Extended Thomas-Fermi

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Module Documentation

4.1 Global parameters

Variables

- real(kind=dp), parameter parameters::pi = 3.1415926535897932_dp

  π
- real(kind=dp), parameter parameters::hbar2_2m = 20.73553_dp

  $\frac{\hbar^2}{2m}$ *for SLy forces*
- real(kind=dp), parameter parameters::rho0 = 0.16_dp

  ρ_0*, nuclear saturation density* $[fm^{-3}]$
- real(kind=dp), parameter parameters::e2 = 1.439978408596513_dp

  e^2*, electric charge squared* $[MeV \cdot fm]$
- real(kind=dp), parameter parameters::mec2 = 0.51099895_dp

  Electron rest mass $[MeV/c^2]$.
- real(kind=dp), parameter parameters::mnc2 = 939.56542052_dp
- real(kind=dp), parameter parameters::mpc2 = 938.27208816_dp
- real(kind=dp), parameter parameters::hbarc = 197.3269804_dp

  $\hbar * c$

4.1.1 Detailed Description

4.1.2 Variable Documentation

4.1.2.1 e2

```
real(kind=dp), parameter parameters::e2 = 1.439978408596513_dp
```

e^2, electric charge squared $[MeV \cdot fm]$

4.1.2.2 hbar2_2m

```
real(kind=dp), parameter parameters::hbar2_2m = 20.73553_dp
```

$\frac{\hbar^2}{2m}$ for SLy forces

4.1.2.3 hbarc

```
real(kind=dp), parameter parameters::hbarc = 197.3269804_dp
```

$\hbar * c$

4.1.2.4 mec2

```
real(kind=dp), parameter parameters::mec2 = 0.51099895_dp
```

Electron rest mass $[MeV/c^2]$.

4.1.2.5 mnc2

```
real(kind=dp), parameter parameters::mnc2 = 939.56542052_dp
```

4.1.2.6 mpc2

```
real(kind=dp), parameter parameters::mpc2 = 938.27208816_dp
```

4.1.2.7 pi

```
real(kind=dp), parameter parameters::pi = 3.1415926535897932_dp
```

π

4.1.2.8 rho0

```
real(kind=dp), parameter parameters::rho0 = 0.16_dp
```

ρ_0, nuclear saturation density $[fm^{-3}]$

4.2 Extra constants for calculatingf$frac{hbar^2}{2m}f$ for BSk forces

Variables

- real(kind=dp), parameter parameters::mamuc2 = 931.49386_dp

  Atomic mass unit u.
- real(kind=dp), parameter parameters::xmh = 7.28896940_dp
- real(kind=dp), parameter parameters::rydb = 13.6056981e-6_dp

  Rydberg constant.
- real(kind=dp), parameter parameters::xmp = xmh - mec2 + rydb
- real(kind=dp), parameter parameters::xmn = 8.07132281_dp

4.2.1 Detailed Description

4.2.2 Variable Documentation

4.2.2.1 mamuc2

```
real(kind=dp), parameter parameters::mamuc2 = 931.49386_dp
```

Atomic mass unit u.

4.2.2.2 rydb

```
real(kind=dp), parameter parameters::rydb = 13.6056981e-6_dp
```

Rydberg constant.

4.2.2.3 xmh

```
real(kind=dp), parameter parameters::xmh = 7.28896940_dp
```

4.2.2.4 xmn

```
real(kind=dp), parameter parameters::xmn = 8.07132281_dp
```

4.2.2.5 xmp

```
real(kind=dp), parameter parameters::xmp = xmh - mec2 + rydb
```

4.3 Numerical fractions

Variables

- real(kind=dp), parameter parameters::fr12 = 1._dp/2
- real(kind=dp), parameter parameters::fr14 = 1._dp/4
- real(kind=dp), parameter parameters::fr18 = 1._dp/8
- real(kind=dp), parameter parameters::fr1_16 = 1._dp/16
- real(kind=dp), parameter parameters::fr1_32 = 1._dp/32
- real(kind=dp), parameter parameters::fr13 = 1._dp/3
- real(kind=dp), parameter parameters::fr16 = 1._dp/6
- real(kind=dp), parameter parameters::fr1_12 = 1._dp/12
- real(kind=dp), parameter parameters::fr1_24 = 1._dp/24
- real(kind=dp), parameter parameters::fr1_36 = 1._dp/36
- real(kind=dp), parameter parameters::fr23 = 2._dp/3
- real(kind=dp), parameter parameters::fr29 = 2._dp/9
- real(kind=dp), parameter parameters::fr32 = 3._dp/2
- real(kind=dp), parameter parameters::fr34 = 3._dp/4
- real(kind=dp), parameter parameters::fr35 = 3._dp/5
- real(kind=dp), parameter parameters::fr38 = 3._dp/8
- real(kind=dp), parameter parameters::fr3_10 = 3._dp/10
- real(kind=dp), parameter parameters::fr43 = 4._dp/3
- real(kind=dp), parameter parameters::fr53 = 5._dp/3
- real(kind=dp), parameter parameters::fr54 = 5._dp/4
- real(kind=dp), parameter parameters::fr83 = 8._dp/3
- real(kind=dp), parameter parameters::fr260_3 = 260._dp/3

4.3.1 Detailed Description

4.3.2 Variable Documentation

4.3.2.1 fr12

```
real(kind=dp), parameter parameters::fr12 = 1._dp/2
```

4.3.2.2 fr13

```
real(kind=dp), parameter parameters::fr13 = 1._dp/3
```

4.3.2.3 fr14

```
real(kind=dp), parameter parameters::fr14 = 1._dp/4
```

4.3.2.4 fr16

```
real(kind=dp), parameter parameters::fr16 = 1._dp/6
```

4.3.2.5 fr18

```
real(kind=dp), parameter parameters::fr18 = 1._dp/8
```

4.3.2.6 fr1_12

```
real(kind=dp), parameter parameters::fr1_12 = 1._dp/12
```

4.3.2.7 fr1_16

```
real(kind=dp), parameter parameters::fr1_16 = 1._dp/16
```

4.3.2.8 fr1_24

```
real(kind=dp), parameter parameters::fr1_24 = 1._dp/24
```

4.3.2.9 fr1_32

```
real(kind=dp), parameter parameters::fr1_32 = 1._dp/32
```

4.3.2.10 fr1_36

```
real(kind=dp), parameter parameters::fr1_36 = 1._dp/36
```

4.3.2.11 fr23

```
real(kind=dp), parameter parameters::fr23 = 2._dp/3
```

4.3.2.12 fr260_3

```
real(kind=dp), parameter parameters::fr260_3 = 260._dp/3
```

