3D ASLDA solver
- status report

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General outlook

Goal: Provide a 3D DFT solver.

Main features:

- Defined on a rectangular spatial lattice (by means of DVR),
- FFT is used for calculations of derivatives,
- No symmetry constraints,
- Able to describe superfluid neutron-proton system with arbitrary spin asymmetry (ASLDA – Asymmetric Superfluid Local Density Approach)
- Solves BdG (HFB) equations.
- Parallelizable.
- Possible extensions: 1D, 2D, other large Fermi systems (ultracold atoms)

Summary (2008)

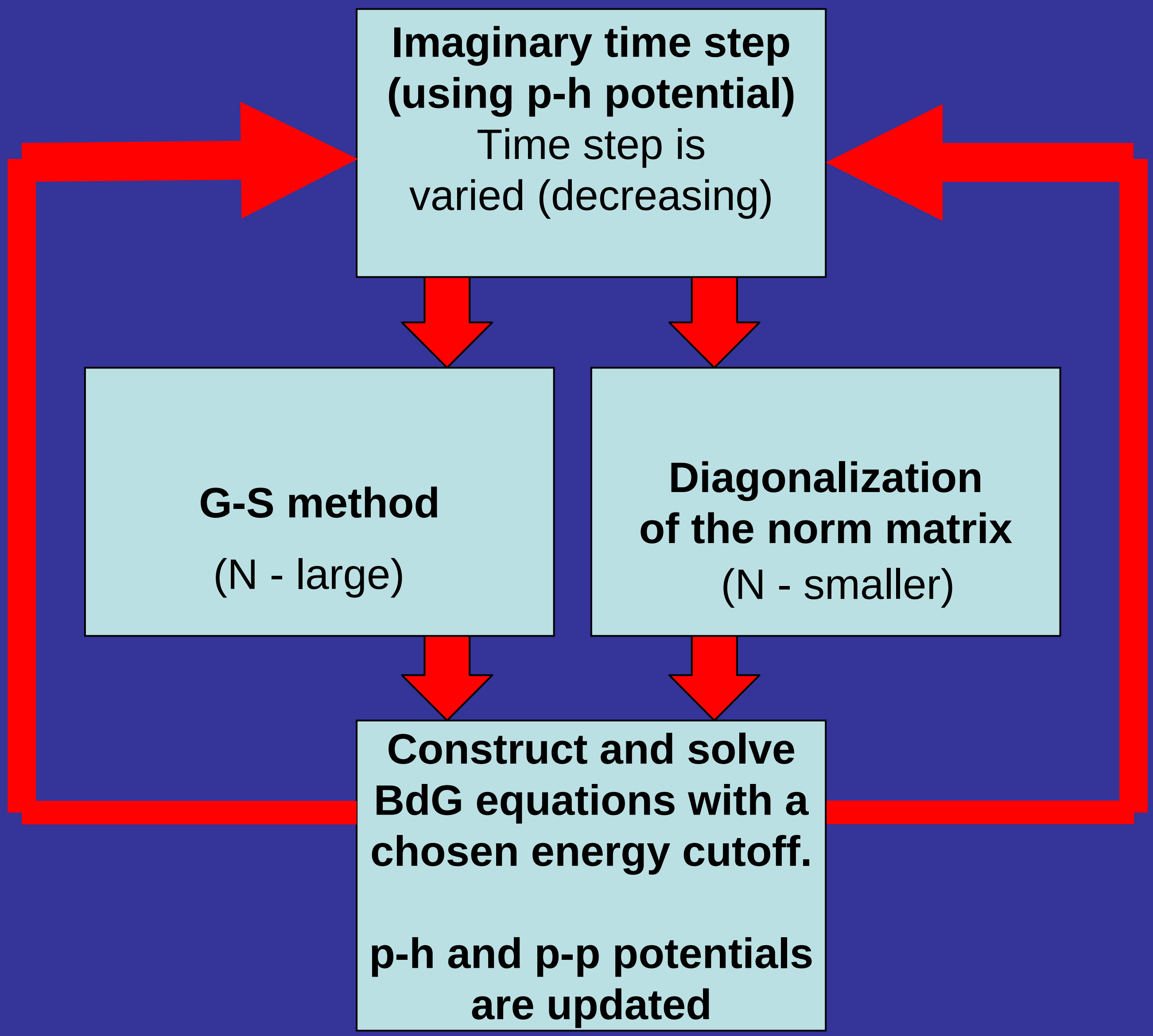
At the moment '*the non-selfconsistent DFT solver*' exist.
It can handle arbitrary shape of potentials in p-h and p-p channels.
The accuracy of the results is stable with respect to variations of the potentials, chemical potentials, energy cutoff, effective masses, etc.

