NSC News 2006:3
National Supercomputer Centre at Linköpings universitet

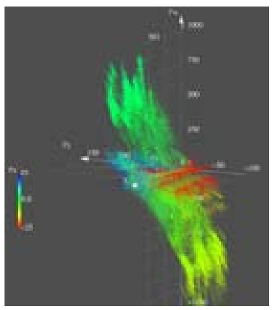
LCSC

Linux Clusters for Supercomputing

For the seventh year in a row, NSC invites you to the Linux Clusters for Supercomputing workshop.

The LCSC workshop will take place on October 17–18 at Linköping University's Campus Valla. We are proud to present professor Thomas Sterling as our key note speaker.

For more information and to register for the event, please visit http://www.nsc.liu.se/lcsc



Cosmic Candles

M. E. Dieckmann and his colleagues B. Eliasson, M. Parviainen and P. K. Shukla are examining plasma wave accelerators as a means to produce cosmic ray particles in the most energetic astrophysical environments. Such accelerators can be modeled numerically by particle-in-cell (PIC) simulations, which are performed on the Monolith cluster at NSC.

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Gamess-UK available

NSC now provides the general *ab initio* quantum chemistry program Gamess-UK 7.0 on Swegrid. The program is made available for a period of one year, after which we will consider prolonging the licence based on the experience of our users. We therefore encourage use of the program with feedback.

For detailed information on how to run the program, see http://www.nsc.liu.se/software/chemistry/gamess-uk/

After Monolith: "Duolith"

Sven Stafström
NSC Director
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NSC is now taking several steps towards becoming a major European HPC center. Just before summer we were granted 35 Mkr for a new capability HPC resource. We are of course very happy that the proposal we sent to SNIC in May was well received. Even though not granted to the full amount, it was given a substantial part of the SNIC budget. The grant is for a new capability resource, which will replace Monolith, the main resource of today, and complement Mozart, the 0.5 TB SMP system at NSC. A few months back we launched the "Duolith" project aimed at testing different (dual-core) processors and different interconnects. Today we have a pretty good picture of the performance profile of the different HPC components available at the market. The Duolith project is led by Niclas Andersson, Peter Kjellström performs most of the hardware testing and the benchmarking is done by Torgny Faxén and Patrick Norman. We are now looking forward to discussions and solutions concerning the design of the full system. Parallel to this development we are starting the construction work on the new computer building at the LiU Campus Valla. With this new building we will more than triple our floor space and cooling capacity and make a further expansion of our services to the national and international HPC communities possible.

Another very positive news item is that the technical faculty at LiU recently approved a proposal to start a new international masters program in Scientific Computing. Behind this initiative are computational intensive research groups in the fields of scientific computing, scientific visualization, structural mechanics, biomechanics, materials science, and bioinformatics. NSC will play an important role in this activity and we are certainly looking forward to welcome a group of international students to learn more about HPC.

As a further example of HPC activities at LiU, the main article in this issue of NSC News is written by Assoc. Prof. Mark Dieckmann working at LiU Campus Norrköping. We also present the Nordic Data Grid Facility (NDGF) and Leif Nixon's role in this organization as national coordinator.

Last but not least, do not forget to register for the Linux Clusters for Super Computing workshop (LCSC) which is advertised on the front page of this issue of NSC News. This year we have a focused workshop in which we present talks about multi-core technology, the exciting new "Cell" processor from IBM, and storage management such as the Lustre and dCache storage systems. As a result of a recent SNIC project focused on storage, both these systems have been introduced at NSC to serve customers with high storage needs such as SMHI, LCG and AMANDA/IceCube.

Looking very much forward to seeing you in Linköping in a couple of weeks!

Yet another acronym

The Nordic Data Grid Facility, NDGF, is a collaboration between four Nordic countries – Denmark, Finland, Norway and Sweden – funded by the national research councils. The goal of NDGF is to coordinate the various grid computing initiatives in the respective countries to create a common computational infrastructure allowing Nordic researchers to take on challenges currently out of reach of each individual country.

One important way for NDGF to facilitate this is to maintain and expand ARC, the middleware stack currently in use by Nordugrid and other Nordic grid projects, and also to develop solutions for interoperability between ARC-based grids and grids based on other middlewares, like gLite. NDGF is currently hiring several software developers for these tasks.