4.3.2.13 fr29

```
real(kind=dp), parameter parameters::fr29 = 2._dp/9
```

4.3.2.14 fr32

```
real(kind=dp), parameter parameters::fr32 = 3._dp/2
```

4.3.2.15 fr34

```
real(kind=dp), parameter parameters::fr34 = 3._dp/4
```

4.3.2.16 fr35

```
real(kind=dp), parameter parameters::fr35 = 3._dp/5
```

4.3.2.17 fr38

```
real(kind=dp), parameter parameters::fr38 = 3._dp/8
```

4.3.2.18 fr3_10

```
real(kind=dp), parameter parameters::fr3_10 = 3._dp/10
```

4.3.2.19 fr43

```
real(kind=dp), parameter parameters::fr43 = 4._dp/3
```

4.3.2.20 fr53

```
real(kind=dp), parameter parameters::fr53 = 5._dp/3
```

4.3.2.21 fr54

```
real(kind=dp), parameter parameters::fr54 = 5._dp/4
```

4.3.2.22 fr83

```
real(kind=dp), parameter parameters::fr83 = 8._dp/3
```

4.4 Skyrme parameters

Variables

- real(kind=dp) parameters::w0

  Spin-orbit strength W_0.
- real(kind=dp) parameters::t0
- real(kind=dp) parameters::x0
- real(kind=dp) parameters::t1
- real(kind=dp) parameters::x1
- real(kind=dp) parameters::t2
- real(kind=dp) parameters::x2
- real(kind=dp) parameters::t3
- real(kind=dp) parameters::x3
- real(kind=dp) parameters::sigma
- real(kind=dp), dimension(0:1) parameters::hbar2_2m_q

  $\frac{\hbar^2}{2m}$ *with isospin dependence, as required by BSk forces*
- logical parameters::j2_terms

  Whether functional uses $\boldsymbol{J}^2$ terms.

4.4.1 Detailed Description

4.4.2 Variable Documentation

4.4.2.1 hbar2_2m_q

```
real(kind=dp), dimension(0:1) parameters::hbar2_2m_q
```

$\frac{\hbar^2}{2m}$ with isospin dependence, as required by BSk forces

4.4.2.2 j2_terms

```
logical parameters::j2_terms
```

Whether functional uses $\mathbf{J}^2$ terms.

4.4.2.3 sigma

```
real(kind=dp) parameters::sigma
```

4.4.2.4 t0

```
real(kind=dp) parameters::t0
```

4.4.2.5 t1

```
real(kind=dp) parameters::t1
```

4.4.2.6 t2

```
real(kind=dp) parameters::t2
```

4.4.2.7 t3

```
real(kind=dp) parameters::t3
```

4.4.2.8 w0

```
real(kind=dp) parameters::w0
```

Spin-orbit strength W_0.

4.4.2.9 x0

```
real(kind=dp) parameters::x0
```

4.4.2.10 x1

```
real(kind=dp) parameters::x1
```

4.4.2.11 x2

```
real(kind=dp) parameters::x2
```

4.4.2.12 x3

```
real(kind=dp) parameters::x3
```

4.5 Skyrme coefficients

Variables

- real(kind=dp) parameters::b1
- real(kind=dp) parameters::b2
- real(kind=dp) parameters::b3
- real(kind=dp) parameters::b4
- real(kind=dp) parameters::b5
- real(kind=dp) parameters::b6
- real(kind=dp) parameters::b7
- real(kind=dp) parameters::b8
- real(kind=dp) parameters::b9
- real(kind=dp) parameters::b10
- real(kind=dp) parameters::b11
- real(kind=dp) parameters::b12
- real(kind=dp) parameters::b13

4.5.1 Detailed Description

4.5.2 Variable Documentation

4.5.2.1 b1

```
real(kind=dp) parameters::b1
```

4.5.2.2 b10

```
real(kind=dp) parameters::b10
```

4.5.2.3 b11

```
real(kind=dp) parameters::b11
```

4.5.2.4 b12

```
real(kind=dp) parameters::b12
```

4.5.2.5 b13

```
real(kind=dp) parameters::b13
```

4.5.2.6 b2

```
real(kind=dp) parameters::b2
```

4.5.2.7 b3

```
real(kind=dp) parameters::b3
```

4.5.2.8 b4

```
real(kind=dp) parameters::b4
```

4.5.2.9 b5

```
real(kind=dp) parameters::b5
```

4.5.2.10 b6

```
real(kind=dp) parameters::b6
```

4.5.2.11 b7

```
real(kind=dp) parameters::b7
```

4.5.2.12 b8

```
real(kind=dp) parameters::b8
```

4.5.2.13 b9

```
real(kind=dp) parameters::b9
```

4.6 Extra parameters for BSk forces

Variables

- real(kind=dp) parameters::alpha
- real(kind=dp) parameters::beta
- real(kind=dp) parameters::gamma
- real(kind=dp) parameters::t4
- real(kind=dp) parameters::x4
- real(kind=dp) parameters::t5
- real(kind=dp) parameters::x5
- real(kind=dp) parameters::fn_pos
- real(kind=dp) parameters::fn_neg
- real(kind=dp) parameters::fp_pos
- real(kind=dp) parameters::fp_neg
- real(kind=dp) parameters::epsilon_lambda

4.6.1 Detailed Description

4.6.2 Variable Documentation

4.6.2.1 alpha

```
real(kind=dp) parameters::alpha
```

4.6.2.2 beta

```
real(kind=dp) parameters::beta
```

4.6.2.3 epsilon_lambda

```
real(kind=dp) parameters::epsilon_lambda
```

4.6.2.4 fn_neg

```
real(kind=dp) parameters::fn_neg
```

4.6.2.5 fn_pos

```
real(kind=dp) parameters::fn_pos
```

4.6.2.6 fp_neg

```
real(kind=dp) parameters::fp_neg
```

4.6.2.7 fp_pos

```
real(kind=dp) parameters::fp_pos
```

4.6.2.8 gamma

```
real(kind=dp) parameters::gamma
```

4.6.2.9 t4

```
real(kind=dp) parameters::t4
```

4.6.2.10 t5

```
real(kind=dp) parameters::t5
```

4.6.2.11 x4

```
real(kind=dp) parameters::x4
```

4.6.2.12 x5

```
real(kind=dp) parameters::x5
```

4.7 Mesh variable

Variables

- real(kind=dp), dimension(:), allocatable parameters::r

  Mesh for r.

