \times 256 (\phi) \times 18 (\gamma)$

Amdahl's law for 99.65% parallel code: 128 CPUs --> speed-up 88.6
256 CPUs --> speed-up 135.3
5 The FEARLESS Cosmic Turbulence Project – Prof. Dr. Jens Niemeyer (Uni Würzburg)
Numerical explosion models

The SN Ta LES code (Garching, Würzburg):

- numerical solution of the (reactive) Euler equations with finite volume method (FVM) on a uniformly expanding grid
- initial model: Chandrasekhar mass C+O white dwarf
- local flame speed is governed by local turbulence intensity (see & Hillebrandt 86, 88)
- turbulence intensity is obtained from subgrid-scale (SGS) model for unresolved turbulent kinetic energy
- uses a level set flame model (Gardner, Hillebrandt & Müller 98)

\[ \alpha = (u x + s_x) \cdot \nabla \alpha \]

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Large Eddy Simulations (LES)

Idea:
- explicitly solve dynamical equations on scales \( \Delta > L \)
- invoke a subgrid-scale model on smaller scales

\[
\begin{align*}
1/L & \quad 1/\Delta & \quad 10/\eta_K \\
\log \kappa &
\end{align*}
\]

energy containing inertial dissipative
resolved subgrid

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Large Eddy Simulations (LES)

Method:
- decomposition of hydro eq. s I eq. for unresolved turbulent energy $k_{res}$
- closure problem I need models for diffusion, dissipation, and production of $k_{res}$

- eddy viscosity closure with localized, dynamical determination of $C_v$
  (Germain 1992, Schmidt, IN Hillebrandt 2005)

Tests of localized closure
(Schmidt, JN, Hillebrandt, subm. to A&A)
Isosurfaces of turbulence energy with contours of the rate of energy transfer:

explicit  localized closure
Numerical Dissipation

Finite volume methods (e.g. PPM) smooth the flow on length scales $\leq 10\Delta$
Kinetic energy is numerically dissipated which mimics the energy transfer from resolved toward subgrid scales

\[
\frac{1}{L} \quad \frac{1}{\Delta}
\]

Problems:
- Overestimation of temperature in adiabatic gas
- Overestimation of compressibility in isothermal gas (turbulence; $\gamma = 5/3$)
- No turbulent transport

thermal energy

$O(1)$ error if cutoff at sonic length

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---

FEARLESS = LES on Adaptive Meshes

Reasons for combining AMR and LES:
1. Flow variables in standard AMR interpreted as smooth quantities; refinement neglects existing velocity fluctuations on small scales $k = \frac{2\pi}{\Delta}$ for large refinement ratios (e.g., star formation) this is the dominant source of fluctuations on small scales
2. Goal: refine on transients, treat stationary turbulence with SGS model
   Local rate of energy transport provides natural refinement criterion

\[
\begin{align*}
&k_1 \quad k_2 \quad k_3 \quad k_4 \\
&\text{refinement} \quad \log k \quad \text{subgrid scale model} \quad \text{thermal energy}
\end{align*}
\]

Challenges:
1. Traditional filtering procedures and closure parameters optimized for uniform grids
   I use localized closure (Gerrero 2002; Schmidt, NIH Hillebrand 2003)
2. Forcing of refined modes I solved "in theory", to be implemented

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Structured Adaptive Mesh Refinement  
(Berger and Colella 1989)

\[ k_0 \gg \sigma_1^2 \]
\[ \sigma_1 \gg k_0^{1/2} \]
\[ k_1 \gg \sigma_2^2 \]
\[ \sigma_2 \gg k_1^{1/2} \]

FEARLESS turbulence simulations

**goal:**
- a toolbox for simulations of intermittent, multiscale, multiphase, turbulent astrophysical flows.

**elements:**
1. current implementation into UCSD’s cosmological hydrocode Enzo (Stone et al. 2008)
   - adaptive mesh refinement à la Berger & Colella
   - PPM hydro + particle-mesh gravity + “chemistry”
   - MPI, HDF5
2. stochastic forcing with autocorrelation time \( T_{\text{corr}} \) and arbitrary combination of solenoidal and dilatational modes (Eswara R. Poesch 1999, Schmidt, 2003)

**under development:**
3. localized subgrid-scale turbulence model including “forcing of refined modes” (Max Schmidt 2018)
4. level-set method for multiphase gas and/or fast reactions (nuclear, atomic, molecular) (Rapke, Schmidt, Jnr)

**computing:**
- currently at SARA/HL as part of the “DEISA Extreame Computing Initiative” (DECI)

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AMR simulations of supersonic turbulence

Kritsuk, Norman & Padoan, astro-ph/0411626:
- AMR simulation of MW turbulence using Enzo
  with effective resolution of 18243
- power spectra and velocity structure functions of
  uniform grid simulations reproduced with AMR, but
  results are sensitive to refinement criteria

DEISA and/or HiBB-2 simulations:
work in progress (quasi-DNS):
- comparison of supersonic turbulence in isothermal
  and adiabatic EOS, various forcing schemes,
  uniform and AMR, database for SGS runs

planned (PEARLESS):
- application of PEARLESS to contemporary
  systems and primordial star formation (e.g., as well as
  galaxy cluster turbulence expected)

The role of turbulence in star formation

Issues:
1. formation of Brown Dwarfs by
   turbulent fragmentation (e.g., Padoan, Kritsuk, Norman, Reddell) or
   gravitational disc fragmentation (e.g., Bai, Bonnell)?
2. do turbulent cores fragment (Bonnell, Cohl) or form massive stars
   (Mckee, Tan)?
3. disagreement between SPH and
   Eulerian AMR simulations on small scales.

Potential PEARLESS contribution:
- SGS turbulence will stiffen the EOS
  reduced compressibility of molecular clouds
- "Taming of refined modes" more fluctuations on small scales than standard AMR but
  perhaps less than SPH; noise level at grid scale given by local turbulence intensity.
Galactic scales: a subgrid model for turbulence-regulated star formation


- Assumptions:
  1. Star formation in virialised, supersonically turbulent GMCs
  2. Density PDF is lognormal
  3. Gas collapse in regions where local $|F_{\text{circ}}| > F_{\text{th}}$

- SFR is given by:

$$\dot{M} \propto SF R_{\text{ff}} \frac{k_{\text{sgs}} \Omega_{\text{vir}}}{t_{\text{ff}}} \frac{M_{\text{gas}}}{t_{\text{ff}}}$$

FEARLESS projects:

1. Calibrate SFR$_{\text{ff}}$ with DECI simulations of supersonic turbulence
2. Use SSS turbulent energy as input for local SFR in subgrid model for star formation; compare with alternative approaches (cf. Spiegel & Hernquist 2002)

---

The First Star Revisited

Abel, Bryan & Norman (2001)

Motivation for revisiting primordial star formation with FEARLESS:

- Astrophysical and cosmological importance, well-defined problem
- ABN provided well-studied testbed for comparison
- Large refinement ratio: strong test for "forcing of refined models"
- Subgrid-scale turbulent transport important for heat and angular momentum transport during protostar formation
Galaxy Cluster Turbulence

Major issues:
1. observability (Sunyaev, Niemeyer, Bressan, unfortunately not with Suzaku/XMM)
2. production of turbulence during cluster formation and major mergers
3. volume filling factor of turbulence from substructure wakes
4. turbulence from buoyant plasma plumes (e.g., Bregman; Enßlin, Heinzen, Knorre et al.)
5. B-field amplification with fluctuation dynamo (e.g., Raga, Afanasyev et al.; Sunara, Shiokawa; Enßlin, e.g.)
6. cosmic ray acceleration
7. cluster core heating
8. numerical dependence on method (e.g., Dolag et al.) and refinement criteria

FEARLESS projects:
1. comparison of refinement criteria on turbulence production/location, volume filling factor, spectra, etc.
2. with level-set and/or MHD: non-diffusive plasma plumes; SGS turbulent dynamo

Instead of conclusions: Suggestions

1. increased sharing of expertise within the German CFD/turbulence community
   “turbulence working group” under framework of KONWIHR?

2. database of turbulence DNS and LES
   unified analysis tools
   facilitate comparison of methods, codes, physics
Localized SGS model for turbulence

Model assumption:
- mean rate of energy transfer $\Sigma$ is asymptotically scale invariant in the inertial subrange. I use a local test filter to compute $\Sigma$.

It does not assume:
1. stationarity
2. incompressibility

.. image:: figure.png
   :alt: Localized SGS model for turbulence

W. Schmidt
Evidence for Kolmogorov turbulence in SNOB simulation

Compensated power spectra show Kolmogorov scaling:

W. Schmidt

Turbulence Simulations with Adaptive Mesh Refinement (AMR)

AMR and turbulence - potential problems:
- structures not sufficiently localized | global refinement needed
- spurious creation of vorticity at level boundaries (Pewaj)
- dissipative scales still unresolvable in most cases | LES required

Promising properties of turbulence for AMR (Kitsuk, Honkan, Patao 2004):
- dissipative structures not volume-filling (vortex filaments or shock sheets | fractal dimension of cascade carriers 0 - 1 or 2)
- since N \sim \text{Re}^{0.8}, the no. of degrees of freedom might be significantly reduced by AMR with adequate refinement criterion
Simulations of Black Holes in Numerical General Relativity

Solve the Einstein equations on the computer.

In particular, solve the two-body problem of general relativity, compute gravitational waves.

Black Holes and Grav. Waves = “vacuum”

Black holes are out there

Gas Disk in Nucleus of Active Galaxy M87
The two-body problem of general relativity is unsolved: 

\[ t_{\text{numerical}} = \begin{cases} 7M, & '97 \\ 30M, & '99 \\ 100M, & '01 \\ 200M, & '04 \end{cases} \]

(in merger regime)

- inspiral post-Newtonian approx.
- plunge/merger full numerical relativity
- ring-down close limit approx.