1. **Is your Year-2 plan well on track?**
   Absolutely.
2. **What are the aspects of your science that require high-performance computing?**
   Data and computational complexity.
3. **Plan for Year-2 and Year-3:**
   - profile current code.
   - parallelization of the code.
   - self-consistent version.
   - interface between TDSLDA code.

Accomplishments since the last meeting:

1) **self-consistent version of the code (Broyden method applied)**
2) **nuclear density functional coded**
3) **interface between TDSLDA code**
4) **2D version of ASLDA (parallelized) for ultracold atomic gas**

Procedure



N – number of evolved wave functions

Skyrme density functional:

$$H_{skyrme} = C^{\rho}\rho_0{}^2 + C^{s}\vec{s}\bullet\vec{s} + C^{\Delta\rho}\rho_0\Delta\rho_0 + C^{\Delta s}\vec{s}\bullet\Delta\vec{s} + C^{\tau}(\rho_0\tau - \vec{j}\bullet\vec{j}) +$$
$$C^{sT}(\vec{s}\bullet\vec{T} - \overleftrightarrow{J}^2) + C^{\nabla J}(\rho_0\nabla\bullet\vec{J} + \vec{s}\bullet(\nabla\times\vec{j}))$$

Particle-hole mean field:

$$\hat{h}(\vec{r}) = -\nabla\bullet B(\vec{r})\nabla + U(\vec{r}) - i\vec{W}(\vec{r})\bullet(\nabla\times\vec{\sigma}) + \vec{S}(\vec{r})\bullet\vec{\sigma} - \nabla\bullet(\vec{\sigma}\bullet\vec{C}(\vec{r}))\nabla + \frac{1}{2i}(\nabla\bullet\vec{A}(\vec{r}) + \vec{A}(\vec{r})\bullet\nabla) =$$
$$= -h^{\Delta}(\vec{r})\Delta - \vec{h}^{\nabla}(\vec{r})\bullet\nabla - i\vec{W}(\vec{r})\bullet(\nabla\times\vec{\sigma}) + V(\vec{r}) = \begin{pmatrix} \hat{h}_{++}(\vec{r}) & \hat{h}_{+-}(\vec{r}) \\ \hat{h}_{-+}(\vec{r}) & \hat{h}_{--}(\vec{r}) \end{pmatrix}$$

$$h^{\Delta}(\vec{r}) = B(\vec{r}) + \vec{\sigma}\bullet C(\vec{r})$$
$$\vec{h}^{\nabla}(\vec{r}) = \nabla B(\vec{r}) - \vec{\sigma}\bullet\nabla C(\vec{r}) + i\vec{A}(\vec{r})$$
$$V(\vec{r}) = U(\vec{r}) + \vec{S}(r)\bullet\vec{\sigma} - \frac{1}{2}i\nabla\bullet\vec{A}(\vec{r}) + V_{ext}(\vec{r})$$

Imaginary time step evolution:

$$\left|\Psi_j^{(n+1)}\right\rangle = e^{-\lambda\hat{h}}\left|\psi_j^{(n)}\right\rangle, \quad j = 1,\ldots,N$$
$$\left|\Psi_j^{(n+1)}\right\rangle \xrightarrow[normalization]{orthogonalization} \left|\psi_j^{(n+1)}\right\rangle$$