4.7.1 Detailed Description

4.7.2 Variable Documentation

4.7.2.1 r

```
real(kind=dp), dimension(:), allocatable parameters::r
```

Mesh for r.

4.8 Global density arrays

Variables

- real(kind=dp), dimension(:,:), allocatable parameters::rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::del2_rho_q
- real(kind=dp), dimension(:), allocatable parameters::rho_t
- real(kind=dp), dimension(:), allocatable parameters::del_rho_t
- real(kind=dp), dimension(:), allocatable parameters::del2_rho_t

4.8.1 Detailed Description

4.8.2 Variable Documentation

4.8.2.1 del2_rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::del2_rho_q
```

4.8.2.2 del2_rho_t

```
real(kind=dp), dimension(:), allocatable parameters::del2_rho_t
```

4.8.2.3 del_rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::del_rho_q
```

4.8.2.4 del_rho_t

```
real(kind=dp), dimension(:), allocatable parameters::del_rho_t
```

4.8.2.5 rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::rho_q
```

4.8.2.6 rho_t

```
real(kind=dp), dimension(:), allocatable parameters::rho_t
```

4.9 Global effective mass arrays

Variables

- real(kind=dp), dimension(:,:), allocatable parameters::f_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::del2_f_q

4.9.1 Detailed Description

4.9.2 Variable Documentation

4.9.2.1 del2_f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::del2_f_q
```

4.9.2.2 del_f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::del_f_q
```

4.9.2.3 f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::f_q
```

4.10 Global arrays for other densities and fields

Variables

- real(kind=dp), dimension(:,:), allocatable parameters::w_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_w_q
- real(kind=dp), dimension(:,:), allocatable parameters::u_q
- real(kind=dp), dimension(:,:), allocatable parameters::j_2_q
- real(kind=dp), dimension(:,:), allocatable parameters::j_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_j_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_j_2_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_j_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_tf_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_2_l_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_2_nl_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_etf_q
- real(kind=dp), dimension(:), allocatable parameters::j_t
- real(kind=dp), dimension(:), allocatable parameters::del_j_t
- real(kind=dp), dimension(:), allocatable parameters::div_j_t
- real(kind=dp), dimension(:), allocatable parameters::tau_etf_t
- real(kind=dp), dimension(:), allocatable parameters::e_density_field
- real(kind=dp), dimension(:), allocatable parameters::e_density_sky
- real(kind=dp), dimension(:), allocatable parameters::v_c_di
- real(kind=dp), dimension(:), allocatable parameters::v_c_ex
- real(kind=dp), dimension(:), allocatable parameters::e_density_c_di
- real(kind=dp), dimension(:), allocatable parameters::e_density_c_ex
- real(kind=dp), dimension(:), allocatable parameters::v_c_pe
- real(kind=dp), dimension(:,:,:), allocatable parameters::tau_2_cont_q
- real(kind=dp), dimension(:), allocatable parameters::rho_ch

  Charge density.

4.10.1 Detailed Description

4.10.2 Variable Documentation

4.10.2.1 del_j_q

```
real(kind=dp), dimension(:,:), allocatable parameters::del_j_q
```

4.10.2.2 del_j_t

```
real(kind=dp), dimension(:), allocatable parameters::del_j_t
```

4.10.2.3 div_j_2_q

```
real(kind=dp), dimension(:,:), allocatable parameters::div_j_2_q
```

4.10.2.4 div_j_q

```
real(kind=dp), dimension(:,:), allocatable parameters::div_j_q
```

4.10.2.5 div_j_t

```
real(kind=dp), dimension(:), allocatable parameters::div_j_t
```

4.10.2.6 div_w_q

```
real(kind=dp), dimension(:,:), allocatable parameters::div_w_q
```

4.10.2.7 e_density_c_di

```
real(kind=dp), dimension(:), allocatable parameters::e_density_c_di
```

4.10.2.8 e_density_c_ex

```
real(kind=dp), dimension(:), allocatable parameters::e_density_c_ex
```

4.10.2.9 e_density_field

```
real(kind=dp), dimension(:), allocatable parameters::e_density_field
```

4.10.2.10 e_density_sky

```
real(kind=dp), dimension(:), allocatable parameters::e_density_sky
```

4.10.2.11 j_2_q

```
real(kind=dp), dimension(:,:), allocatable parameters::j_2_q
```

4.10.2.12 j_q

```
real(kind=dp), dimension(:,:), allocatable parameters::j_q
```

4.10.2.13 j_t

```
real(kind=dp), dimension(:), allocatable parameters::j_t
```

4.10.2.14 rho_ch

```
real(kind=dp), dimension(:), allocatable parameters::rho_ch
```

Charge density.

4.10.2.15 tau_2_cont_q

```
real(kind=dp), dimension(:,:,:), allocatable parameters::tau_2_cont_q
```

4.10.2.16 tau_2_l_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_2_l_q
```

4.10.2.17 tau_2_nl_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_2_nl_q
```

4.10.2.18 tau_etf_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_etf_q
```

4.10.2.19 tau_etf_t

```
real(kind=dp), dimension(:), allocatable parameters::tau_etf_t
```

4.10.2.20 tau_tf_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_tf_q
```

4.10.2.21 u_q

```
real(kind=dp), dimension(:,:), allocatable parameters::u_q
```

4.10.2.22 v_c_di

```
real(kind=dp), dimension(:), allocatable parameters::v_c_di
```

4.10.2.23 v_c_ex

```
real(kind=dp), dimension(:), allocatable parameters::v_c_ex
```

4.10.2.24 v_c_pe

```
real(kind=dp), dimension(:), allocatable parameters::v_c_pe
```

4.10.2.25 w_q

```
real(kind=dp), dimension(:,:), allocatable parameters::w_q
```