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SFB/TrReg 7  
http://www.tpi.uni-jena.de
(3+1)D General Relativity (ADM 62)

- 3+1: \[ 4M = R \times 3\Sigma \]
  \[ ds^2 = -(\alpha^2 - \beta^\alpha \beta_\alpha) dt^2 + 2\beta_\alpha dx^\alpha dt + g_{ab} dx^a dx^b \]
  metric \[ g_{ab}(t, x) \]
  extrinsic curvature \[ K_{ab}(t, x) \]

- Einstein equations
  \[ \rightarrow \text{evolution} \]
  \[ \rightarrow \text{constraints} \]

\[ \begin{align*}
0 &= \nabla_b (K^{ab} - g^{ab} K) \equiv D^a \\
0 &= R + K^2 - K_{ab} K^{ab} \equiv H \\
\partial_t g_{ab} &= -2\alpha K_{ab} + \nabla_a \beta_b + \nabla_b \beta_a \\
\partial_t K_{ab} &= -\nabla_a \nabla_b \alpha + \alpha (R_{ab} + K_{ab} K - 2 K_{ac} K^{c}) \\
&\quad + \beta^c \nabla_c K_{ab} + K_{ca} \nabla_b \beta^c + K_{cb} \nabla_a \beta^c
\end{align*} \]

---

Brief summary of brief 3d binary black hole evolutions

Black hole simulations tend to go unstable and “crash” at infinities.

The field is young:
- 1995: 3d Schwarzschild
- 1999: grazing collision inside ISCO
- 2001: plunge from ISCO/pre-ISCO
- 2004: first last orbit

Traditional merger simulations used to last for no more than \( t = 30-40M \) before merger.

Orbit simulations for large separations typically last for less than 10% of an orbit.

For the “last orbit” of the inspiral roughly \( t = 100M \) is required.
Brief history of brief 3d binary black hole evolutions

Schwarzschild: Aminios, Camarda, Massó, Seidel, Suen, Towns 95; Daues 96 (shift)
BB 96 (PMR, excision); Alcubierre, BB 00 (stable 3+1 evolution)
Kidder, Scheel, Teukolsky 01 (spectral)

single black hole: Allen, Camarda, Seidel 98 (3d dist)
Cook, Huq, Klasky, Scheel, Grand Challenge 98 (Cauchy evolution, excision)
Gomez, Mara, Lehner, Winicour, Grand Challenge 98 (stable characteristic evolution)
e.g. Duez, Shapiro, Yo 04; Rezzolla et al. 04 (matter collapse)

axisymmetric collision: Baker, BB, Campanelli, Lousto 00 (Lazarus); AEI 03

non-axisym, black hole binary, grazing collision:
BB 97, 99 (BAM, punctures); AEI 00-04 (Cactus, waves)
Pitt-PSU-Texas 00-04 (Maya, excision)

plunge, "pre-ISCO" through ring-down
Baker, BB, Campanelli, Lousto, Takahashi 01; Baker, Campanelli, Lousto, ...
(Lazarus)
AEI 01, 04 (merger, corotation)

orbit
BB, Tichy, Jansen 04; Pretorius 05

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SFB/Transregio 7
http://www.tpi.uni-jena.de

Sonderforschungsbereich/Transregio 7
Gravitational Wave Astronomy

Orbiting Black Holes
Numerical Relativity
Jena

Jose Gonzalez
Mark Hannam
Sascha Husa
Ulrich Sperhake
Niels Lohmann
Lucia Santamaria

A collaboration of 50 scientists including 27 Ph.Ds in 14 projects.
1.5 MEuro/year since 1.1.2003, funded by the German Science Foundation.
Grazing Collision: spins aligned/zero/antialigned with orbit

Numerically zero

$3 \times 10^{-4}$
Resources for black hole orbit simulations

Example:
Finite Differencing on Cartesian grids
Mostly explicit time stepping, no elliptic solves
Memory requirement grows as $3^n$ power with resolution, flops as $4^n$ power

Need about $1000^3 = 10^9$ grid points
100 to 160 variables per grid point, 8 bytes/variable/point, 1 kB/point
Total memory of $10^{23}$ bytes = 1 TB
Orbit near merger requires about 2000 time steps, want 10 orbits or 20000 steps
5000 flops per point per timestep means $10^8$ flops/point for 10 orbits

10 orbits require $10^8$ Teraflop and 1 Terabyte
= 1 data point out of a template set of more than $10^9$
resources are getting there, so far 768x768x384 for 1/4 of an orbit
use AMR for better accuracy
Resources for black hole orbit simulations

Machines:
SGI Origin 2000, starting 1997, 32 cpus locally, 256 at NCSA
T3Es at Garching and Berlin
Hitachi SR8000-F1, LRZ, 2000-02, Seidel and BB, 1100000 cpu hours
NPAC/NRAC 2002/3, Seidel, BB et al 1000000 cpu hours
Penn State, Linux Cluster, 40 nodes
Jena, Linux Cluster, 24 nodes (Megware)
Cray, Opteron (Strider) HLRS

BAM (‘bifunctional adaptive mesh’, BB 96, 97, 99, 03, Jansen, Tichy 04, Gonzalez 05)

Light-weight, small group code

- Explicit finite difference schemes on 3d Cartesian grids
- Multigrid elliptic solver
- Programmed in C
- Tensor equations are compiled into C using Mathematica (and MathTensor)
- Basic cell based adaptive mesh refinement
- MPI parallelization by domain decomposition
- Plug-and-play modularity

```
~/bam/exe> bam
Welcome to bam. BAM or proof, that is the question.
Usage: bam name.par
Thank you for running bam.
~/bam/exe>
```

Status 12/05:
- BBH initial data
- stable single black hole
- BBH orbit to 150M

New:
- fixed mesh refinement for Schwarzschild and BBH orbits (reasonable up to 128 processors) (BB 96, 99, Luminati 99; Schnetter, Hawley, Hawke 04; Centrella et al 04, Pretorius 04)
First benchmarks

Iris Chistadler

Altix2: out of the box performance
4 - 6% of peak, 260 - 530 MFlops/s
Optimization planned!

Altix2 (SGI)
64 Itanium
1.6GHz, 4GB/cpu

Ikon (SUN):
80 dual Opteron
2.4GHz, 4GB/cpu
Infiniband, gcc

Fixed Mesh
Refinement
5x80^2 = 3.7 GB
5x128^2 = 15 GB
Summary

- Numerical relativity is closing in on a long-standing goal: astrophysical information for BH mergers
- There are many research and job opportunities, astrophysical – analytical – numerical – computational

1995: Schwarzschild in 3d
1999: Grazing Collision
2002: S0M for plunge from ISCO
   - Ps4 in x-y plane
   - lapse based excision mask
   - corotating coordinates
   - AEP/PSTU/NNK
2004: one orbit

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7 Simulation of Lattice QCD at Physical Quark Masses – Prof. Gerrit Schierholz (DESY)

Simulation of Lattice QCD at Physical Quark Masses

G. Schierholz
Deutsches Elektronen-Synchrotron DESY

– QCDSF Collaboration –

(Berlin-DESY-Edinburgh-Leipzig-Liverpool-München-Regensburg)

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DESY
Lexington
ZIB Berlin
FU Berlin
Edinburgh

DFG

ComHP

FOR 465
QCD

Quantum Chromodynamics is considered to be the theory of the strong interactions. It binds quarks and gluons, the smallest building blocks of matter, to nucleons and mesons, and these to nuclei. The forces are so strong, that quarks and gluons are not observed in isolation. This phenomenon is called quark confinement.

\[
\text{Force } \approx 10^t
\]

Task

- To solve QCD from first principles without any model assumption
- To understand the mechanism of quark confinement and dynamical symmetry breaking (mass generation)

This is prerequisite to any understanding of dynamical symmetry breaking in the electroweak sector of the Standard Model (Higgs mechanism) and in Grand Unified Theories (GUT).
In particular

- Fundamental constants of QCD
  - $\Lambda_{QCD}$, $\alpha_s(Q^2)$
  - Quark masses

- Light hadron spectrum
  - Baryon spectrum, pentaquarks
  - Glueballs, hybrids, exotics

- Decay constants

- Hadron structure
  - Form factors, parton distributions
  - Generalized parton distributions

- Weak matrix elements
  - CKMM, $\epsilon'/\epsilon$

- QCD vacuum
  - Condensates

Many of these quantities are needed to interpret ongoing and future experiments at DESY, CERN, SLAC, RHIC, TJNAF, FERMILAB, GSI, etc., and to put them on a sound theoretical basis.

---

**Lattice QCD**

$$\mathcal{P}(U^{(0)}_\mu) \propto \int \prod_x D\bar{\psi}(x) D\psi(x) e^{-S_F - S_G}$$

$$= \det\left(D(U^{(0)}_\mu) + am\right) e^{-S_G}$$

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^N \mathcal{O}(U^{(0)}_\mu)$$

Generate sequence of configurations - HMC
Preferred fermionic actions

**$O(a)$ improved Wilson fermions**

$$S_F = \sum_x \bar{\psi}(x) (D_W + m_0) \psi(x)$$

$$-\frac{1}{4} c_{SW} g^2 a \sum_x \bar{\psi}(x) d_{sw} F_{\mu\nu}(x) \psi(x)$$

Transfer matrix, local $\checkmark$

Breaks all chiral symmetries on the lattice – restoration to $O(a^2)$ feasible

**Overlap fermions**

$$S_F = \sum_x \bar{\psi}(x) \left[ \left( \frac{D}{a} - \frac{m}{2} \right) \left( 1 + \frac{X}{\sqrt{X^2 X}} \right) + m \right] \psi(x)$$

$$X = D_W - \frac{\rho}{a}$$

$U(N_f) \times U(N_f)$ chiral symmetry on the lattice

$O(100)$ times more CPU-time consuming

---

**Present Status**

$O(a)$ improved Wilson fermions $N_f = 2$

![Graph showing the present status](image)

$0.07 \, \text{fm} \leq a \leq 0.12 \, \text{fm}$,  $1 \, \text{fm} \leq L \leq 2.2 \, \text{fm}$

Hitachi SR8000
A representative result

**Generalized parton distribution** \( H_u(x, b^2, Q^2) \)

**Probability of finding a \( u \)-quark with fractional energy \( x \) in the proton at impact parameter \( b \).**

Similar results are obtained for spin & transversity distribution in the fast moving polarized nucleon.