λ - imaginary time step

$$e^{-\lambda\hat{h}} = 1 + \sum_{i=1}^{n} \frac{(-\lambda)^i}{i!}\hat{h}^i + O(\lambda^{n+1})$$

Usually used for n=1

Drawbacks: - slow convergence.
- divergent for too large imaginary time step.
- numerically costly for n>1.

$$\hat{h}(\vec{r}) = -h^{\Delta}(\vec{r})\Delta + V(\vec{r}) - \vec{h}^{\nabla}(\vec{r})\bullet\nabla - i\vec{W}(\vec{r})\bullet(\nabla\times\vec{\sigma})$$

$$e^{-\lambda\hat{h}} = e^{-\frac{\lambda}{2}\hat{T}} e^{-\frac{\lambda}{2}\hat{V}} \left(1 - \lambda\hat{M} + \frac{\lambda^2}{2}\hat{M}^2\right) e^{-\frac{\lambda}{2}\hat{V}} e^{-\frac{\lambda}{2}\hat{T}} + O(\lambda^3),$$ - second order method

where

$\hat{T}$ - is local in momentum space

$\hat{V}$ - is local in space

$\hat{M}$ -contains mixed terms (e.g. spin-orbit)

The above expansions are particularly useful if the Hamiltonian can be expressed as a sum of terms either local in the coordinate space (potential), or in the momentum space (kinetic energy).
In such a case one is adviced to use Fast Fourier Transform algorithm during the evolution of the wave function.

$$e^{-\lambda \hat{T}}\psi(\vec{p}) = e^{-\lambda \frac{p^2}{2m}}\psi(\vec{p})$$

$$e^{-\lambda \hat{V}}\psi(\vec{r}) = e^{-\lambda V(\vec{r})}\psi(\vec{r})$$

REAL SPACE ⇔ *FFT* ⇔ **MOMENTUM SPACE**

Advantages:

- Much faster convergence (**order of magnitude** difference between the first order and the second order method).
- The methods **do not diverge** even for large time steps.
- The low cost of **FFT** instead of matrix multiplication.

$$\hat{h}(\vec{r}) = -h^{\Delta}(\vec{r})\Delta + V(\vec{r}) - \vec{h}^{\nabla}(\vec{r}) \bullet \nabla - i\vec{W}(\vec{r}) \bullet (\nabla \times \vec{\sigma})$$

How to decrease magnitude of mixed terms:

$$\hat{h}(\vec{r})\psi_n(\vec{r}) = e^{-\alpha(\vec{r})}\left(-\tilde{h}^{\Delta}(\vec{r})\Delta + \tilde{V}(\vec{r}) - \tilde{\vec{h}}^{\nabla}(\vec{r}) \bullet \nabla - i\tilde{\vec{W}}(\vec{r}) \bullet (\nabla \times \vec{\sigma})\right) e^{\alpha(\vec{r})}\psi_n(\vec{r})$$

where

$$\tilde{h}^{\Delta}(\vec{r}) = h^{\Delta}(\vec{r})$$

$$\tilde{\vec{h}}^{\nabla}(\vec{r}) = \vec{h}^{\nabla}(\vec{r}) + 2h^{\Delta}(\vec{r})\nabla\alpha(\vec{r})$$

$$\tilde{V}(\vec{r}) = V(\vec{r}) + h^{\Delta}(\vec{r})\left(\left(\nabla\alpha(\vec{r})\right)^2 - \Delta\alpha(\vec{r})\right) - \vec{h}^{\nabla}(\vec{r}) \bullet \nabla\alpha(\vec{r})$$

then

$$e^{-\lambda\hat{h}}\psi_n(\vec{r}) = e^{-\alpha(\vec{r})}e^{-\lambda\hat{h}'}\psi'_n(\vec{r}), \quad \psi'_n(\vec{r}) = e^{\alpha(\vec{r})}\psi_n(\vec{r})$$

In particular transformation:

$$\psi'_n(\vec{r}) = \sqrt{\frac{m^*(\vec{r})}{m}}\psi_n(\vec{r})$$

allows to get rid of the effective mass term.