4.11 Global arrays for densities and fields for 4th-order terms

4.12 Variables for storing properties of Wigner-Seitz cell

Variables

- real(kind=dp), dimension(0:1) parameters::n_q

  Number of neutrons and protons.
- real(kind=dp) parameters::n_t

  Total number of particles.
- real(kind=dp) parameters::e_field

  Field energy.
- real(kind=dp) parameters::e_skyrme

  Skyrme energy.
- real(kind=dp), dimension(0:1) parameters::e_kinetic_q

  Kinetic energy for neutron and protons.
- real(kind=dp) parameters::e_kinetic_t

  Total kinetic energy.
- real(kind=dp) parameters::e_so

  Spin-orbit energy.
- real(kind=dp) parameters::e_coulomb_di

  Direct Coulomb energy.
- real(kind=dp) parameters::e_coulomb_ex

  Exhange Coulomb energy.
- real(kind=dp) parameters::e_coulomb

  Total Coulomb energy.
- real(kind=dp) parameters::e_total

  Total energy.
- real(kind=dp), dimension(0:1) parameters::mu_q

  Neutron and proton chemical potential.
- real(kind=dp) parameters::mu_e

  Electron chemical potential.
- real(kind=dp) parameters::mu_c

  Coulomb interaction contribution to electron chemical potential.
- real(kind=dp) parameters::delta_mu

  Overall chemical potential (beta-equilibrium condition)
- real(kind=dp) parameters::pressure_nucl

  Nuclear pressure.
- real(kind=dp) parameters::pressure_e

  Electron pressure.
- real(kind=dp) parameters::pressure_ex

  Coulomb exchange pressure.
- real(kind=dp) parameters::pressure_t

  Total pressure.

4.12.1 Detailed Description

4.12.2 Variable Documentation

4.12.2.1 delta_mu

```
real(kind=dp) parameters::delta_mu
```

Overall chemical potential (beta-equilibrium condition)

4.12.2.2 e_coulomb

```
real(kind=dp) parameters::e_coulomb
```

Total Coulomb energy.

4.12.2.3 e_coulomb_di

```
real(kind=dp) parameters::e_coulomb_di
```

Direct Coulomb energy.

4.12.2.4 e_coulomb_ex

```
real(kind=dp) parameters::e_coulomb_ex
```

Exhange Coulomb energy.

4.12.2.5 e_field

```
real(kind=dp) parameters::e_field
```

Field energy.

4.12.2.6 e_kinetic_q

```
real(kind=dp), dimension(0:1) parameters::e_kinetic_q
```

Kinetic energy for neutron and protons.

4.12.2.7 e_kinetic_t

```
real(kind=dp) parameters::e_kinetic_t
```

Total kinetic energy.

4.12.2.8 e_skyrme

```
real(kind=dp) parameters::e_skyrme
```

Skyrme energy.

4.12.2.9 e_so

```
real(kind=dp) parameters::e_so
```

Spin-orbit energy.

4.12.2.10 e_total

```
real(kind=dp) parameters::e_total
```

Total energy.

4.12.2.11 mu_c

```
real(kind=dp) parameters::mu_c
```

Coulomb interaction contribution to electron chemical potential.

4.12.2.12 mu_e

```
real(kind=dp) parameters::mu_e
```

Electron chemical potential.

4.12.2.13 mu_q

```
real(kind=dp), dimension(0:1) parameters::mu_q
```

Neutron and proton chemical potential.

4.12.2.14 n_q

```
real(kind=dp), dimension(0:1) parameters::n_q
```

Number of neutrons and protons.

4.12.2.15 n_t

```
real(kind=dp) parameters::n_t
```

Total number of particles.

4.12.2.16 pressure_e

```
real(kind=dp) parameters::pressure_e
```

Electron pressure.

4.12.2.17 pressure_ex

```
real(kind=dp) parameters::pressure_ex
```

Coulomb exchange pressure.

4.12.2.18 pressure_nucl

```
real(kind=dp) parameters::pressure_nucl
```

Nuclear pressure.

4.12.2.19 pressure_t

```
real(kind=dp) parameters::pressure_t
```

Total pressure.

4.13 Input parameters

Variables

- integer parameters::run_mode

  Mode to run code in (normal, test)
- logical parameters::verbose

  Whether to print all extra messages about run.
- real(kind=dp) parameters::dr

  Mesh spacing of r (fm).
- logical parameters::profile_r_max

  Whether to take "r_max" from "r_ws".
- real(kind=dp) parameters::r_max

  Max value of r (fm).
- logical parameters::specify_n

  Whether to specify "n" instead of "dr".
- integer parameters::n

  Number of mesh points.
- integer parameters::force

  Force to use.
- integer parameters::etf_order

  Order at which to calculate kinetic energy densities.
- logical parameters::coulomb_on

  Use Coulomb interaction or not.
- logical parameters::electrons_on

  Add electrons.
- integer parameters::nmaxstate

  Number of states that can be stored.
- integer parameters::lmax

  Maximum angular momentum of states to find.
- logical parameters::calc_chem_pots

  Calculate chemical potentials.
- logical, dimension(0:1) parameters::strutinsky_on

  Use Strutinsky Integral (SI) correction for neutrons and protons.
- real(kind=dp) parameters::strut_r_max

  Max value of r to use for box for single particle states (fm).
- logical parameters::emax0_mod

  Whether to modify "emax0" to always = 0.
- integer parameters::neutron_pairing

  Type of pairing calculation to perform for neutrons.
- logical parameters::proton_bcs

  Whether to do BCS for protons.
- real(kind=dp) parameters::pair_qp_cut

  Cut-off for quasiparticle energy for solving gap equation.
- logical parameters::smooth_qp_cut

  Whether to use smooth cut-off on quasiparticle energy.
- real(kind=dp) parameters::pair_k_max

  Maximum momentum for integral in gap equation.
- real(kind=dp) parameters::pair_v0

  Interaction strength parameter.

- real(kind=dp) parameters::pair_eta

  Interaction parameter eta.
- real(kind=dp) parameters::pair_alpha

  Interaction parameter alpha.
- real(kind=dp) parameters::pair_tol

  Gap equation self-consistency tolerance.
- real(kind=dp) parameters::pair_mix

  Mix of previous iteration in gap equation self-consistency loop.
- real(kind=dp) parameters::pair_dk

  Step size in integral in gap equation.
- real(kind=dp) parameters::pair_del_init

  Initial guess for pairing gap.
- integer parameters::pair_max_iters

  Maximum iterations for gap equation self-consistency loop.
- real(kind=dp) parameters::pair_num_tol

  BCS number equation self-consistency tolerance.