---

**Extrapolation to physical limit by \( \chi^P T \) + Hemmert**

For a controlled error estimate: \( m_\pi \lesssim 400 \text{ MeV} \)
Algorithm and Performance

Lattices

\[ 24^3 \times 48, \ 32^3 \times 64, \ldots \]

Hybrid Monte Carlo (HMC) algorithm

- Molecular Dynamics integration to propose new configuration
- Acceptance/reject step every time the whole system is updated

Kernel \( \approx 80\% \) of CPU time

- Conjugate gradient
- Multiplcation of fermion matrix (M) times vector (V)
- M sparse: connects nearest neighbors only
- Essentially \( V \times V \)
- Domain decomposition: small local volumes, large demand on communication
- Elements of M and V are \( 4 \times 3 \) and \( 3 \times 3 \) complex matrices

Algorithmic improvements

Sexton & Weingarten

Hasenbusch

QCDSF

Further improvement: HMC \( \rightarrow \) RHMC

\[ Y = 24 \times 48 \]
\[ a = 0.07 \text{ fm} \]
- CP-PACS
- Staggered
Performance on Altix 3700

- Matrix times vector multiplication
  \( M \times V \) programmed in Assembler
- Local volume fits into L3 cache
- Single CPU performance 5.2 Gflops
- Communication method
  - `shmem pointers & prefetch`: 1.22 Gflops/CPU
  - `shmem_get`: 1.28 Gflops/CPU
  - `shmem_put`: 1.97 Gflops/CPU
  - `fastcopy`: 1.97 Gflops/CPU
- Overall performance
  - 8 CPUs: 2.63 Gflops/CPU
  - 16 CPUs: 2.24 Gflops/CPU
  - 32 CPUs: 2.16 Gflops/CPU
- \( \mathcal{O}(10\%) \) of peak performance

Expect to increase the performance on Altix 4700 (and in particular on Montecito processor)

---

Plans

\( \mathcal{O}(\alpha) \) improved Wilson fermions \( N_f = 2 \)

\( L = 2 \text{ fm} \) 1000 Configurations

\( L = 3 \text{ fm} \) 1000 Configurations

\( m_c/m_b = 0.3 \iff m_\pi \approx 250 \text{ MeV} \)

\( \iff \text{Well within convergence radius of NNLO } \chiPT \)
Anticipated results

![Graph showing relationship between $m_B$ and $m_\pi^2$ with quenched overlap legend.]

Reduce errors on hadronic observables to 5% and better.

CPU-time Request

| Year  | Expected 
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
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<tbody>
<tr>
<td>2006</td>
<td>$O(10)$ T\text{flops} x year</td>
</tr>
<tr>
<td>2007</td>
<td>$O(30)$ T\text{flops} x year</td>
</tr>
<tr>
<td>2007++</td>
<td>$O(100)$ T\text{flops} x year</td>
</tr>
</tbody>
</table>
8 Lattice QCD with chirally improved quarks (for the Bern-Graz-Regensburg collaboration) – Prof. C. Gattringer (Universität Graz)

Main topics addressed in the last 4 years:

Example: Formula for calculation of pion mass $m$

$$\int D[U] \left\| D_{t,0}^{-1}[U] \right\|^2 e^{-S[U]} \det(D[U])^{\frac{1}{n!}} = ae^{-mt} + be^{-Mt} \ldots$$

- Development of Dirac operators with good chiral properties: CI and FP.
- Chiral properties of QCD: $\Sigma$, $\chi_{top}$, $m_t$, $m_s$, $f_s$, $F_\pi$ ... .
- Spectroscopy of excited hadrons for light quarks.
- Analysis of topological excitations in the QCD vacuum.
- Algorithmus for simulations with dynamical CI and FP fermions.
Type of calculations/algorithms used in Lattice QCD

\[ \int D[U] \| D_{t_0}^{-1}[U] \|^2 \ e^{-S[U]} \ det (D[u])^{N_t} \]

- Markov chain evolution of \( U \) according to \( e^{-S[U]} \ det (D[U])^{N_t} \).
- Molecular dynamics evolution for calculation of \( det (D[U])^{N_t} \).
- \( D \) is a matrix of size: \( \mathcal{O}(10^6 \times 10^6) \) – \( \mathcal{O}(10^7 \times 10^7) \).
  \( \Rightarrow \) linear algebra with very large matrices.
- Calculation of \( D^{-1} \) with, e.g., conjugate gradient.

Previous results, Example 1: Topological excitations of the QCD vacuum

Without filtering a gluon field configuration is dominated by quantum fluctuations.

The low-lying eigenvectors of the Dirac operator are a filter for the relevant infrared structures.
Previous results, Example 2: Excited hadrons on the lattice

- Excited states correspond to subleading terms $\Rightarrow$ very weak signal.
- New techniques for more realistic wave functions were developed.

Achievements:

- 21 Publications in refereed journals (NPB, PLB, PRD, PRL), with an average citation of 20.8, and 18 contributions to proceedings.
- >60 Presentations (colloquiums, seminars, invited talks ...)
- 8 PhD Theses, 10 Diploma Theses.
- Project is integral part of the DFG Forschergruppe Gitter Hadronen Phänomenologie.
Central goal for the next period: QCD with dynamical sea quarks

- Many of our results were obtained in the *quenched approximation*, which neglects sea quarks by setting $\text{det}D[U] \equiv 1$.

- The main objective for the near future is the incorporation of light dynamical sea quarks.

- Physics perspectives (build on existing expertise):
  - Compare to other chiral formulations of QCD.
  - QCD at small quark masses.
  - Spectroscopy of excited hadrons.
  - Excitations of the QCD vacuum.

Current status of algorithmic development

- **Standard HMC update with suitable adjustments.**

- Both the CI and FP operators extend over several lattice sites.  
  - Terms must be pre-calculated and stored.

- Smearing with stout links.  
  - Differentiable action.

- Calculation of fermionic force in the MD evolution is hard coded.

- All steps are parallelized via domain decomposition of the lattice.

- Algorithm is working and is currently tested on $12^3 \times 24$ lattices (upcoming publication is in preparation).
Example results from current test runs on small volumes

The algorithm decorrelates the configurations well and we observe frequent tunneling to different topological sectors also for our smaller quark masses.

Anticipated achievements and resources needed

In 3 years from now we aim at results for:

- QCD with dynamical quarks on a volume of $(2 \text{ fm})^3 \times 4 \text{ fm}$.
- At least 2 different lattice spacings, with 4 quark masses each.
- Pion masses well below 300 MeV $\Rightarrow$ chiral perturbation applicable.
- Similar observables as studied in the quenched approximation $\Rightarrow$ systematic analysis of quenching effects.

Based on our experience with the currently running code we estimate the cost to be 8 TFlop Years, distributed over 3 years (2006 $\sim$ 2 TFY, 2007 $\sim$ 2 TFY, 2008 $\sim$ 4 TFY).
Many-body dynamics in quantum optical systems – Dr. Andreas Buchleitner (MPI für Physik komplexer Systeme)

Many-body dynamics in quantum optical systems

Andreas Buchleitner

Max-Planck-Institut für Physik komplexer Systeme, Dresden

Garching, 7 December 2006
In Collaboration with . . .

D. Delande (Paris)  C. Eltschka (Regensburg)  B. Grémaud (Paris)
L. Hilico (Paris)    K. Hornberger (München)   A. Krug (Erlangen)
J. Madroñero (München)  P. Schlagheck (Regensburg)  K. Taylor (Belfast)

funded by DAAD, European Union, European Science Foundation,
DFG, VolkswagenStiftung, Bavarian Academy of Sciences, RZG

Research Lines

• Highly excited atoms in strong external fields

• Quantum transport phenomena with (ultra)cold atoms

• Scaling issues in quantum information

• common ground: complex quantum dynamics in terms of (resonance) spectrum •

Guiding principle for computational physics:
The quest for quantitative precision is as arduous as it is important.
Bertrand Russell, ABC of Relativity
**Universal ionization threshold of one electron Rydberg states**

**PhD Andreas Krug 2001 – now Siemens Erlangen**

Identical parameters in theory and experiment – for H, Li, Na, Rb

\[ n_0 = 28 \ldots 80, \omega/2\pi = 36 \text{ GHz}, t = 327 \times 2\pi/\omega \]

\[ F_0 = F \times n_0^2 \] and \[ \omega_0 = \omega \times n_0 \]

Experimental evidence of universal threshold in T.F. Gallagher’s group! Experiments in contact with theory under way!