To coordinate the Nordic grid activities NDGF is hiring one national coordinator per country to act as liaison with the national projects and to maintain NDGF's various core grid services. The Swedish coordinator is NSC's Leif Nixon.

NDGF will also host the Nordic Tier-1 centre within the CERN-led WLCG collaboration for storing and processing the huge amounts of data that the Large Hadron Collider at CERN will produce when it comes online during 2007.

Apply for time from SNAC

It is now time to apply for allocations of high end computing capacity for 2007 through the Swedish National Allocation Committee (SNAC). Proposed projects should be submitted via the SNAC on-line application procedure at http://www.snac.vr.se/. The deadline for SNAC proposal submission this fall is November 2 at 16:00. At that time, all access to the on-line application system will be closed. Incomplete or late proposals will be discarded.

The Fast and the Ferocious

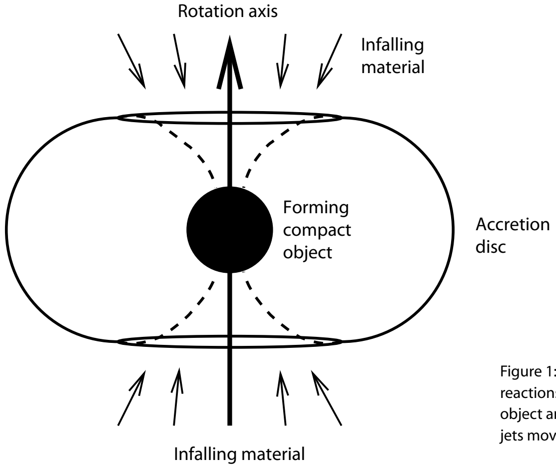


Figure 1: A massive star implodes once the internal nuclear reactions cease. Some stellar material forms the compact object and other is sometimes ejected (not shown), to form jets moving along the rotation axis.

Violent eruptions in the universe are attributed to forming, colliding or accreting compact objects, i.e. neutron stars and black holes. Compact objects are formed during supernovæ, as sketched in Fig. 1. Supernovæ are powerful enough to outshine their host galaxy, in particular if they trigger an ultraenergetic shower of cosmic rays: a Gamma Ray Burst (GRB)[1, 2]. GRBs are thought to be driven by the internal thermalization of an ultrarelativistic jet that erupts out of the imploding star, and which expands into the ambient medium with a bulk Lorentz factor above 100. Relativistic flows within the jet accelerate particles by previously unknown mechanisms and yield the prompt GRB emissions [1]. The beamed radiation of the collimated GRB jets can be observed even at cosmological distances. Their rapid changes in the emission spectrum on subsecond time scales and their sheer intensity, implies that the underlying physical processes must be fast and ferocious.

Energy source and cosmic ray generation

The emissions of accreting compact objects are powered by plasma and hydrodynamic instabilities, which convert the gravitational energy of the accreted material into plasma outflows and energetic particle- and electromagnetic (cosmic ray) radiation. We consider the interaction of electrons and protons with plasma waves and magnetic fields as a means to transfer energy from gravity-driven bulk plasma flow into cosmic ray emissions and jet flow. We invoke relativistic beams of charged particles [1] as energy sources. In contrast to dense collisional fluids like water, collisionless astrophysical plasma can sustain particle beams for long times and they relax through electromagnetic fields. A typical scenario is shown in Fig. 2. The beam relaxation gives rise to a range of wave modes. We consider the electrostatic two-stream instability driven by a proton beam, even though it is not the fastest growing one [3]. Its electrostatic potential can, however, (almost) elastically reflect charged particles (no synchrotron radiation). Elastic head-on collisions of particles with a relativistically fast potential results in enormous particle energies.

Extreme electrostatic potential

Two-stream instabilities saturate by their nonlinear interaction with the

Mats S Andersson retires

The grand old man at NSC, Mats Andersson, is retiring and will therefore leave NSC. NSC was founded in 1989, and Mats joined the centre shortly after that in February, 1992. In the beginning he shared his time between NSC and the Department of Computer and Information Science (IDA) working in the group of Professor Erik Sandewall.

Since 1996 he has been working full time at NSC. Mats has been the Technical Director at NSC from 1992 and he is very well known to most of us who have been using HPC resources in Sweden since the "good old" Cray days. He was actively involved in the procurement and the set up of the Cray XMP, YMP, C90 and T3E systems. Mats has also been particularly active in NSC:s relations to our partners Saab and SMHI and in the relations to many of the HPC vendors.