4.13.1 Detailed Description

4.13.2 Variable Documentation

4.13.2.1 calc_chem_pots

```
logical parameters::calc_chem_pots
```

Calculate chemical potentials.

4.13.2.2 coulomb_on

```
logical parameters::coulomb_on
```

Use Coulomb interaction or not.

4.13.2.3 dr

```
real(kind=dp) parameters::dr
```

Mesh spacing of r (fm).

4.13.2.4 electrons_on

```
logical parameters::electrons_on
```

Add electrons.

4.13.2.5 emax0_mod

```
logical parameters::emax0_mod
```

Whether to modify "emax0" to always = 0.

4.13.2.6 etf_order

```
integer parameters::etf_order
```

Order at which to calculate kinetic energy densities.

4.13.2.7 force

```
integer parameters::force
```

Force to use.

4.13.2.8 lmax

```
integer parameters::lmax
```

Maximum angular momentum of states to find.

4.13.2.9 n

```
integer parameters::n
```

Number of mesh points.

4.13.2.10 neutron_pairing

```
integer parameters::neutron_pairing
```

Type of pairing calculation to perform for neutrons.

4.13.2.11 nmaxstate

```
integer parameters::nmaxstate
```

Number of states that can be stored.

4.13.2.12 pair_alpha

```
real(kind=dp) parameters::pair_alpha
```

Interaction parameter alpha.

4.13.2.13 pair_del_init

```
real(kind=dp) parameters::pair_del_init
```

Initial guess for pairing gap.

4.13.2.14 pair_dk

```
real(kind=dp) parameters::pair_dk
```

Step size in integral in gap equation.

4.13.2.15 pair_eta

```
real(kind=dp) parameters::pair_eta
```

Interaction parameter eta.

4.13.2.16 pair_k_max

```
real(kind=dp) parameters::pair_k_max
```

Maximum momentum for integral in gap equation.

4.13.2.17 pair_max_iters

```
integer parameters::pair_max_iters
```

Maximum iterations for gap equation self-consistency loop.

4.13.2.18 pair_mix

```
real(kind=dp) parameters::pair_mix
```

Mix of previous iteration in gap equation self-consistency loop.

4.13.2.19 pair_num_tol

```
real(kind=dp) parameters::pair_num_tol
```

BCS number equation self-consistency tolerance.

4.13.2.20 pair_qp_cut

```
real(kind=dp) parameters::pair_qp_cut
```

Cut-off for quasiparticle energy for solving gap equation.

4.13.2.21 pair_tol

```
real(kind=dp) parameters::pair_tol
```

Gap equation self-consistency tolerance.

4.13.2.22 pair_v0

```
real(kind=dp) parameters::pair_v0
```

Interaction strength parameter.

4.13.2.23 profile_r_max

```
logical parameters::profile_r_max
```

Whether to take "r_max" from "r_ws".

4.13.2.24 proton_bcs

```
logical parameters::proton_bcs
```

Whether to do BCS for protons.

4.13.2.25 r_max

```
real(kind=dp) parameters::r_max
```

Max value of r (fm).

4.13.2.26 run_mode

```
integer parameters::run_mode
```

Mode to run code in (normal, test)

4.13.2.27 smooth_qp_cut

```
logical parameters::smooth_qp_cut
```

Whether to use smooth cut-off on quasiparticle energy.

4.13.2.28 specify_n

```
logical parameters::specify_n
```

Whether to specify "n" instead of "dr".

4.13.2.29 strut_r_max

```
real(kind=dp) parameters::strut_r_max
```

Max value of r to use for box for single particle states (fm).

4.13.2.30 strutinsky_on

```
logical, dimension(0:1) parameters::strutinsky_on
```

Use Strutinsky Integral (SI) correction for neutrons and protons.

4.13.2.31 verbose

```
logical parameters::verbose
```

Whether to print all extra messages about run.

4.14 External profiles

Variables

- real(kind=dp), dimension(5) parameters::n_profile
- real(kind=dp), dimension(5) parameters::p_profile
- real(kind=dp) parameters::num_n
- integer parameters::num_p
- real(kind=dp) parameters::r_ws

4.14.1 Detailed Description

4.14.2 Variable Documentation

4.14.2.1 n_profile

```
real(kind=dp), dimension(5) parameters::n_profile
```

4.14.2.2 num_n

```
real(kind=dp) parameters::num_n
```

4.14.2.3 num_p

```
integer parameters::num_p
```

4.14.2.4 p_profile

```
real(kind=dp), dimension(5) parameters::p_profile
```

4.14.2.5 r_ws

```
real(kind=dp) parameters::r_ws
```

4.15 Format statements

Variables

- character(18), dimension(10) parameters::n_floats = (/'(1(es24.16e3,1x))','(2(es24.16e3,1x))','(3(es24.↩ 16e3,1x))', '(4(es24.16e3,1x))','(5(es24.16e3,1x))','(6(es24.16e3,1x))','(7(es24.16e3,1x))', '(8(es24.↩ 16e3,1x))','(9(es24.16e3,1x))','(10(es24.16e3,1x))'/)
- character(27) parameters::info_format = '(a27,1x,a1,1x,es24.16e3)'

4.15.1 Detailed Description

4.15.2 Variable Documentation

4.15.2.1 info_format

```
character(27) parameters::info_format = '(a27,1x,a1,1x,es24.16e3)'
```

4.15.2.2 n_floats

```
character(18), dimension(10) parameters::n_floats = (/'( 1(es24.16e3,1x))','( 2(es24.16e3,1x))','(
3(es24.16e3,1x))', '( 4(es24.16e3,1x))','( 5(es24.16e3,1x))','( 6(es24.16e3,1x))','( 7(es24.↩
16e3,1x))', '( 8(es24.16e3,1x))','( 9(es24.16e3,1x))','(10(es24.16e3,1x))'/)
```

4.16 Global strings for printing output

Variables

- character(8) parameters::force_string
- character(80), parameter parameters::line_break = '##

    Separating output.
- character(62), parameter parameters::table_string = '---------------------------+------------------------'
- character(1), dimension(0:1), parameter parameters::iso_string = (/'n','p'/)

    Isospin labels.
- character(4), parameter parameters::space4 = ' '

    Whitespace of length 4.