---

**Anderson localization of the ionization yield**

- **Anderson**: subsequent transmission and reflection events
- **atoms**:
  - transmission → absorption
  - reflection → emission
  - disorder → detuning
  - configuration space → energy

Quantum suppression of diffusive transport (here in energy space)

**ATOMS CEASE TO ABSORB PHOTONS!**

Analogous phenomena with cold kicked atoms, photons in random media, electrons in disordered solids
Driven helium
PhD Javier Madroñero 2004 – now TU München

Non-integrable
- high dimensional Hamiltonian chaos
- sequential vs. nonsequential ionization under strong laser pulses
- multidimensional tunneling effects

The Hamiltonian of planar helium
Representation in creation and annihilation operators

Unperturbed Hamiltonian $H_0$ - 433
Jacobian $J$ - 1411
Field term $F$ - 5472
Nondispersive wave packets in driven 2D helium

wave packets in phase space (projection along field polarization axis)

field-free autonization rates

\[ \omega_k = \ldots n/2 \ldots n \quad (\text{left to right}) \quad N = 6 \]

life times approx. 700...1000 field cycles

N excitation of the inner electron

dimension does matter!

generalizes nondispersive wave packets in one electron systems

novel tool of coherent control

Research Lines

- Highly excited atoms in strong external fields

- Quantum transport phenomena with (ultra)cold atoms

- Scaling issues in quantum information
**Many particle interactions**

**ultracold atoms**

**compound nuclei**

*TODAY: CONTROLLED INTERACTIONS WITH ULTRACOLD ATOMS IN OPTICAL LATTICES*

---

**Research Lines**

- Highly excited atoms in strong external fields
- Quantum transport phenomena with (ultra)cold atoms
- Scaling issues in quantum information
Entanglement in composite, open quantum systems

Key challenges

- Entanglement, a central resource of quantum information processing
  \[ |\Psi\rangle \neq |\phi\rangle \otimes |\chi\rangle \]

- How does "entanglement" scale with the number of system components?

Research Lines – Perspectives

- Grand challenges in atomic physics
  - control of atomic/molecular fragmentation processes; 3D He

- Quantum transport phenomena with (ultra)cold atoms
  - microscopic/spectral understanding of quantum statistics
    - how few are "many" particles?

- Scaling issues in quantum information
  - macroscopic/multipartite limit of entanglement

[Anand, Horberger, Zilinger, Physics World 2005]

All this cooks down to solving high-dimensional eigenvalue problems!
Estimated resources

- formal problem: spectral theory
  - generalized eigenvalue problem
  - complex or hermitian
  - sparse banded or sparse

- computational approach
  - Larezos algorithm, MPI portable (T3E, Hitachi SR8000, IBM regatta, Beowulf cluster Université Paris 6)
  - not all eigenvalues but only those in the energetically relevant range are required
  - crucial limitation is memory space rather than computation time, due to polynomially (or even exponentially) increasing dimension of matrices to be diagonalized

- anticipated needs over the next three years
  - memory 1...20(40) TB
  - CPU time (very) approx. 800000 hours

---

!!!THANKS VERY MUCH,
FOR SPLENDID SUPPORT DURING THE LAST YEARS,
TO THE LRZ AND RZG CREWS!!!
10 Simulation of Ultrafast Chemical Reactions – Dr. Irmgard Frank (Institut für physikalische Chemie, LMU)

Simulation of Ultrafast Chemical Reactions

Irmgard Frank

Department Chemie und Biochemie
Ludwig-Maximilians-Universität München

Chemical reactions: motion on potential surfaces

Number of points of potential surface = Number of points / (number of dimensions)
Full determination of potential surface not possible for medium size molecules. 0 dynamics 'on the fly'

Department Chemie und
Car-Parrinello molecular dynamics

- Electronic structure: density-functional theory
  (standard functionals: LDA, BLYP, BP, ...)
- Valence electrons: plane waves, periodic boundary conditions (also surfaces, solids)
- Inner electrons: pseudopotentials
- Motion of nuclei: Newton dynamics ‘on the fly’
  according to the Car-Parrinello equations
- Description of chemical reactions (breaking and formation of bonds)
- Limitations (1 processor):
  about 100 atoms, 1 nm³, 10 ps

Highly reactive systems

- Destabilised by mechanical stress:
  silicone materials under strain (project h0622)
- Activated by electronic excitation (photoreactions):
  cis-trans isomerisation in rhodopsin (project h0621)
- Reactive mixtures
Siloxanes under tensile stress: why do they break that easily?
(in collaboration with Wacker Chemie GmbH)

Long siloxanes: formation of ions

Short siloxanes: proton transfer, neutral products

Ongoing CPMD Simulations of Siloxane Materials under Tensile Stress

Breaking of single polymer: more statistics
Influence of environment: Hydrolysis by surrounding water molecules, no influence of HMD

Polymer covalently attached to surface: Influence of surface, comparison to actual AFM single molecule experiments

Next step: Simulation of crack propagation
K. Lipton, C. Niereboeck, B. Artieres, J. Wei.
Simulation of excited state reactions

- Photoreactions are fast, in many cases accessible to unconstrained on-the-fly simulations
- Need for a method that is suitable for excited state simulations: such a method should
  - be fast
  - have a simple gradient
  - be robust
  - be free of Hartree-Fock exchange (for use with plane waves)
  - be simple to use

Systematics of single-configuration methods

<table>
<thead>
<tr>
<th></th>
<th>Hartree-Fock</th>
<th>Kohn-Sham</th>
</tr>
</thead>
<tbody>
<tr>
<td>closed-shell</td>
<td>(R)HF</td>
<td>LDA</td>
</tr>
<tr>
<td>open-shell,</td>
<td>UHF</td>
<td>LSD</td>
</tr>
<tr>
<td>unrestricted</td>
<td></td>
<td></td>
</tr>
<tr>
<td>open-shell,</td>
<td>ROHF</td>
<td>ROKS</td>
</tr>
<tr>
<td>restricted</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Butadiene: dimerisation vs excitation transfer


Larger systems: ROKS plus QM-MM
(U. F. Ruhig, I. Frank, J. Buttner, A. Laib, J. Vandervondele, U. Röthlisberger,

QM: quantum mechanical description
(MM: classical molecular mechanics)

Rhodopsin

- ROKS description of the chromophore and counterion.
  The presence of the anionic counterion significantly lowers the rotational barrier in the excited state (C. Molteri, I. Frank, M. Paminello, J. Am. Chem. Soc., 121, 12177 (1999)).
- Construction of a model in membrane-mimetic environment (25000 Atoms, stable without constraints).
**Rhodopsin**

- Chromophore
- 'Membranes'
- Protein
- Water with a physiological amount of NaCl

**Excited state motion of the chromophore**
*(elevated temperature)*

- $C_{11}-C_{12}$ bond
**Rhodopsin: before and after rotation to 90 degrees**


**Unidirectional 360 degrees rotation in a chiral nanorotor**

Outlook

Siloxanes: CRACK PROPAGATION

Photoreactions: DNA PHOTODEGRADATION

OTHER REACTION TYPES

(in part in collaboration with W. Domcke, TU)

CPU time: 300,000 – 700,000 CPU hours
64 processors or more, preferably permanent use

Dr. Elisabeth Lupton
Dr. Christel Nonnenberg
Stephan Grimn
Konstantina Danianos

Dr. Carla Moltani
Ute Bührig
Dr. Leonardo Guidoni
Dr. Alessandro Luisi
Prof. Dr. Ursula Röhlberger
Prof. Dr. Jürg Hutter
Prof. Dr. Michele Parrinello

Prof. Dr. Christoph Bräuche

Center for Nanoscience
Deutsche Forschungsgemeinschaft (SFB 486)
Fonds der Chemischen Industrie
Forschungszentrum Jülich
Leibniz-Rechenzentrum (HLR) project h0621 and h0622
Volkswagen-Stiftung
Wacker-Chemie GmbH
Comparison to other methods

Polyenes, excitation energies

Comparison with multi-reference methods and experiment

Comparison with TEDFT

* Triplet energies are lower, singlet energies are red-shifted (leading to a too low Franck-Condon region)

Department Chemie und

Comparison to other methods

Hexatriene, Rotation about Double Bonds

* Good results for double bond rotations and for open-shell ground states
* Conservation of orbital symmetry is guaranteed during an MD

Department Chemie und

LMU
**Butadiene: Isomerisation**


**Hexadiene: Ring opening**

---

**Rhodopsin excited state simulation**

11 Reconstructing a Tree of Life from DNA Sequence Data by High Performance Computing – Dr. Harald Meier (TU München)

Reconstructing a tree of life from DNA sequence data by HPC

Harald Meier, Michael Ott, K.H. Schleifer and Arndt Bode
Lehrstuhl für Rechnertechnik und Rechnerorganisation, Institut für Informatik, Technische Universität München; Lehrstuhl für Mikrobiologie, Technische Universität München

OUTLINE

1. Molecular Phylogenetic treeing

2. Maximum Likelihood + Phylogenetic Treeing

3. Previous Results

4. Future Projects / Requirements

5. Importance / Impact
OUTLINE

1. Molecular Phylogenetic treeing

5. Importance / Impact

2. Maximum Likelihood + Phylogenetic Treeing

4. Future Projects / Requirements

3. Previous Results

Why Molecular Phylogenetic Trees?

- Molecular sequence → precise information
- Phenotype insufficient for inferring phylogeny of microorganisms
- Inferring relationships of very different organisms
- Universal Marker (EF-Tu, ribosomal RNA genes, ...)
- Sequence availability ( > 100,000 rRNA gene sequences)
A Phylogenetic Tree from Gene Sequence Data

Edge (Branch)  Leaf

Branching  Root

OTU1  AC6GT C---AATCCTTTATGATGTTAAGGA...
OTU2  AC6GT C---AATCCCTTTATGATGTTAAGGA...
OTU3  AC6GT C--CCATCCAGATGACGATTAGGA6A...
OTU4  AC6GT C--GATCCACATGACGATTAGGA...
OTU5  AC6GT CCG6ATCCGGATGGACGATTAGGA...

ssu rRNA gene

Motivation: Towards a „Tree of Life“

Where we are:

- > 100,000 sequences available,

...
Motivation: Towards a "Tree of Life"

Where we want to go:
- > 100,000 sequences available
- future trees

OUTLINE

1. Molecular Phylogenetic treeing
2. Maximum Likelihood + Phylogenetic Treeing
3. Previous Results
4. Future Projects / Requirements
5. Importance / Impact
Maximum Likelihood Based Tree

- OTU1: ACATCTGAAGCTTAAAGGGT
- OTU2: ACATCTGAAGCTTAAAGGGT
- OTU3: CATCTGAAGCTTAAAGGGT
- OTU4: CATCTGAAGCTTAAAGGGT
- OTU5: CATCTGAAGCTTAAAGGGT

How Probable?