In the basis $\psi_n(\vec r) = \begin{bmatrix} \psi_{n+}(\vec r) \\ \psi_{n-}(\vec r) \end{bmatrix}$ **one solves BdG(HFB) eq.**

$$\begin{pmatrix} h & \Delta \\ \Delta^\dagger & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix}$$

$$h_{nn'} = \langle \psi_n | \hat h - \begin{pmatrix} \mu_+ & 0 \\ 0 & \mu_- \end{pmatrix} | \psi_{n'} \rangle \delta_{nn'}$$

$$\Delta_{nn'} = \int \left(\psi^*_{n+}(r) \quad \psi^*_{n-}(r) \right) \begin{pmatrix} 0 & \Delta_{+-}(\vec r) \\ \Delta_{-+}(\vec r) & 0 \end{pmatrix} \begin{pmatrix} \psi^*_{n'+}(r) \\ \psi^*_{n'-}(r) \end{pmatrix} d^3 r$$

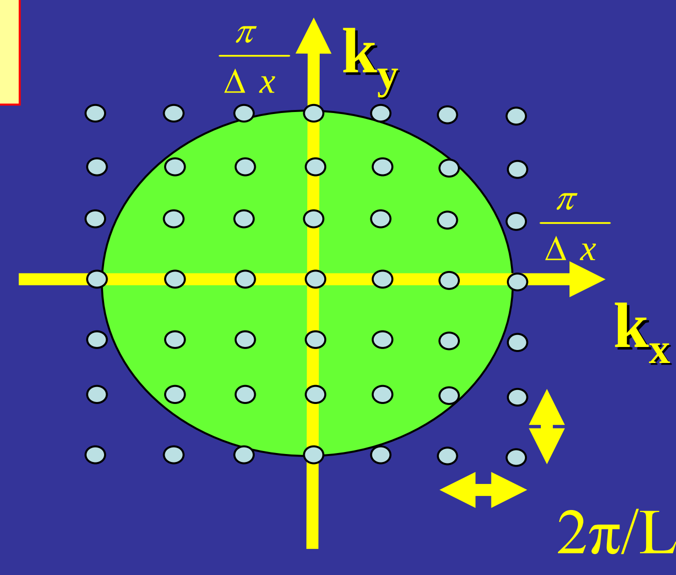
$$\rho(r) = \sum_{k,k'} \left(V^* V^T \right)_{kk'} \begin{pmatrix} \psi_{k+}(\vec r)\psi^*_{k'+}(\vec r) & \psi_{k+}(\vec r)\psi^*_{k'-}(\vec r) \\ \psi_{k-}(\vec r)\psi^*_{k'+}(\vec r) & \psi_{k-}(\vec r)\psi^*_{k'-}(\vec r) \end{pmatrix};$$

$$\chi(\vec r) = \sum_{k,k'} \left(V^* U^T \right)_{kk'} \begin{pmatrix} 0 & \psi_{k+}(\vec r)\psi_{k'-}(\vec r\,') \\ \psi_{k-}(\vec r)\psi_{k'+}(\vec r\,') & 0 \end{pmatrix}$$

$$\Delta_{+-}(\vec r) = -g\,\chi_{+-}(\vec r) \frac{1}{1 - \dfrac{g\,(k_{cut} - k_0/2)}{4\pi^2 \left(\dfrac{\hbar^2}{2m} + C^\tau \rho_0 \right)} \log\left(\dfrac{k_{cut} + k_0}{k_{cut} - k_0} \right)}$$

$$k_0(\vec r) = \sqrt{\frac{-V(\vec r)}{\dfrac{\hbar^2}{2m} + C^\tau \rho_0}}$$

$$k_{cut}(\vec r) = \sqrt{\frac{E_{cut} - V(\vec r)}{\dfrac{\hbar^2}{2m} + C^\tau \rho_0}}$$