4.16.1 Detailed Description

4.16.2 Variable Documentation

4.16.2.1 force_string

```
character(8) parameters::force_string
```

4.16.2.2 iso_string

```
character(1), dimension(0:1), parameter parameters::iso_string = (/'n','p'/)
```

Isospin labels.

4.16.2.3 line_break

```
character(80), parameter parameters::line_break = '##########################################################
```

Separating output.

4.16.2.4 space4

```
character(4), parameter parameters::space4 = ' '
```

Whitespace of length 4.

4.16.2.5 table_string

```
character(62), parameter parameters::table_string = '---------------------------+------------------------'
```

4.17 Variables for use in strutinsky module

Variables

- integer parameters::strut_n
- real(kind=dp), dimension(:,:), allocatable parameters::dhmen
- real(kind=dp), dimension(:,:), allocatable parameters::d2hmen
- real(kind=dp), dimension(:,:), allocatable parameters::hb2m
- real(kind=dp), dimension(:,:), allocatable parameters::vpot
- real(kind=dp), dimension(:,:), allocatable parameters::vso
- real(kind=dp), dimension(0:1) parameters::ecut

  Cutoff energies for neutrons and protons.
- real(kind=dp), dimension(:,:), allocatable parameters::ps

  Storage for single particle wavefunctions.
- integer parameters::nnst

  Number of states found within cutoff energy.
- integer, dimension(:), allocatable parameters::jjp

  Storage for J of states found.
- integer, dimension(:), allocatable parameters::lp

  Storage for L of states found.
- real(kind=dp), dimension(:), allocatable parameters::ep

  Storage for energy of states found.
- real(kind=dp), dimension(0:1) parameters::e_sc_q

  Storage for shell correction energies.
- real(kind=dp) parameters::e_sc_t

  Storage for total shell correction energy.

4.17.1 Detailed Description

4.17.2 Variable Documentation

4.17.2.1 d2hmen

```
real(kind=dp), dimension(:,:), allocatable parameters::d2hmen
```

4.17.2.2 dhmen

```
real(kind=dp), dimension(:,:), allocatable parameters::dhmen
```

4.17.2.3 e_sc_q

```
real(kind=dp), dimension(0:1) parameters::e_sc_q
```

Storage for shell correction energies.

4.17.2.4 e_sc_t

```
real(kind=dp) parameters::e_sc_t
```

Storage for total shell correction energy.

4.17.2.5 ecut

```
real(kind=dp), dimension(0:1) parameters::ecut
```

Cutoff energies for neutrons and protons.

4.17.2.6 ep

```
real(kind=dp), dimension(:), allocatable parameters::ep
```

Storage for energy of states found.

4.17.2.7 hb2m

```
real(kind=dp), dimension(:,:), allocatable parameters::hb2m
```

4.17.2.8 jjp

```
integer, dimension(:), allocatable parameters::jjp
```

Storage for J of states found.

4.17.2.9 lp

```
integer, dimension(:), allocatable parameters::lp
```

Storage for L of states found.

4.17.2.10 nnst

```
integer parameters::nnst
```

Number of states found within cutoff energy.

4.17.2.11 ps

```
real(kind=dp), dimension(:,:), allocatable parameters::ps
```

Storage for single particle wavefunctions.

4.17.2.12 strut_n

```
integer parameters::strut_n
```

4.17.2.13 vpot

```
real(kind=dp), dimension(:,:), allocatable parameters::vpot
```

4.17.2.14 vso

```
real(kind=dp), dimension(:,:), allocatable parameters::vso
```

4.18 Variables for use in pairing module

Variables

- real(kind=dp), dimension(:), allocatable parameters::pair_gap_n

  Neutron pairing gap.
- real(kind=dp), dimension(:), allocatable parameters::delta_n

  Neutron pairing field.
- real(kind=dp), dimension(:), allocatable parameters::pair_gap_p

  Proton pairing gap.
- real(kind=dp), dimension(:), allocatable parameters::delta_p

  Proton pairing field.
- real(kind=dp), dimension(:), allocatable parameters::rho_p_bcs

  Proton density (from wavefunctions)
- real(kind=dp), dimension(:), allocatable parameters::rho_anom_p_bcs

  Anomalous density.
- real(kind=dp), dimension(:), allocatable parameters::strength_bcs

  Interaction strength for protons.
- real(kind=dp), dimension(:), allocatable parameters::occ_v

  Particle occupation probabilities.
- real(kind=dp), dimension(:), allocatable parameters::occ_u

  Hole occupation probabilities.
- real(kind=dp), dimension(:), allocatable parameters::e_qp_p

  Quasiparticle energies.
- real(kind=dp) parameters::num_p_bcs

  Number of protons calculated from occupations.
- real(kind=dp) parameters::e_pair_bcs

  BCS pairing energy.
- real(kind=dp), dimension(0:1) parameters::e_pair_q

  Storage for pairing condensation energies.
- real(kind=dp) parameters::e_pair_t

  Storage for total pairing condensation energy.

4.18.1 Detailed Description

4.18.2 Variable Documentation

4.18.2.1 delta_n

```
real(kind=dp), dimension(:), allocatable parameters::delta_n
```

Neutron pairing field.

4.18.2.2 delta_p

```
real(kind=dp), dimension(:), allocatable parameters::delta_p
```

Proton pairing field.

4.18.2.3 e_pair_bcs

```
real(kind=dp) parameters::e_pair_bcs
```

BCS pairing energy.

4.18.2.4 e_pair_q

```
real(kind=dp), dimension(0:1) parameters::e_pair_q
```

Storage for pairing condensation energies.

4.18.2.5 e_pair_t

```
real(kind=dp) parameters::e_pair_t
```

Storage for total pairing condensation energy.

4.18.2.6 e_qp_p

```
real(kind=dp), dimension(:), allocatable parameters::e_qp_p
```

Quasiparticle energies.

4.18.2.7 num_p_bcs

```
real(kind=dp) parameters::num_p_bcs
```

Number of protons calculated from occupations.

4.18.2.8 occ_u

```
real(kind=dp), dimension(:), allocatable parameters::occ_u
```

Hole occupation probabilities.