Evolutionary Model

ML - Method

Maximum Likelihood calculates:
2. Topologies
3. Branch lengths \( v[i] \)
4. Log Likelihood \( L \) of the tree

Goal: Find tree topology which maximizes likelihood

Problem I: Number of possible topologies is exponential in \( n \)

Problem II: Computation of likelihood value + branch length optimization is expensive

Solution:
1. New Heuristics + HPC
2. Algorithmic and Technical Optimizations
**OUTLINE**

1. Molecular Phylogenetic Trees

2. Maximum Likelihood + Phylogenetic Trees

3. Previous Results

4. Future Projects / Requirements

5. Importance / Impact

---

**RAxML (Randomized Accelerated ML)**

- **RAxML**
  - Phase I - Parsimony starting tree
    - stepwise addition
    - distinct starting trees
  - Phase II - Starting Tree Optimization
    - Subtree rearrangements
    - Accelerated ML - hill climbing

- **Best ML-phylogenetic analysis program**
  (Stamatakis, Ludwig and Meier, Bioinformatics, 2005)

- **MPI-based parallel RAxML Version 2**
Improved RAxML-VI

- Lazy Subtree Rearrangements (LSR)
- Automatic Determination of a good rearrangement distance
- Reduced number of tree store/restore operations
- Memory-efficient design:

<table>
<thead>
<tr>
<th>Dataset (Organisms, Baspairs)</th>
<th>RAxML</th>
<th>PHYML</th>
<th>IQPNNI</th>
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<tbody>
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<td>1000,5547</td>
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<td>8780,1217</td>
<td>930 MB</td>
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<td>2.8 GB</td>
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<td>25057,1463</td>
<td>2.7 GB</td>
<td>18.8 GB</td>
<td>7.4 GB</td>
</tr>
</tbody>
</table>
Improved RAxML-VI

RAxML/OMP: Parallelization

\begin{align*}
P[i] &= f(g(Q[i]), g(R[i])) \\
P[i+1] &= f(g(Q[i+1]), g(R[i+1]))
\end{align*}
OUTLINE

1. Molecular Phylogenetic Treeing

2. Maximum Likelihood + Phylogenetic Treeing

3. Previous Results

4. Future Projects / Requirements

5. Importance / Impact
Hybrid OpenMP/MPI parallelization

- MPI processes work on disjoint subtrees
- OpenMP parallelism within MPI processes on likelihood-vectors

Future Work - Informatics

- Hybrid OpenMP/MPI parallelization of RAxML
- Optimization for the Intel Itanium Architecture
Future Work – Phylogenetic Analysis

- Molecular Maximum Likelihood Tree of Life
  - Gene Alignment (30,000 OTUs, alignment length ~ 40,000)
  - Genome Alignment (~325 OTUs, ~100,000 bp)
  - Evaluation of ML-Topology (data-robustness, data quality)

- Comparative phylogenetic analysis

Required Resources

- 2 million CPU hours

- Memory-consumption depends on:
  - Number of sequences/organisms
  - Alignment length
  - Number of MPI-processes

- Partitioning into shared memory nodes and MPI processes will depend on dataset

- 8 GB memory per MPI process

- Personal Funding (→ KONWIHR 2)
OUTLINE

1. Molecular Phylogenetic Treeing

5. Scientific Impact

2. Maximum Likelihood + Phylogenetic Treeing

4. Future Projects / Requirements

3. Previous Results

Molecular Tree of Life – Scientific Impact

- Evolutionary Science
- Taxonomy in Biology (i.e. Bacteria + Archaea)
- Molecular Identification by Phylogeny
- Molecular Phylogenetic Signatures
- Graphical representation of molecular databases
Thank you

Dr. Harald Meier (meierh@ntum.de)

Dipl. Informat. Michael Ott,
Lehrstuhl für Rechnertechnik und Rechnerorganisation,
Institut für Informatik, TU München

Prof. Dr. Karlheinz Schleifer, Dr. Wolfgang Ludwig,
Lehrstuhl für Mikrobiologie, TU München

Foreign Partner:
Dr. Alexandos Stamatakis, IFORTH, Crete, Greece
Direct Numerical Simulations of Transitional Flow in Turbomachinery

Jan Wissink and Wolfgang Rodi

wissink@ifh.uni-karlsruhe.de

Computational details

- Simulations are performed using a second-order accurate central finite-volume discretisation with curvilinear coordinates.
- A collocated variable arrangement is used.
- Time integration is performed using a three-stage Runge-Kutta scheme.
- The code is parallelised by splitting the computational domain into several blocks of equal size.
- Each block is assigned to its own processor achieving a near-optimal load-balancing.
- Communication between processors is done using the MPI protocol.
Brief overview of current research

- LES of flow in the T106 turbine cascade with periodically oncoming wakes
  - Study of the capability of LES to reproduce experimental / DNS data
  - LES performed at both a low Reynolds number with large inflow angle and a more realistic Reynolds number with an “in-design” inflow angle.

- DNS of flow in turbine-like geometries
  - Will be discussed in more detail in this presentation.

Flow in turbine-like geometries

- Periodic unsteadiness caused by rotor-stator interaction
- Relatively low Reynolds numbers
- Both phenomena directly affect blade boundary-layer transition, tendency to separation, heat transfer and losses
Overview of the Calculations

- Flow very complex and difficult to predict with RANS
- Phenomena need to be understood and reliable data need to be generated for improving transition models
- Because of low Re - this is possible with DNS – and calculations are summarized here:
  (i) Flat plate boundary layer separation with oscillating inflow
  (ii) Flow around turbine blades
    - Separating flow past T106 blade
    - Flow and heat transfer in a MTU cascade

Flat plate boundary layer separation

Geometry

Periodic boundary conditions in spanwise direction
Reynolds number, $Re=60 000$, is based on the mean inflow velocity $U_i$ and the length-scale $L$ (see figure).
Structure of a Laminar Separation Bubble

Dividing Streamline

Transition

Laminar boundary layer
Dead-air region
Reverse flow vortex
Redeveloping turbulent boundary layer

Separating flow affected by inflow oscillations

Simulations performed

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Grid</th>
<th>Size span</th>
<th>Amplitude</th>
<th>Period</th>
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</thead>
<tbody>
<tr>
<td>O1</td>
<td>966x226x128</td>
<td>0.12L</td>
<td>0.20</td>
<td>0.01</td>
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<tr>
<td>O2</td>
<td>1286x310x128</td>
<td>0.08L</td>
<td>0.10</td>
<td>0.30</td>
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<tr>
<td>O3</td>
<td>966x226x128</td>
<td>0.12L</td>
<td>0.05</td>
<td>0.30</td>
</tr>
</tbody>
</table>
Separating flow affected by inflow oscillations (3D film)

Simulation O2

Iso-surface of the spanwise vorticity at $\alpha = 150$

Separation flow affected by inflow oscillations

Space-time plots showing the location of flow-separation

Sim. O1

Sim. O2

Sim. O3

M: Location of maximum reverse flow

Region I corresponds to the spanwise roll of turbulent flow that is shed

Region II corresponds to the remains of the re-circulation zone

Note: Increasing amplitude of oscillation results in a faster roll-up of the shear layer and a smaller separation bubble. (Compare Sim. O2 to Sim. O3)
**Separating flow affected by inflow oscillations (spectra)**

In all simulations, the most unstable frequency of the Kelvin-Helmholtz instability is approx. $f = 6.5 U_L$.

**Location of $P_1 - P_4$ in Simulation O1**

---

**DNS of a separating flow affected by inflow oscillations**

**Summary of Results**

- The basic instability is a (2D inviscid) Kelvin-Helmholtz (KH) instability of the separated boundary layer.

- This instability is triggered by the inflow oscillation.

- The frequency of the most unstable (KH) mode is found to correspond to one of the higher harmonics of the inflow oscillation frequency.

- Increasing the amplitude of the inflow oscillation results in a stronger triggering of the KH instability.
DNS of Separating Flow in a T106A Turbine Cascade at Re = 51,831

Periodic boundary conditions in the spanwise direction
Reynolds number is based on the inflow velocity U
and the length scale L (see figure)

DNS of Flow in a T106A Turbine Cascade at Re = 51,831

Simulations performed

<table>
<thead>
<tr>
<th>Simulation</th>
<th>grid</th>
<th>Span</th>
<th>WVD</th>
<th>WHW</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>$771 \times 262 \times 128$</td>
<td>0.25L</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>T2</td>
<td>$1014 \times 266 \times 64$</td>
<td>0.20L</td>
<td>25%</td>
<td>0.03L</td>
</tr>
</tbody>
</table>

WVD: Mean wake velocity deficit
WHW: Wake half-width
DNS of Flow in a T106A Turbine Cascade at Re=51831 with Periodically Passing Wakes

Close-up of Suction Side Separation near Trailing Edge

Illustration of Kelvin-Helmholtz Instability

DNS of Flow in a T106A Turbine Cascade at Re=51831 with Periodically Passing Wakes

Vortical Structures at the Pressure Side

\( \tau / T = 13.30 \)
Summary of Results

- The Pressure side boundary layer remains laminar at all times.
- Elongated vortical structures are found along the pressure side.
- A large separation bubble is intermittently found to be present along the downstream half of the suction side.
- As a consequence separation induced transition is observed somewhat upstream of the trailing edge.
- The separation bubble is periodically suppressed by the impinging wakes.
Conclusions

- DNS of transitional flow over turbine blades is possible
  - Still limited to moderate Ra and simplified geometries (2D)
- Calculations are very expensive
  - Up to 100 Mio. grid points, Dt $\sim 10^4$ L/U
  - Several months of clock time on supercomputers
- DNS not for practical applications, but increasingly important tool for studying transitional flows
  - Allows to extract all flow details
  - Provides valuable data for developing more economic/accurate transition models
- Further increase in computational power will allow to handle more complex geometries

Future Research/Computational needs

Investigation of the effect of integral length-scale of free-stream turbulence on laminar heat transfer.