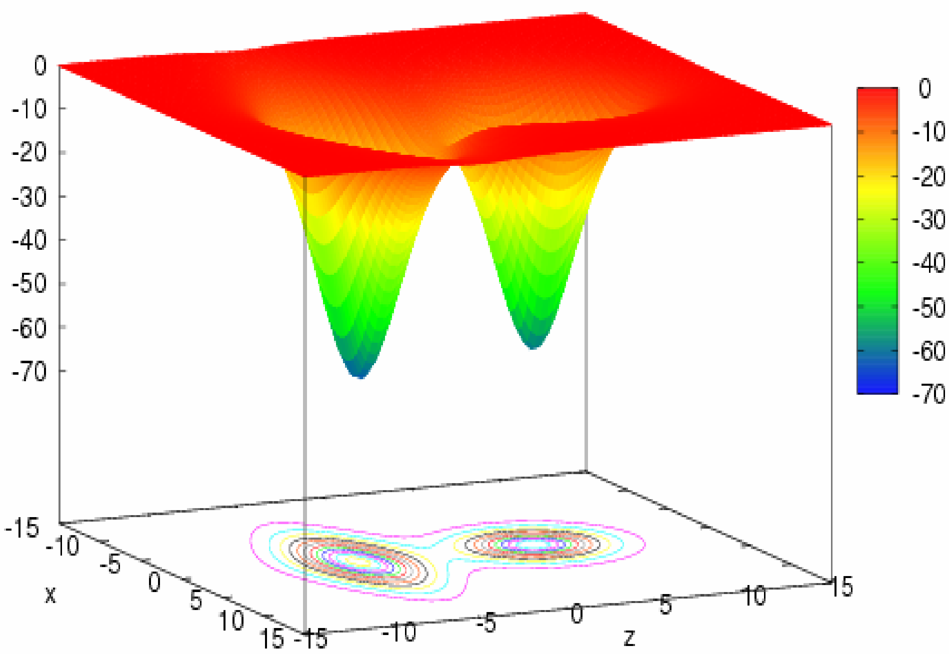
External potential in p-h channel

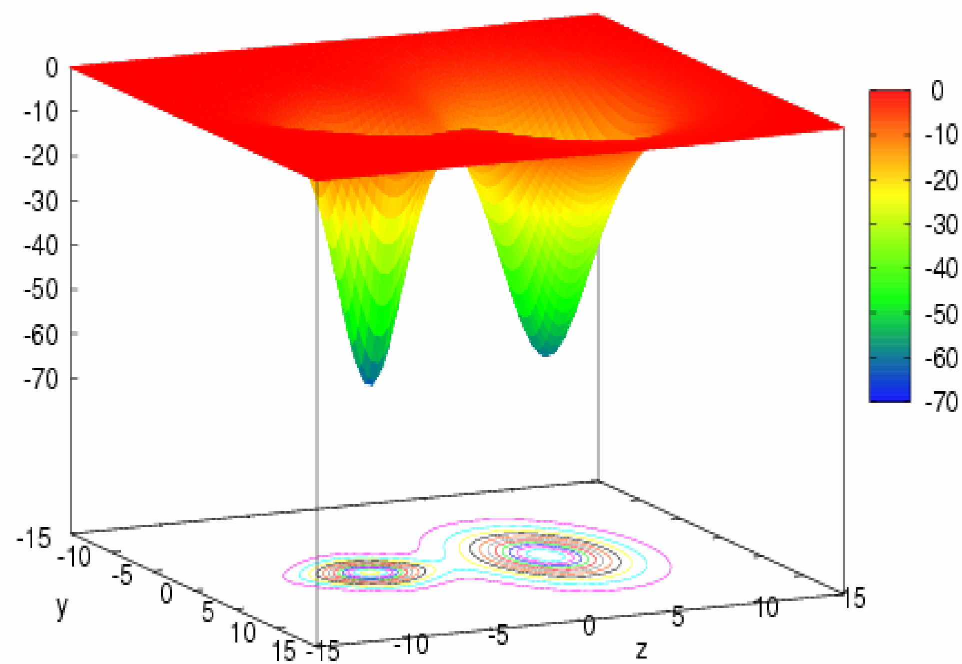
$$V_{ext}(\vec{r}) = \frac{V_1}{1+\cosh\left(\frac{r_1}{a}\right)} + \frac{V_2}{\left(1+\cosh\left(\frac{r_{xy}}{b}\right)\right)\left(1+\cosh\left(\frac{z+\xi}{b}\right)\right)}$$