4.18.2.9 occ_v

```
real(kind=dp), dimension(:), allocatable parameters::occ_v
```

Particle occupation probabilities.

4.18.2.10 pair_gap_n

```
real(kind=dp), dimension(:), allocatable parameters::pair_gap_n
```

Neutron pairing gap.

4.18.2.11 pair_gap_p

```
real(kind=dp), dimension(:), allocatable parameters::pair_gap_p
```

Proton pairing gap.

4.18.2.12 rho_anom_p_bcs

```
real(kind=dp), dimension(:), allocatable parameters::rho_anom_p_bcs
```

Anomalous density.

4.18.2.13 rho_p_bcs

```
real(kind=dp), dimension(:), allocatable parameters::rho_p_bcs
```

Proton density (from wavefunctions)

4.18.2.14 strength_bcs

```
real(kind=dp), dimension(:), allocatable parameters::strength_bcs
```

Interaction strength for protons.

4.19 Variables for electron contributions

Variables

- real(kind=dp) parameters::rho_e

    Electron density.
- real(kind=dp) parameters::e_kinetic_e

    Total electron kinetic energy.
- real(kind=dp) parameters::e_coulomb_e

    Total electron-electron potential energy from Coulomb interaction.
- real(kind=dp) parameters::e_coulomb_pe

    Total proton-electron potential energy from Coulomb interaction.

4.19.1 Detailed Description

4.19.2 Variable Documentation

4.19.2.1 e_coulomb_e

```
real(kind=dp) parameters::e_coulomb_e
```

Total electron-electron potential energy from Coulomb interaction.

4.19.2.2 e_coulomb_pe

```
real(kind=dp) parameters::e_coulomb_pe
```

Total proton-electron potential energy from Coulomb interaction.

4.19.2.3 e_kinetic_e

```
real(kind=dp) parameters::e_kinetic_e
```

Total electron kinetic energy.

4.19.2.4 rho_e

```
real(kind=dp) parameters::rho_e
```

Electron density.

Chapter 5

Module Documentation

5.1 pairing Module Reference

Module to hold routines for carrying out Strutinsky correction.

Functions/Subroutines

- subroutine calc_e_pair ()

  Subroutine to calculate the pairing energy for the WS cell, using the method specified in "input.in".
- real(kind=dp) function calc_gap (r, rhon, rhop, fq, mu)

  Function to calculate the pairing gap in infinite neutron matter, for specified density and effective mass.
- subroutine bcs_protons ()

  Subroutine to perform BCS for protons.
- real(kind=dp) function calc_bcs_num_p (mu_p)

  Function to solve gap equation at given chemical potential "mu_p", returning the (BCS) number of protons.
- real(kind=dp) function interazchamelanalyt (rhon, rhop, hbm, itz)

  Function to calculate the interaction strength for the effective contact pairing force. Modified by M. Shelley.
- real(kind=dp) function llambda (x)

  Function to calculate the pairing cutoff for the effective contact pairing force.
- real(kind=dp) function delta_parametric (kf, YY, itz, xk0)

  Function to calculate the pairing gap using the analytical BSk expression. Modified by M. Shelley.

5.1.1 Detailed Description

Module to hold routines for carrying out Strutinsky correction.

Author

M. Shelley

5.1.2 Function/Subroutine Documentation

5.1.2.1 bcs_protons()

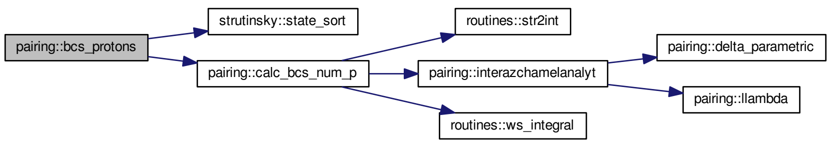
```
subroutine pairing::bcs_protons ( )
```

Subroutine to perform BCS for protons.

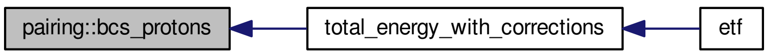
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.1.2.2 calc_bcs_num_p()

```
real(kind=dp) function pairing::calc_bcs_num_p (
              real(kind=dp), intent(in) mu_p )
```

Function to solve gap equation at given chemical potential "mu_p", returning the (BCS) number of protons.

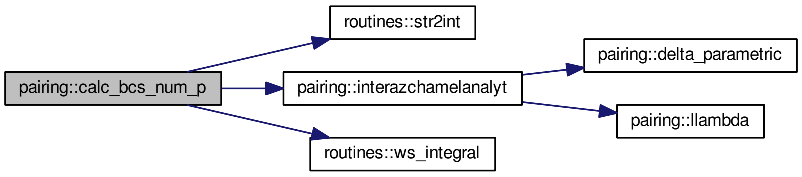
Author

M. Shelley, A. Pastore

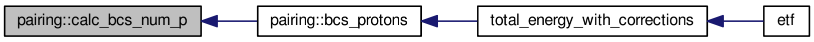
Parameters

in	*mu_p*	Proton chemical potential

Here is the call graph for this function:



Here is the caller graph for this function:



5.1.2.3 calc_e_pair()

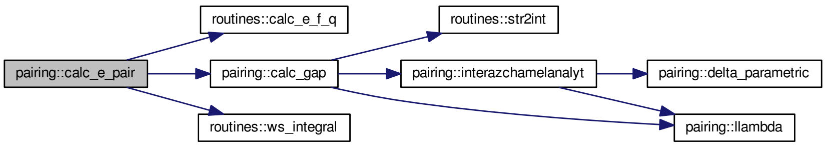
```
subroutine pairing::calc_e_pair ( )
```

Subroutine to calculate the pairing energy for the WS cell, using the method specified in "input.in".

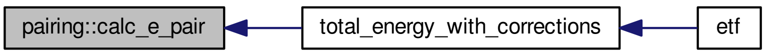
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.1.2.4 calc_gap()

```
real(kind=dp) function pairing::calc_gap (
            real(kind=dp), intent(in) r,
            real(kind=dp), intent(in) rhon,
            real(kind=dp), intent(in) rhop,
            real(kind=dp), intent(in) fq,
            real(kind=dp), intent(in) mu )
```

Function to calculate the pairing gap in infinite neutron matter, for specified density and effective mass.

