A Light for Science

ESRF

European Synchrotron Radiation Facility

Simulation Needs

Alessandro Mirone, SCISOFT

We present a digest of programs for the simulation of spectroscopic properties (Resonant reflectivity, Phonon calculations, ab-initio simulations, multiplet calculations) (Small input, Big calculation)

How do they fit to the GRID?

What does the GRID need to host them?

Plans for the future

Important keywords

Domain (ω, k) decomposability -> coarse parallelisation(Condor)

System decomposability -> fine parallelisation (MPI)

Band-pass requirements , scalability

Temporary files (for example eigenvectors ...) , their size, their distributibility

Benefits from GPU

Audience : consolidated Audience, market Audience

In house competences

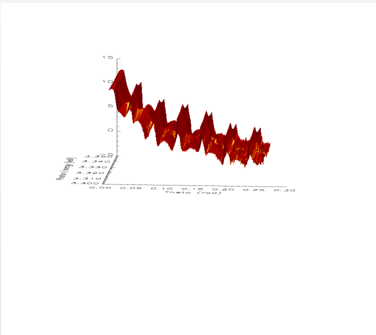
Selected programs

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
PPM	multilayer SXRD	ω, Q (MPI)	Just the error function	None	********	*** *****	Main developper
OpenPhonon	HRIXS	Q (Condor)	Just the error function	1E8bytes distributed	? (lapack 20x20)	** ****	Main developper
WIEN	Phonons, XAS	K (Condor) System (MPI)	temporary files Huge (dense matrices)	50Gb NFS	? (LAPACK) ?(SCALAPACK)	***********	Inst. f. Materials Chemistry TU Vienna
FDMNES	XANES, DAFS	ω (MPI)	Just the spectra	None	?(LAPACK)	******	Yves Joly CNRS, Scisoft maintenance
Hilbert++	multiplets, correlated systems	System (MPI)	Huge (random connectivity)	~2Gb	? (Sparse Matrices)	** ****	Main developper
FEMTO	XANES	System(MPI)	Small (zone borders)	~1Gb distrib.	(Sparse Matrices)	* *****	Main developper
BigDFT	DFT (Pseudopot.)	MPI	Wavefunctions	None	Huge, (beta)	ABINIT	Luigi Genovese (Theory Group)

PPM: Pythonic Programming for Multilayers

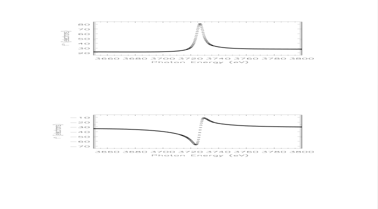
Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
PPM	multilayer SXRD	ω, Q (MPI)	Just the error function	None	********	*** *****	Main developper

[U9 Å /Fe34 Å]×30 multilayer

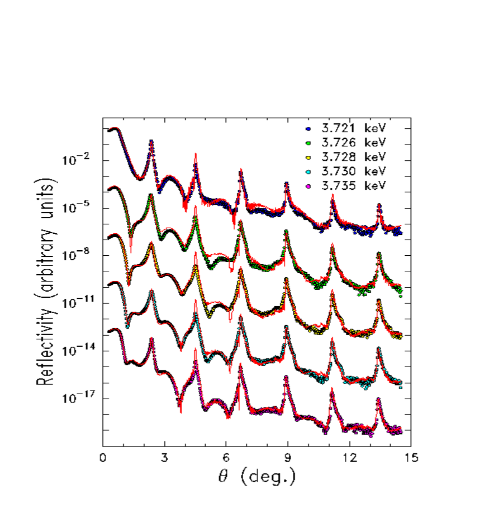


specular reflectivity fitted on a grid of incident angle and energy across resonances

Goal : retrieval of optical constants as a function of multilayer depth, respecting dispersion relations
composition/magnetisation profiles inside layers
Automatic fit.



synthetised U optical constants



GPU advantages for both scalar and magnetic calculations
So far used MPI for parallelisation
Condor could be used but latency must remain small.
The model is described by an XML file

*Phys. Rev. B **77** 014427 (2008)*

OpenPhonon : Lattice Dynamics Calculations: Fit of parametrised forces to HRIXS spectra

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
OpenPhonon	HR RIXS	Q (Condor)	Just the error function	1E8bytes	? (lapack 20x20)**	****	Main developper