$$r_1 = \sqrt{x^2 + 0.4y^2 + (z-\xi)^2}; r_{xy} = \sqrt{0.2x^2 + y^2}$$

$$V_1 = -120 MeV \ , V_2 = -250 MeV, \ a = 3.5\ fm, \ b = 2.0\ fm, \ \xi = 5\ fm$$

External potential in p-p channel: $\Delta_{ext}(\vec{r}) = 2MeV$

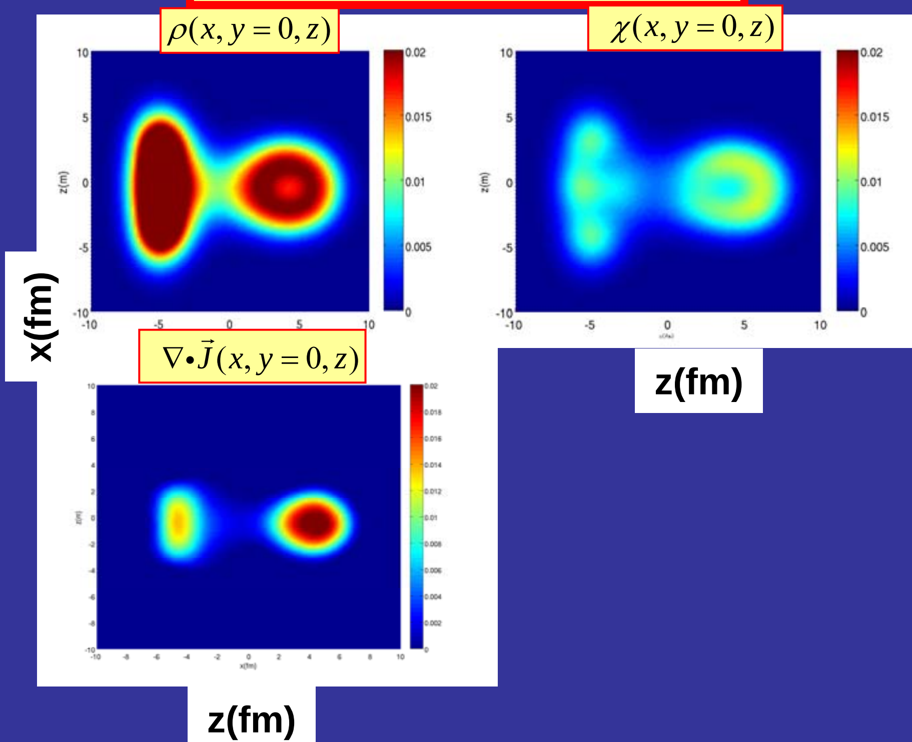




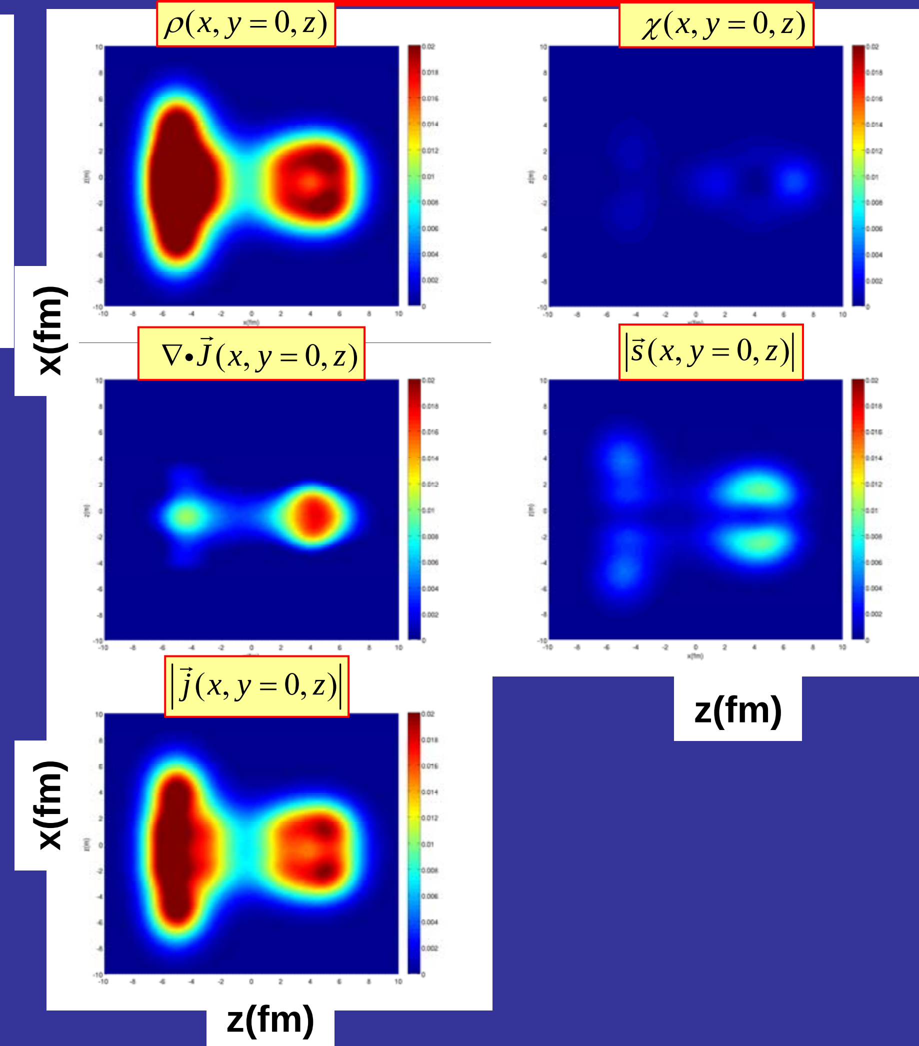
Preliminary results (neutrons – SkM*):