- Study concerns accelerating laminar boundary layer flows with free-stream turbulence.
- Because of the large integral length-scales the typical spanwise size is significantly larger than the spanwise size used in previous simulations.
- As a result, the typical number of grid points needed is up to four times as large, i.e. up to 400 Mio. per simulation.
- Typical time-step will remain unchanged.
Future Research/Computational needs

Various simulations are planned, such as:

- Free-stream grid-turbulence and wakes impinging on an accelerating flat plate boundary layer.
- The wake of a small cylinder impinging on a large cylinder placed downstream.
- Simulation of heat transfer in a turbine cascade with incoming wakes.
  - Similar simulation has been performed before employing artificial wakes which have a different integral length-scale than the real wakes stemming from a circular cylinder.

Example

Flow over and heat transfer to a flat plate with free-stream turbulence

Computational domain
Flow over and heat transfer to a flat plate with free-stream turbulence

Contours of the instantaneous spanwise velocity:

Nusselt number distribution for various integral length-scales $\Lambda$. 
13 Direct Numerical Simulation (DNS) of zero pressure gradient turbulent boundary layer flow – Ph.D. George Khujadze (TU Darmstadt)
14 Adaptive Hochleistungssimulationen zur Kurzzeitprognose von Überflutungseignissen - Prof. Manfred Krafczyk (TU Braunschweig)

HPC-based adaptive simulations for short-term prediction of flood disasters

Manfred Krafczyk
Institute for Computer Applications in Civil Engineering

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overview

• introduction to the problem
• overview of previous results
• description of the planned work
• algorithms and parallelization strategy
• anticipated results
• required computer and software resources
• summary

07.12.2005 Perspective of High End Computing slide 2
Introduction to the problem 1

TSUNAMIS, STORM SURGES AND DAM-BREAKS
- involve the large-scale movement of solids and fluids
- are often irregular in timing and thus difficult to observe and measure
- involve multiple types of physical processes
  on a broad range of spatial and temporal scales

Computational modelling can play an important role both in helping to
- understand the nature of the fundamental processes involved and in
- predicting the detailed outcomes of various types of events in specific
  locations.

State-of-the-art is 1D/2D modeling / simulation of (potential type) flows

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New Orleans:
red lines indicate flooded area after "impact" of hurrican Kathrina

---
Introduction to the problem III

Alps flood 8/2005 following massive precipitation:

Average fill level exceeds river bank level:

Genuine 3D effect

Introduction to the problem II

Glacier – sea interaction
project idea:
support / optimization of evacuation / rescue / damage minimization measures by short term HPC simulation
overview of previous results I

base tool: research prototype Lattice-Boltzmann CFD solver

**Virtual Fluids**

- 3D
- transient
- adaptive
- multiphase / free surface
- LES
- parallel
- second-order accurate in space and time
- MPI

07.12.2005  Perspectives of High End Computing  slide 9

overview of previous results

code performance on Hitachi SR-8000:
- ~30% of theoretical peak performance per node
- parallel efficiency ~90% on 32 nodes

code performance on CAB’s Opteron cluster
(120 processors, 500 GB RAM, Myrinet):
- parallel efficiency ~95% on 120 processors
- up to 1 billion grid points (uniform grid)

07.12.2005  Perspectives of High End Computing  slide 10
drainage / imbibition process in porous media (Hitachi):

Sand CT: resolution ~ 330,000,000 Voxel
(coop. ETH Zürich - CAB TUBS - PSI)
LES-flow around sphere at $Re = 6.5 \times 10^6$

- $1.25 \times 10^8$ grid nodes
- $2.3 \times 10^7$ DOF
- parallel efficiency >95%

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**LB-simulation of turbulent flows**

**LB-LES validation**

M. Krafczyk, J. Tölke, L.-S. Luo

Large-eddy simulations with a multiple-relaxation-time LBE model


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Rodt et al.: Status of LES:

~3 CPU hours on a fast PC

course resolution simulation of wave impact on a shore line
Development of a space adaptive CFD prototype for short-term 3D flood/tsunami prediction based on automatic GIS data input to support evacuation/rescue/damage minimization measures.
Virtual Fluids

Input:
- flow BC
- GIS database (surface mesh)

3D - SST
CFD simulation
$\geq 10^{10} \text{DOF}$

Simulation cycle:
few hours

Algorithm and parallelization strategy

Bozmann equation
$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \Omega(f, f)$$

Chapman-Enskog-Expansion

Navier-Stokes equations
$$\frac{\partial \bar{u}}{\partial t} + (\bar{v} \cdot \nabla) \bar{u} = -\frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \Delta \bar{u}$$
continuity equation
$$\frac{\partial p}{\partial t} + \nabla (\bar{v} \bar{u}) = 0$$

BGK-Approximation (Bolttner, Gross, Krolik)

Lattice Boltzmann equation (LBGK)
$$f_i(t+\Delta t, \bar{x}+\xi\Delta t) = f_i(t, \bar{x}) - \frac{\Delta t}{\tau} \left( f_i(t, \bar{x}), f_i(0)(t, \bar{x}) \right)$$

Taylor + Chapman-Enskog-Expansion
algorithms and parallelization strategy II

The LB-equation

\[ f_i(t+\Delta t, x+\xi_i \Delta t) = f_i(t, x) - \frac{\Delta t}{\tau} \left( f_i(t, x), f_i^{(0)}(t, x) \right) \]

structural advantages:
- linear and exact advection operator
- conservative scheme for mass and momentum
- no numerical viscosity

algorithms and parallelization strategy III

computational aspects
- no Poisson equation is solved for the pressure
- Cartesian grid (automatic 3D grid generation)
- convergence properties:
  - LBE can be tuned to second-order accuracy with respect to the corresponding solution of incompressible Navier-Stokes flow
  - because of their explicit nature and local stencil LB models are perfect candidates for efficient parallelization
- stress tensor locally available (turbulence modelling)
algorithms and parallelization strategy IV

Optimized data structures for general geometries

- top: Peano-Hilbert, U-ordering
- bottom: Morton, N-ordering

(M. J. Albors et al., Applications of Space-Filling Curves to Cartesian Methods for CFD, AIAA-2004-1232)

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algorithms and parallelization strategy V

second order accuracy in space

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Gittergenerierung

algorithms and parallelization strategy VI

Automatic 3D grid generation

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Domain decomposition: (PAR)METIS

07.12.2005 Perspectives of High End Computing slide 28
Virtual Fluids

- Multi Relaxation Time
- second order BC
- local grid refinement
- efficient data structures
- asynchronous communication

anticipated results

feasibility proof of short term prediction / analysis of catastrophic flood events based on 3D CFD modeling and automatic input of GIS / satellite based topographic data
required computer and software resources

minimum requirements:

- sufficient (short-term) CPU share ~10 TFlops (-> 1 TFlop week)
- 1 TB byte RAM
- 10 TB byte Disk space
- F90 / C++ compiler
- parallel Debugger
- MPI 2.x?

outlook: fluid-structure interaction, debris flow

erosion, sedimentation, scouring
Summary

- The purpose of this research project is twofold:

  - In terms of **engineering** we want to develop a 3D simulation prototype for short term prediction/analysis of catastrophic flood events based on HPC-based 3D-CFD modeling.

  - In terms of **modeling / numerical methods / computer science** we want to study and optimize the performance of an adaptive kinetic CFD solution environment including pre- and postprocessing issues on massively parallel hardware.
Large three-dimensional direct numerical simulations of convective turbulence – Dr. Wolf-Christian Müller (Max-Planck-Institut für Plasmaphysik)

Large-scale simulation of three-dimensional convective turbulence

Wolf-Christian Müller, Dan Škandera
Independent Max-Planck Junior Research Group
Max-Planck-Institut für Plasmaphysik, 85748 Garching, Germany

Turbulent Convection

- mean temperature gradient common source of turbulence in the atmosphere and planetary/stellar interiors
- in plasmas possibly leads to generation of magnetic fields (turbulent dynamo effect)
- basics of convective turbulence only partially/phenomenologically understood
- inherent properties should be universal (independent of, e.g., additional physics and geometry)
- phenomenologies need to be scrutinized via direct numerical simulations
- open questions when comparing 2D/3D numerical simulations with experimental findings (Rayleigh-Bénard)
Some Basic Issues

Turbulence seemingly chaotic mixture of velocity/temperature/magnetic-field fluctuations over wide range of spatial scales → high numerical resolution

Under idealized conditions (statistical stationarity/homogeneity, $Re \sim \frac{\text{Domain}}{\text{VISCOSITY}} \rightarrow \infty$)

$\langle f(\lambda \ell) \rangle = \lambda^{\alpha} \langle f(\ell) \rangle \Rightarrow$ Power-law behavior $\langle f(\ell) \rangle \sim \ell^{\alpha}$

→ periodic boundary conditions → Fourier representation

Starting point for mostly phenomenological theories dealing with

- temporal/spectral evolution of low-order statistical moments,
  e.g. magnetic and kinetic energies, helicities, associated spectral fluxes
- spatially intermittent structure of turbulent fields/dissipation

---

Kolmogorov-Richardson Picture

Energy ($\omega$, $\omega^{3}$/m)

Large eddies

$10^{3}$

$10^{2}$

$10^{1}$

$10^{0}$

Direct cascade

$10^{0}$

Inverse cascade

$10^{-1}$

$10^{-2}$

$10^{-3}$

Drive range

Inertial range

Small-scale structures

Dissipation range

$k$ (m, mm, nm)
Incompressible Boussinesq-Magnetohydrodynamics (MHD)