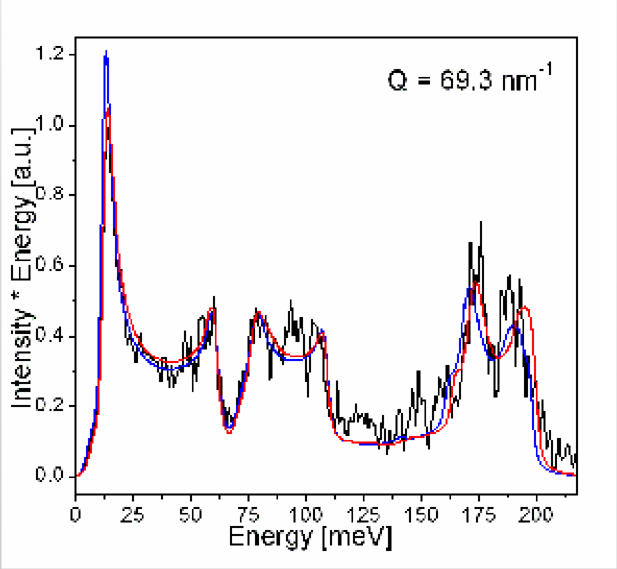
Orientation average and calculation of polycrystalline IXS spectra

Polycrystalline IXS data, collected over a large momentum transfer range

K space decomposition
Condor parallelisation
GPU : eigenvectors for ~20x20 might be a problem
latency : some seconds
eigenvectors are stored on disk (local)

Least squares fitting routine, refining model

single crystal dispersion, thermodynamic & elastic properties



Irmengard FISCHER's Thesis

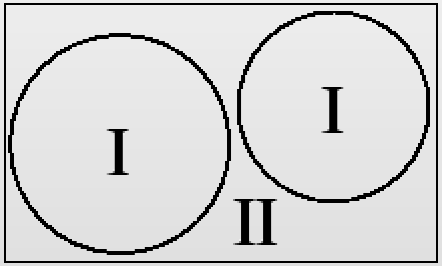
WIEN2k Blaha et al. Inst. f. Materials Chemistry, TU Vienna

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
WIEN	Phonons, XAS	K (Condor) System (MPI)	temporary files Huge (dense matrices)	50Gb NFS	? (LAPACK) ?(SCALAPACK)	***********	Vienna

Applications

electronic structure calculations of solids using DFT

Phonons calculations, pre-edge spectra, struct. relax.



Method

Linearized augmented plane waves (LAPW)

Full potential

I) $$\phi_{k_n} = \sum_{lm}[A_{lm}u_l(r,E_l) + B_{lm}\dot{u}_l(r,E_l)]Y_{lm}(\hat{r})$$

Computing Aspects

K points parallelisation : rsh or Condor

Distributed memory(MPI) : band-pass limitations

II) $$\phi_{k_n} = \frac{1}{\sqrt{\omega}}e^{ik_n r}$$

FDMNES: XANES beyond muffin-tin approximation

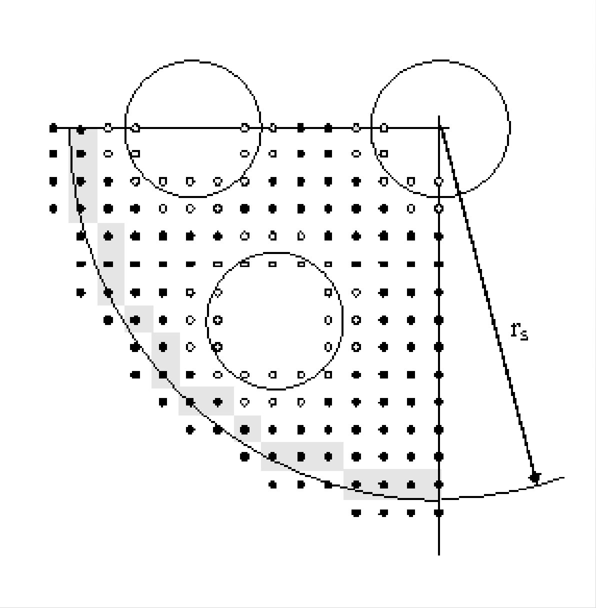
Yves Joly, Laboratoire de Cristallographie, Grenoble

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
FDMNES	XANES, DAFS	ω (MPI)	Just the spectra	None	?(LAPACK)	******	Yves Joly CNRS, Scisoft maintenance

Applications

XANES study of selected atoms environment.

DAFS study of long range order parameters.



Method

Finite differences Schroedinger equation

Atomic wave-functions

Spherical Bessel outside Rs

Computing Aspects

ω parallelisation : mpi (better Condor)

Dense matrix : inverse by Lapack

memory and time explode with Rs

FEMTO: XANES beyond muffin-tin approximation. Linear scalability

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
FEMTO	XANES	System(MPI)	Small (zone borders)	~1Gb distrib.	Grahm-Schmidt *	*******	Main developper

Applications

XANES study of selected atoms environment.