At NSC we will miss Mats, not only for his professional skills but also for his kind personality and his good sense of humor. As a highly appreciated goodbye gift to us and to other people he has been working with, Mats presented a lunch concert, where

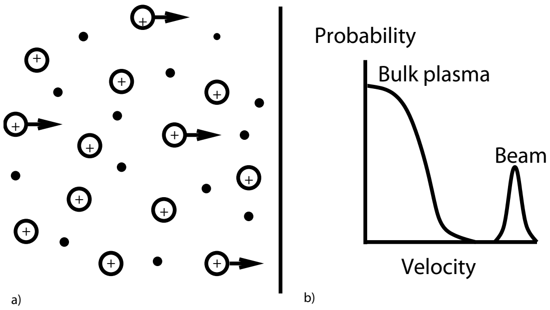


Figure 2: A plasma consists of mobile free charges, e.g. protons and electrons (small circles), as shown in panel a). Some protons move relative to the plasma, as indicated by the arrows. In panel b) a probability distribution of proton velocities representative for a) is shown, which is unstable to the two-stream instability.

electrons. The massive protons are only weakly affected. In the absence of a magnetic field, the electron speed is limited. The electrons can reach Lorentz factors $\Gamma(v) = (1 - v^2/c^2)^{-1/2}$ of about 100, if the proton beam $\Gamma = 7$ [4]. A perpendicular magnetic field component boosts the electrons to a $\Gamma \approx m_p/m_e$, where m_p/m_e is the proton-to-electron mass ratio [5, 6], as Fig. 3 demonstrates. Nevertheless, comparatively little energy can be transferred by the two-stream instability from the proton beam to the electrons. We have, however, shown recently [8] that the remaining free energy is released, when bunches of ultrarelativistic electrons modulate the proton beam velocity. This destabilizes the beam and a relativistic proton phase space hole [7] forms, which we show in Fig. 4. Its electrostatic field can accelerate electrons to $\Gamma \approx 6\times10^4$, for an initial proton beam Lorentz factor $\Gamma = 10$ [8].

The event chain we propose in Ref. [8] has remarkable properties: (1) It can be driven by moderately relativistic beams of protons. (2) All processes develop on the fast electron time scale. (3) The proton phase space hole thermalizes the relativistic proton beam on short spatio-temporal scales. (4) Energy equipartition between electrons and protons is established ⇒ the electrons can radiate away the energy much more easily than protons. (5) Electrostatic bremsstrahlung may replace synchrotron emission, which would require strong large-scale magnetic fields and a yet unknown mechanism that generates these [1]. (6) The evolution time is robust with respect to the plasma density [8] ⇒ we obtain an unambigous time estimate that can be compared with experimental observations. For plasma parameters that are representative for the ultrarelativistic GRB jets, we obtain a duration time of the order seconds [8]. This matches the characteristic time scale of the prompt GRB emissions [1]. Our simulation work has thus established a

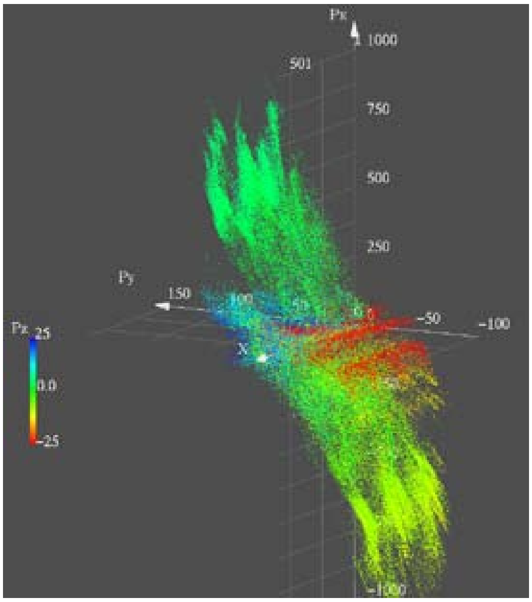
This destabilizes the beam and a relativistic proton phase space hole forms…

he played the piano accompanied by some jazz friends; this was indeed a memorable moment!

