Ilian Todorov

I.T.Todorov@dl.ac.uk
Advanced Research Computing (A31)
Computational Science & Engineering Department
STFC Daresbury Laboratory, Daresbury
Warrington, Cheshire, WA4 4AD, United Kingdom

Employment & Education

STFC Daresbury Laboratory / University of Cambridge
Since 2003 :
HPC Software Engineer using Fortran90, MPI, shell scripting, C and XML. Work includes managing DL_POLY_3, the flagship UK science application for Molecular Dynamics.

1999 – 2002 University of Bristol, School of Chemistry, Bristol (ORS scholar)
PhD in Computational Chemistry.
1997 – 1999 University of Hull, Chemistry Department, Hull (TEMPUS scholar)
MSc Degree in Chemistry (by research) via Joint European Project.
1996 – 1997 Military School "P. Volov", Shoumen, Bulgaria
Radiolocation Officer – graduated top of class with Distinction.
Served as a lieutenant in the Bulgarian Air Force.
1991 – 1996 University of Sofia, Faculty of Physics, Eurika foundation and State scholar
MSci (Hons) Degree in Physics: First Class with Distinction.
1986 – 1991 Secondary School, OMG-Plovdiv, Bulgaria (State scholar)
Silver Medal, by the Ministry of Education for in Physics and Maths Olympiads.

Scientific Work & Experience

Directly involved in parallel and distributed memory programming to aid cutting edge research in HPC: domain decomposition, advanced domain mapping and memory distribution, variable timestep, linked-cells and particle tracking. Implementation of a range of Trotter derived velocity Verlet integration algorithms for various ensembles to provide symplecticity, improved numerical stability and superior performance to that of leapfrog Verlet integrations. Also: FORTRAN90 software modularisation, factorisation, code quality, portability, parallel performance and scaling.

Directly involved in cutting edge MD simulation research on materials reaction upon irradiation with groups at the University of Cambridge (in collaboration with e-Minerals) and University of Bristol to investigate materials resistance and self-healing (damage recoverability) to high energy irradiation doses. The work provides drive for development of DL_POLY_3 to speed up simulations and enhance the analysis of damaged states by defects detection during evolution, which the experiments cannot provide (help to amorphisation theories).

Work on embedding trans-membrane proteins in lipid bilayers and investigating local environment conditions influence on ion-channelling stimulation using molecular dynamics.

1999–2002: research on disordered compounds and solid solutions by analysing computational results based on current best practices and implementing novel algorithms for statistical analysis of order/disorder in binary oxide systems. The work involved several development environments to enhance the analysis of leading mathematical and scientific problems (statistical averaging over limited number of representative states, extraction of complete phase diagrams of binary solids at wide interval of temperatures and pressures, prediction of phase diagrams at Earth core like pressures, at which experiments are not feasible, to help geological theories). The research required maintaining a strong collaboration in Bristol, Norway and Argentina.