Simplified incompressible fluid model:

\[ \partial_t \mathbf{v} = - (\mathbf{v} \cdot \nabla) \mathbf{v} - \nabla p - \mathbf{b} \times (\nabla \times \mathbf{b}) - \Gamma \mathbf{e}_z + \mu \Delta \mathbf{v} \]
\[ \partial_t \theta = \nabla \cdot (\mathbf{v} \cdot \nabla) \theta + \mathbf{e}_z \cdot \mathbf{e}_z + \kappa \Delta \theta \]
\[ \partial_t \mathbf{b} = \nabla \times (\mathbf{v} \times \mathbf{b}) + \eta \Delta \mathbf{b} \]
\[ \nabla \cdot \mathbf{v} = \nabla \cdot \mathbf{b} = 0. \]

- Thermal driving parameterized by Rayleigh number: \( \Gamma = \frac{\beta \Delta T^4}{\nu} \)
- Thermal diffusivity \( \kappa \)
- Kinetic and magnetic Reynolds number: \( \text{Re} := \frac{\rho \theta_0}{\mu} \quad \text{Rm} := \frac{\rho \theta_0}{\eta} \)
- Kinematic viscosity \( \mu \), magnetic diffusivity \( \eta \)
- Turbulence, if \( \text{Re, Rm} \gg 1 \), corresponds to \( \Gamma \gg 1 \)

Energy Cascade Phenomenology

- **Kolmogorov (K41)**
  - Turbulent eddies break up into successively smaller structures
  - Time-scale: \( \tau_{K1} \sim \ell / \nu_2 \) (Eddy turnover)
  - Energy flux \( v_2^3 / \tau_{NL} \sim \varepsilon \sim \text{const} \)
    - Energy spectrum \( E^E(k) \sim k^{-5/3} \)
    - Entropy spectrum \( E^T(k) \sim k^{-5/3} \) (passive scalar)

- **Bogliano-Obukhov (BO)**
  - Time-scale: \( \tau_{BO} \sim (\ell / \Gamma \theta_2)^{1/2} \) (Eucyancy)
  - Entropy flux \( \theta_2^3 / \tau_{BO} \sim N \sim \text{const} \)
    - Entropy spectrum \( E^T(k) \sim k^{-7/5} \)
  - Kinetic energy flux \( v_2^3 / \tau_{BO} \sim v_2 \theta_2 \sim \text{const} \)
    - Energy spectrum \( E^E(k) \sim k^{-11/5} \)

3D-simulations \( \rightarrow \) K41-scaling
2D-simulations/RE-experiments \( \rightarrow \) BO-scaling
**Velocity and Temperature Fluctuations**

512³ direct numerical simulation of Navier-Stokes convection \( \Gamma \sim 10^7, \text{Re} \sim 10^9 \)

**Energy/Entropy spectrum**

1024³ pseudospectral simulation (Navier-Stokes, Re \( \sim 10^9 \), \( \Gamma \sim 10^9 \))

Observed state closer to K41 than to BO

Higher Rayleigh number needed \( \sim 10^{11} \) \( \Rightarrow \) Higher Resolution \( 2048^3 \) collocation points
Simulation Code

- Pseudospectral scheme with explicit time-integration (trapezoidal leapfrog)
- Fortran90, MPI parallelisation
- scales on Cray T3E, IBM Regatta, and SGI Altix (speed-up of $\approx 1.8$ up to 1024 processors on IBM Regatta, problem size $1024^3$)
- slab-distributed memory layout (due to FFTW fast Fourier transform)
- various implemented extensions (magnetic fields, system rotation, Lagrangian tracers)
- Planned: Grid size $2048^3$, 6-16 TB Memory

Summary

- Pseudospectral parallel single-fluid code (MPI) for hydro- and magnetohydrodynamics
- Performance strongly communication dependent (→ Altix)
- Application: study of two-point statistics in turbulence
- Planned: High-resolution run with $2048^3$ to verify phenomenological fundamentals
- Planned: Magneto-convection (with/without rotation)
Numerical aerodynamic research activities at the Lehrstuhl für Aerodynamik at the TU München

Dr. Christian Stemmer, Xiangyu Hu Ph.D., Stefan Hickel, Maxim Loginov, Prof. Dr. Nikolaus A. Adams
Lehrstuhl für Aerodynamik
Technische Universität München

Numerical aerodynamic research activities

Code development and application of highly accurate numerical methods for Navier-Stokes equations for applications in the following areas:
Numerical aerodynamic research activities

Computational Fluid Dynamics on various architectures:
- Notebook
- AMD64 Workstations
- LINUX Cluster
- ALTIX 330 parallel Server
- NEC SX8 (HLRS) parallel/Vector System
- LRZ HLRE-2 massive parallel

Microfluidics I

Microfluidics:
- Small scale (0.1 μm < d < 1 mm) complex flows with surface tension and wetting effects on solid wall
- Mesoscopic complex flow involving embedded nanostructures such as colloids or DNA molecules

Applications:
- medical research, biotechnology, sensor design, lab-on-a-chip,...
Microfluidics II: Applications

A micro-mixer

in general: development of micro-mechanical systems
understanding the flow physics in small-scale devices
design of devices for tailored applications in medical devices,
control devices, measurement units, ...

Microfluidics III: A typical model problem

moving contact line problem
- Two fluids with surface tension draining in a wetting or non-wetting channel

Simulation objective
- Relation between flow speed and dynamical contact angle

Numerical method
- Smoothed particle hydrodynamics (SPH)
**Microfluidics IV: Current computational challenges**

SPH is similar to molecular dynamics (follow small particles in stead of molecules)

- High flexibilities
- High computational cost

**characteristic problem size**

- particle number for simulation N
  - current limitation on a desktop computer: \( \approx 10000 \)
  - real experiments: \( >> 100000 \)

- Ratio between numerical interface width \( h \) and domain size \( H \):
  - current limitation on a desktop computer: \( H/h \approx 10 \)
  - real experiments: \( H/h >> 100 \)

---

**Microfluidics V: Required computational power**

Small scale complex flows:

- Objective oriented MPI environment
- moderate number of parallel processors (20-30)
- 2 GB and more main memory size

Mesoscopic complex flow with DNA molecules

- 3D simulations are indispensable
- increased computing resources needed by one or two orders of magnitude

**Turbulent channel flow**
**Turbulent channel flow I**

Direct Numerical Simulation (DNS) solves the Navier Stokes equations directly without model assumptions of any kind

\[
\frac{\partial u_j}{\partial t} + \frac{\partial u_j u_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \rho}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j}
\]

Large Eddy Simulations (LES) solves the filtered Navier Stokes equations for the large scale structures and models the contribution of the small scales

\[
\frac{\partial \bar{u}_j}{\partial t} + \bar{u}_j \frac{\partial \bar{u}_i}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_j} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial \tau_{ij}}{\partial x_j}
\]

mit \[\tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j\]

**Turbulent channel flow II**

To allow for faster simulations with less points with the same quality of the results as relevant, energy carrying scales are resolved

\[\Rightarrow\] resolution requirements for DNS scale with \[Re^9\]

\[\Rightarrow\] turbulence at \[Re=10 \times 10^6\] requires simulations exceeding the capabilities of any existing supercomputer by several orders of magnitude

Development of fast and efficient numerical methods for the application in complex wall-bounded flows in technical and aeronautical applications
Turbulent channel flow III

Test case
- channel flow at $Re_x = 395$, $Re_{e,a} = 6875$
- reference DNS available for verification
- reference LES with dynamic Smagorinsky model

Grid
- $N_x = 64$, $N_y = 68$, $N_z = 48$
- stretching $y^+ = \frac{1}{\text{tanh}(C_f y)} \text{tanh} \left( C_{e,2} y \right)$

Turbulent channel flow VI

\begin{align*}
\text{original ALDM} & \quad \text{ALDM with van Driest damping} \\
\text{dynamic Smagorinsky model} & \quad \text{DNS Moser et al.}
\end{align*}
Turbulent channel flow V: Periodic hill flow

Test case
- channel with periodic restrictions (periodic hill flow)
- $L_x = 9h$, $L_y = 3.035h$, $L_z = 4.5h$
- $Re_{bulk} = 10595$ (bulk velocity and hill height)
- geometry-induced separation and reattachment
- separated shear layer and recirculation zone

Instantaneous pressure fluctuation and streamlines:

Turbulent channel flow VI: Periodic hill flow

Grid
- Cartesian grid
- $3.2 \times 10^6$ cells within fluid domain

$\rightarrow$ DNS would require $> 1 \times 10^9$ points for the same quality of the results
- no-slip walls approximated by blocking technique.
Turbulent channel flow VI: Periodic hill flow

Vortical structures on the downhill side of the periodic hill

Turbulent channel flow VII: Periodic hill flow

Good agreement with reference LES data. ALDM performs better than the dynamic Smagorinsky model.
Turbulent compressible corner flow

Motivation:
- Investigate for the development of turbulence in a corner flow
- Ramp configuration is important in engine inlets in supersonic flight as a passive compression stage
- Interaction of shock/boundary layer/turbulence
- Fundamental understanding of the flow physics

Sketch of the flowfield:
- Undisturbed boundary layer
- Shock system with \( \lambda \)-configuration
- Separation region
- Expansion in Prandtl–Mayer waves
- Reynolds number based on incoming boundary layer thickness \( \text{Re}_{in} = 63560 \)
- Mach number \( M_a = 2.95 \)
- Free-stream parameters match experimentally studied case
compressible corner flow II: computational setup

domain and grid (every 10th line is shown):
- domain size $28.66_0 \times 4.28_0 \times 4.18_0$
- gridsize $701 \times 132 \times 201$
- gridsteps in wall unit: $h_\tau^+ \approx 30-18$; $h_\gamma^+ \approx 17$; $h_\beta^+ \approx 1$ (first gridpoint)
- size in spanwise direction chosen wide enough to capture Görtler-type vortices

- 4000 CPUh on vector-parallel NEC SX-5/8 platform (OpenMP – MPI)
- 9 GB memory usage
- 200 GB of data for post processing

compressible corner flow III: results -- density distribution

spanwise averaged density field
compressible corner flow VI: results – 3D structures

colored lines: streamlines
red & blue isosurface: vortices
grey isosurface: shock (p=0.1)

compressible corner flow V: Schlieren-type visualization

density gradient averaged in spanwise direction
(Schlieren-type visualisation):
shocklets cause high turbulence intensity in outer flow

shock foot motion distance is about 1.3 \( \delta_o \)
Turbulent channel flow VI: comparison to experimental data

direct comparison of skin friction with experimentally observed oil footprint of Görtler vortices.
• experimental Re is twice as larger as in current computation
• vortex width growing towards the wall

Aerothermodynamics

Motivation:
• Wind-tunnel experiments for high Mach numbers are extremely difficult to undertake. Free-flight conditions cannot be attained in the tunnel (Darikohler number).