Mats job as technical director is now taken over by Niclas Andersson, but I am sure that Mats will come and visit us also in the future and follow the activities at NSC from a slightly more relaxed position. See you then Mats!

SVEN STAFSTRÖM

Mats S Andersson



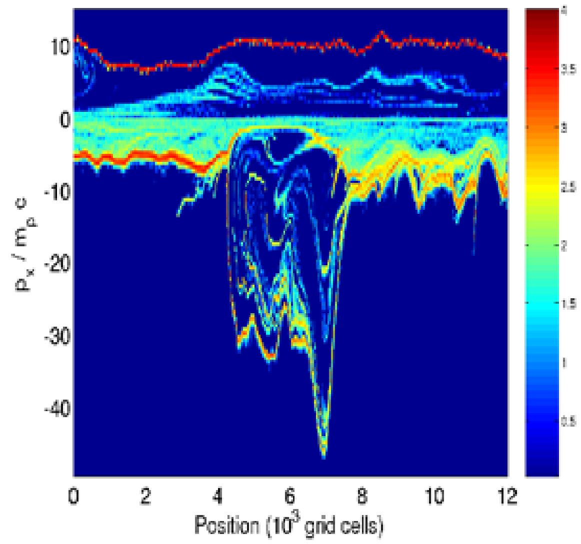


Figure 3: A typical electron phase space distribution, resulting from particle interactions with electric and magnetic fields. The coordinate system represents one position and two momentum coordinates and the third coordinate is mapped into colour. The electron momenta are given in units of $m_e c$ (Image taken from [6]).

Figure 4: An ultrarelativistic proton phase space hole forming in our PIC simulation (Image taken from [8]). The momentum is given in $m_p c$. The x-direction is in units of simulation grid cells, each about one Debye length of the plasma.

novel mechanism that can explain the prompt emissions of GRBs.

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Mark Dieckmann is senior lecturer at the department of science and technology (ITN) at Linköping University. He got his PhD in plasma physics at the physics departement of the University of Warwick in 1999. He has held postdoc positions at Warwick and LiU as well as positions as visiting researcher at the Ruhr-University Bochum and the Dublin Institute of Advanced Studies. He is currently on leave of absence from ITN for a position as research associate at the Ruhr-University Bochum.

UPCOMING EVENTS

LCSC; 7th Annual Workshop on Linux Clusters for Supercomputing

October 17–18, 2006, Linköping, Sweden.
http://www.nsc.liu.se/lcsc/

SC 06; International Conference for High Performance Computing, Networking, Storage and Analysis

November 11–17, 2006, Tampa, USA.
http://sc06.supercomputing.org/

GCE 2006; The Second International Workshop on Grid Computing Environments

November 12, 2006. (held in conjunction with SC06)
http://www.cogkit.org/GCE06/

HiPC 2006; 13th IEEE International Conference on High Performance Computing

December 18–21, 2006, Bangalore, India.
http://www.hipc.org/

IPDPS 2007; 21st IEEE International Parallel & Distributed Processing Symposium

March 26–30, 2007.Long Beach, California, USA.
http://www.ipdps.org//

CAC 2007; The Workshop on Communication Architecture for Clusters

March 26–30, 2007. Long Beach, California, USA. (held in conjunction with IPDPS 2007)
http://www.c3.lanl.gov/cac2007/

CCGrid07; 7th IEEE International Symposium on Cluster Computing and the Grid

May 14–17, 2007, Rio de Janeiro, Brasil.
http://ccgrid07.lncc.br/

ISC 2007; International Supercomputer Conference

June 26-29, 2007. Dresden, Germany.
http://www.supercomp.de/isc2007/

HPDC 2007; IEEE International Symposium on High Performance Distributed Computing

June 27–29, 2007. Monterey Bay, California, USA.
http://www.isi.edu/hpdc2007/

ParCo2007; Parallel Computing 2007

September 4–7, 2007. Juelich and Aachen, Germany.
http://www.fz-juelich.de/parco2007/

ICPP 2007; 2007 International Conference on Parallel Processing

September 10-14, 2007. XiAn, China.
http://www.cse.ohio-state.edu/~icpp2007/

24th IEEE MSST2007 Conference on Mass Storage Systems and Technologies

September 24–27, 2007. San Diego, CA, USA.
http://storageconference.org/2007/

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