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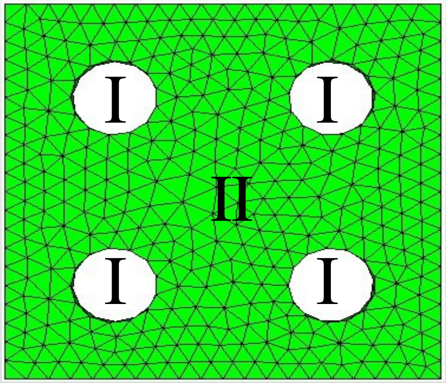
Method

Finite Elements + atomic function expansion

Variational principle ==> Hermitian Form

Generalised Lanczos tridiagonalisation =>continued fraction



I) atomic wave functions and derivative

II) first order shape functions

Computing Aspects

System : mpi

3D decomposition : low bandpass

Huge systems

BigDFT: Ab initio simulation of large systems
Luigi Genovese , Theory Group

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
BigDFT	DFT (Pseudopot.)	MPI	Wavefunctions	None	Huge, (beta)	ABINIT	Luigi Genovese (Theory Group)

Applications

DFT of large systems, surfaces, nanostructures

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Method

Wavelets basis

LDA+xc

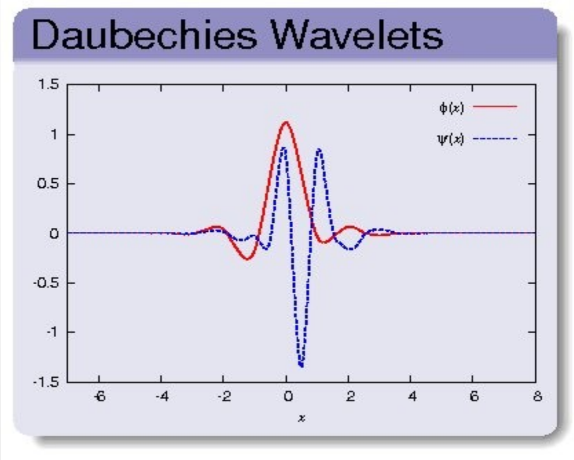
pseudo-potentials

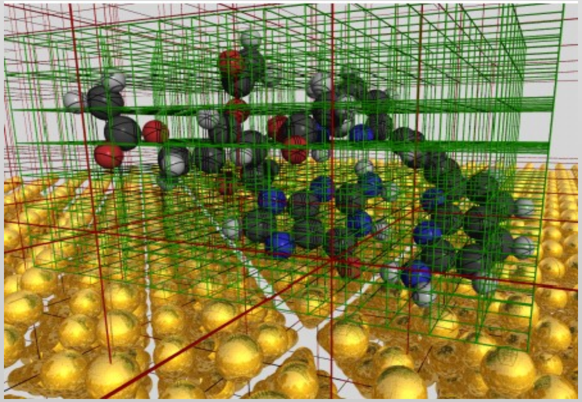
Computing Aspects

System : mpi

3D decomposition : low bandpass

Huge systems





Hilbert++

Code	Applications	decomposability	Band Pass	Temporary files	GPU's Benefits	Audience	In House Competences
Hilbert++	multiplets, correlated systems	System (MPI)	Huge (random connectivity)	~2Gb	? (Sparse Matrices)	** ****	Main developper

Applications

Many-body effects in pre-edge XAS, RIXS, SXRD

Method

Start from a model Hamiltonian in second quantisation

Using 2nd quantisation operators to develop

Hilbert space, and obtain Sparsa Matrices

Eigenvalues and spectra by Lanczos method

and tridiagonalisation =>continued fraction

2nd quantisation

$$e = c_i^{+} c_k^{+} \dots c_l^{+} |\square\rangle$$

quantum states in memory :

e.val= ...010..10.........10....

e.signs = ..001..10....01.....

Computing Aspects

System : mpi

N dimension : High bandpass

Small Clusters (exponential complexity)

Other Programs

AB INITIO	MonteCarlo	Molecular Dynamics
Abinit	GEANT4	Moldy
Vasp	Penelope	GROMACS
ADF	MCNPX	
StoBe	EGS4	
Siesta		
Orca		
Gamess-UK		
Crystal		

Conclusion

Different Applications with different requirements

Users could access to in-house Applications through the GRID, releaving the developers and the user from replicating installations at each external institution .

Applications in continuous evolution : GRID could ease updating issues and reduce maintenance labour.

GRID could trigger positive interactions in the scientific community.