• Free-flight experiments are extremely expensive, happen very seldom and the exact conditions are difficult to control

• Transition prediction indispensable to predict heat load (heat transfer) for any kind of (re-)entry into atmospheres to design appropriate heat protection for space traveling vehicles
**Mars atmosphere entry – ESA Expert vehicle (test vehicle for research)**

NASA's first heat shields were dimensioned with a safety margin of 3 A "tile" from the shuttle in the size of a full-size suitcase weighs ≈ 15 pounds.

The appropriate dimensioning of the heat shield can provide a great potential for the increase in payload.

---

**Space Shuttle (needs to be replaced after 2010/12)**

Space Shuttle during reentry:

© NASA artworks © NASA Ames Division IN

temperatures above ~2000 K ongoing for about 90 sec.

failure of prediction can be catastrophic
Governing equations and chemical model

Direct Numerical Simulation – DNS

Solving the Navier-Stokes equations without model assumptions of any kind, including the continuity and the energy equation and an additional equation for the vibrational energy (including a new variable: vibrational temperature).

5 additional continuity equations for the species densities (concentrations):

\[ \frac{\partial \rho_i}{\partial t} + \frac{\partial (\rho_i u_j)}{\partial x_j} = C.S.T. \]  

(depending on: translational + vibrational temp.)


Park's 5-Element Model

- \( N_2 + M \Rightarrow N + N + M \)
- \( O_3 + M \Rightarrow O + O + M \)
- \( NO + M \Rightarrow N + O + M \)
- \( N_2 + O \Rightarrow NO + N \)
- \( NO + O \Rightarrow N + O_3 \)

17 reactions

Plettner's thermodynamic properties

\[ \mu_i = 0.1 \cdot \exp \left[ C_{\mu_i} + \left( \ln T \left( B_{\mu_i} + \ln T \cdot A_{\mu_i} \right) \right] \]

\[ \kappa_i = \mu_i \left( \frac{5}{2} \kappa_{\mu,i} + \kappa_{\lambda,i} \right) \]

\[ \kappa_{\lambda,i} = \mu_i \cdot \kappa_{\lambda,i} \]

Wilkes' mixing rule for mixture properties

\[ 5 \times 5 \] mixing terms per property per grid point

---

Species concentrations inside the boundary layer - equilibrium

Species concentration at \( x = 5.5 \) m

The species concentrations show highest rates of dissipation inside the boundary layer where highest temperatures are present (\( y \approx 0.05 \) m)

- \( \cdots \cdots \cdots \cdots \cdots c_{O_2} \)
- \( \cdots \cdots \cdots \cdots \cdots c_{N_2} \)
- \( \cdots \cdots \cdots \cdots \cdots \cdots c_0 \)
- \( \cdots \cdots \cdots \cdots \cdots \cdots E \times c_N \)

\( 10 \times c_{NO} \)
species concentrations inside the boundary layer - nonequilibrium

the dissipation is now highest closer to the wall at y=0.05m

Temperature inside the boundary layer: ideal gas ↔ non-equilibrium

ideal gas $T_{\text{max}} \approx 4900$K

non-equilibrium $T_{\text{max}} \approx 4400$K

Vibrational temperature decreases to $T \approx 2000$K
temperature development for reacting flow

Time-dependent evolution of the disturbance temperature inside the boundary layer:

Computational performance on a parallel-vector machine NEC SX8

- Vector operation ratio: 90.4%
- Average vector length: 252.9 (of 256)
- Grid size: 1001 x 15 x 255 (3.8 x 10^6 points)
- Main memory size: 11.07 GB

Time per grid point and full time step:
- 10.38 µs (>40% for thermodynamic coefficients)
- MFLOPS/Proc.: 3979 MFLOPS
- MFLOPS/Conc.: 20587 MFLOPS (speedup 6.7x)

The rate for the MOPS is 5000/Proc and 40000/8 Proc.s

Micro-multitasking capabilities (equivalent to OpenMP) of the SX FL compiler is employed (FDIR PARDISO...
### Computational needs for future full resolution projects

- **typical grid size:** 2000x64x511 (>50 Mio. points)
- **main memory size:** 100-200 GB
- **disc storage needs:** 1-2 TB
- **parallel CPUs:** ~50 CPUs with OpenMP and MPI
- **software resources:** Intel Fortran compiler – MKL lib.
  - self developed research codes

### High-speed boundary-layer transition: outlook

**future work:**

compare three-dimensional simulations at \(M=20\) of possible transition scenarios for:

- Frozen conditions
- Chemical non-equilibrium
- Thermal non-equilibrium

include further chemical & physical effects as i.e.

- catalytic surface as a boundary condition
- surface imperfections (due to impact or loss of material)

quantitative comparison with stability calculations by Johnson & Candler taking into account chemical reactions

qualitative comparison to experiments by Mironov & Maslov through harmonic point-source disturbances
17 Challenges in computational Seismology: Earthquakes and the Structure of the Deep Interior – Michael Ewald (Geophysics Section, LMU)
Numerical methods

- Finite Differences
- Spectral elements
- ADER-DG
- Parallelization using MPI (message passing interface)

Some general statements

- There is a wide gap between theoretical/numerical and observational seismology
- Computational power is now such that 3D numerical approaches to wave propagation could enter routine data fitting procedures (e.g., source or structural imaging) or monitoring
- The scientific value of 3D simulation data is continuously increasing (e.g., earthquake scenario simulations, global wave propagation) -> (some) simulations should be seen with the same priority as observations
Earthquake scenarios

- Accurate calculation of strong ground motion for regional earthquake scenarios
- Accurate prediction of hazard and risk scenarios for specific regions and time intervals
- Incorporation of earthquake scenario simulations into probabilistic hazard analysis

Dynamic Rupture

- Understanding the earthquake process
- Understanding the controlling mechanisms of earthquakes (frictional properties, strength, heterogeneities, material interfaces, etc.)
- Resulting power of seismic observations with respect to (dynamic) source parameters
- Regional conditions (intraplate, interplate, subduction zones, normal, strike, etc.)
Global Seismology

scientific objectives

- 3D wave effects of structures like plumes, subduction zones, lower mantle structure
- High resolution imaging of global earth structure (geodynamics)
- Development of 3D reference models

Volcano seismology

scientific objectives

- Monitoring volcanic activity through observation and modeling of observed seismic wave fields
- Recovering structural changes in volcanoes over time
- Monitoring changes in seismic source mechanisms
- Understanding the relation between seismic sources and the eruptive state of a volcanic system
Recent results

**Global wave propagation**: wave propagation through physically consistent Earth models
- 3D Earth models from high-resolution calculations of mantle flow (thermal convection) plus global wave propagation

**Earthquake scenarios**: towards a quantitative estimation of shaking hazard
- Scenario Modeling
- Numerical Green's functions, multiple earthquake scenarios for major active faults

---

**Global Wave propagation**

How To Build A Physically Consistent Model Planet?

- Mantle Convection Model
- Temperature Field
- Mineral Physics Model
- Velocity Model
- Wave Propagation
Global Wave propagation

Relative Amplitude Variations
3D vs. 1D average Model

Example Seismograms

Scenario Modeling in the Lower Rhine Embayment

Location, Seismicity and Hazard
Scenario Modeling in the Lower Rhine Embayment

Alsford Earthquake

- 22 July 2002
- Magnitude 4.9
- Full Area
- Slight building damage
- Numerous strong motion recordings

Scenario Modeling in the Lower Rhine Embayment

Synthetics vs. Observation

Wiggle-by-Wiggle comparison not possible

Characterize Seismograms

Key Parameters:

- Peak Ground Velocity (PGV)
- Envelope
- Spectral Content
Scenario Modeling in the Lower Rhine Embayment

Spectral Content

**Synthetics**

Amplitude Spectra - Station FLIN

**Observation**

PE, PV - Point Source Elastic
FE, FF - Finite Source Elastic
FV - Finite Source Fissure-Elastic

Scenario Modeling in the Lower Rhine Embayment

Shaking Hazard derived from Synthetics
Numerical Green's Functions

Study Area: Los Angeles Basin
Idealized Newport Inglewood Fault
Velocity Model based on SCEC Version 3
Numerical Green’s Functions

Once the complete set of numerical Green’s functions for a particular fault is calculated, various problems can be investigated with relatively little computational effort. For example:

- Variation of synthetic PGVs depending on slip distribution

Scientific conclusions

**Global seismology**

- We are now capable of **forward** modeling the global wave field through 3D structures
- **Routine calculations** and storage of theoretical seismograms for large earthquake is just starting
- The next step is the incorporation of 3D modelling into the imaging (inverse) problem (possible only with the next generation of supercomputers)

**Earthquakes scenarios**

- A new method was devised that allows the calculation of a large number of earthquake scenarios based on 3D Green’s functions
- This allows to better quantify uncertainties of shaking hazard in realistic situations
- Higher resolution simulations will allow quantitative forecasting of strong ground motions relevant to structures