Number of wave functions: 40
Number of particles: 20
Box size: 24x24x24 fm^3

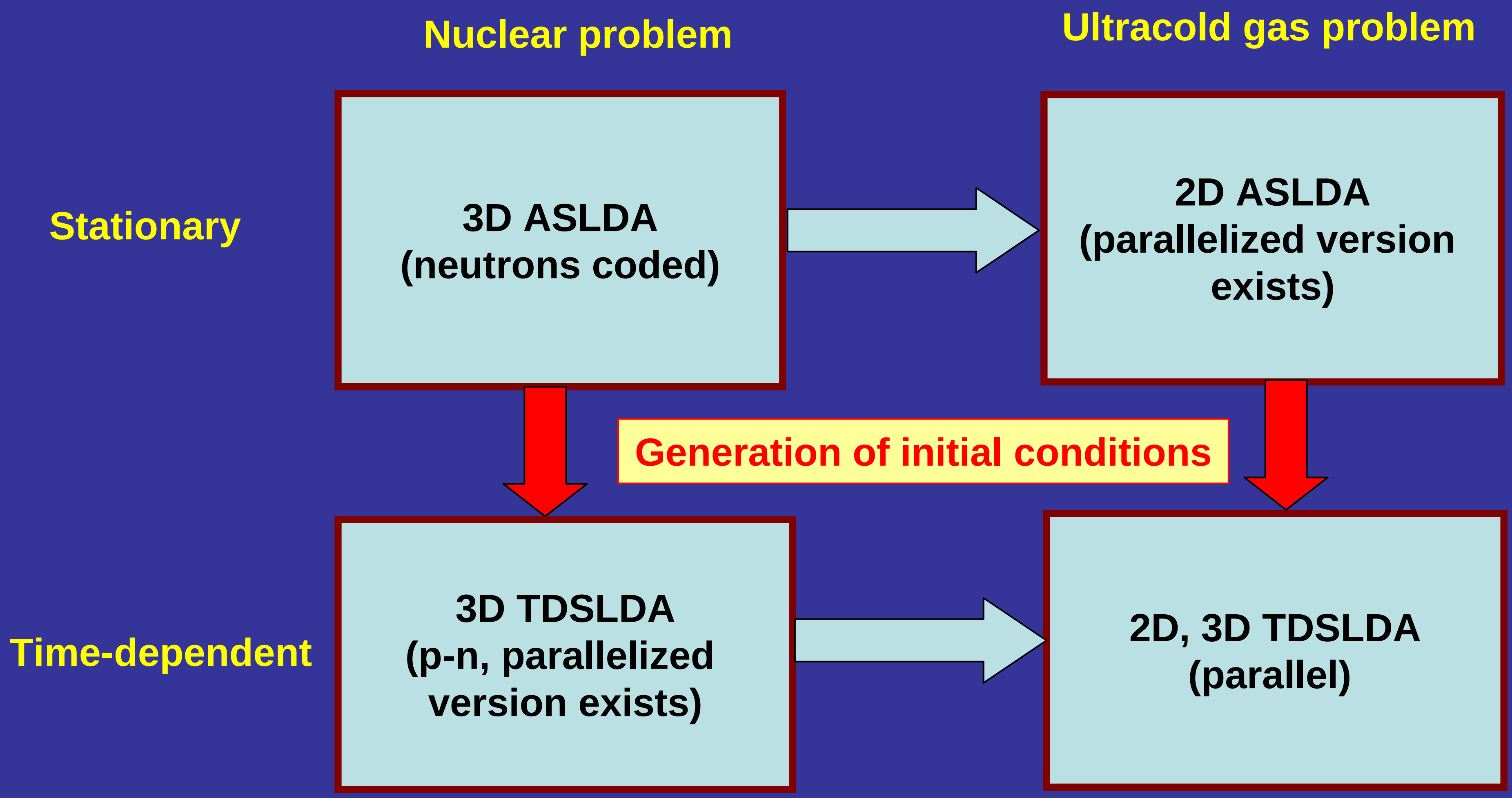
$$\sigma = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = 0 \text{ - spin symmetric system}$$



$$\sigma = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow} = 0.8 \text{ - spin asymmetric system}$$



Relations between the codes (Map of the codes)



See talks of Aurel Bulgac (today), Kenny Roche and Ionel Stetcu (tomorrow)

Summary 2009

Accomplishments since the last meeting:

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2) nuclear density functional coded
3) interface between TDSLDA code
4) 2D version of ASLDA (parallelized) for ultracold Fermi gas

1. Is your Year-3 plan well on track?
   Absolutely.
2. What are the aspects of your science that require high-performance computing?
   Data and computational complexity.
3. Plan for Year-3
   - profile current code.
   - parallelization of the code + proton-neutron extension
   - applications and generation of initial conditions for TDSLDA
4. Plan for Year-4
   - further applications: calculations of odd nuclei, neutron droplets...