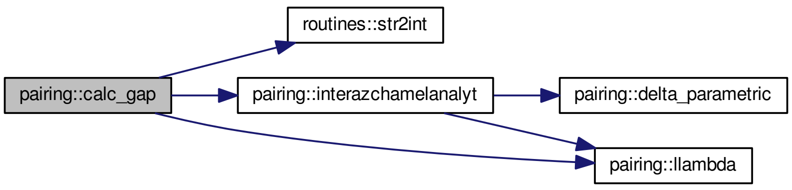
Author

M. Shelley

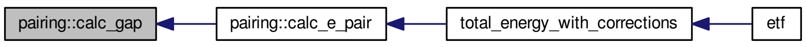
Parameters

in	*r*	Radius
in	*rhon*	Neutron density
in	*rhop*	Proton density
in	*fq*	Effective mass
in	*mu*	Effective chemical potential

Here is the call graph for this function:



Here is the caller graph for this function:



5.1.2.5 delta_parametric()

```
real(kind=dp) function pairing::delta_parametric (
            real(kind=dp), intent(in) kf,
            real(kind=dp), intent(in) YY,
            integer, intent(in) itz,
            real(kind=dp), intent(in) xk0 )
```

Function to calculate the pairing gap using the analytical BSk expression. Modified by M. Shelley.

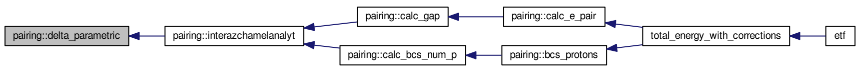
Author

A. Pastore, M. Shelley

Parameters

in	*kf*	Fermi momentum
in	*YY*	Neutron-proton composition
in	*itz*	Isospin
in	*xk0*	"Average" fermi momentum

Here is the caller graph for this function:



5.1.2.6 interazchamelanalyt()

```
real(kind=dp) function pairing::interazchamelanalyt (
          real(kind=dp), intent(in) rhon,
          real(kind=dp), intent(in) rhop,
          real(kind=dp), intent(in) hbm,
          integer, intent(in) itz )
```

Function to calculate the interaction strength for the effective contact pairing force. Modified by M. Shelley.

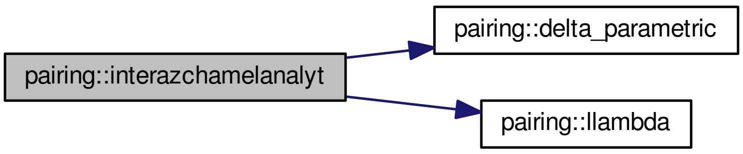
Author

A. Pastore, M. Shelley

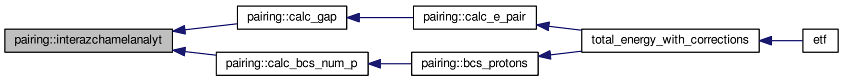
Parameters

in	*rhon*	Neutron density
in	*rhop*	Proton density
in	*hbm*	$\frac{\hbar^2}{2m^*}$
in	*itz*	Isospin

Here is the call graph for this function:



Here is the caller graph for this function:



5.1.2.7 llambda()

```
real(kind=dp) function pairing::llambda (
            real(kind=dp), intent(in) x )
```

Function to calculate the pairing cutoff for the effective contact pairing force.

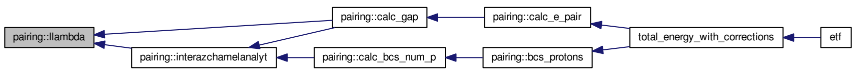
Author

A. Pastore

Parameters

`in`	*x*	(DDCI cutoff) / (Fermi energy)

Here is the caller graph for this function:



5.2 parameters Module Reference

Module to hold global parameters and variables.

Functions/Subroutines

- subroutine force_initialise ()

  Subroutine to initialise Skyrme force parameters with values for a given force specified in 'input.dat'.

Variables

- integer, parameter dp = selected_real_kind(15, 300)

  Precision.
- real(kind=dp), parameter pi = 3.1415926535897932_dp

  π
- real(kind=dp), parameter hbar2_2m = 20.73553_dp

  $\frac{\hbar^2}{2m}$ *for SLy forces*
- real(kind=dp), parameter rho0 = 0.16_dp

  ρ_0*, nuclear saturation density* $[fm^{-3}]$
- real(kind=dp), parameter e2 = 1.439978408596513_dp

  e^2*, electric charge squared* $[MeV \cdot fm]$
- real(kind=dp), parameter mec2 = 0.51099895_dp

  Electron rest mass $[MeV/c^2]$.
- real(kind=dp), parameter mnc2 = 939.56542052_dp
- real(kind=dp), parameter mpc2 = 938.27208816_dp
- real(kind=dp), parameter hbarc = 197.3269804_dp

  $\hbar * c$
- real(kind=dp), parameter mamuc2 = 931.49386_dp

  Atomic mass unit u.
- real(kind=dp), parameter xmh = 7.28896940_dp
- real(kind=dp), parameter rydb = 13.6056981e-6_dp

  Rydberg constant.
- real(kind=dp), parameter xmp = xmh - mec2 + rydb
- real(kind=dp), parameter xmn = 8.07132281_dp
- real(kind=dp), parameter fr12 = 1._dp/2
- real(kind=dp), parameter fr14 = 1._dp/4
- real(kind=dp), parameter fr18 = 1._dp/8
- real(kind=dp), parameter fr1_16 = 1._dp/16
- real(kind=dp), parameter fr1_32 = 1._dp/32
- real(kind=dp), parameter fr13 = 1._dp/3
- real(kind=dp), parameter fr16 = 1._dp/6
- real(kind=dp), parameter fr1_12 = 1._dp/12
- real(kind=dp), parameter fr1_24 = 1._dp/24
- real(kind=dp), parameter fr1_36 = 1._dp/36
- real(kind=dp), parameter fr23 = 2._dp/3
- real(kind=dp), parameter fr29 = 2._dp/9
- real(kind=dp), parameter fr32 = 3._dp/2
- real(kind=dp), parameter fr34 = 3._dp/4
- real(kind=dp), parameter fr35 = 3._dp/5
- real(kind=dp), parameter fr38 = 3._dp/8

- real(kind=dp), parameter fr3_10 = 3._dp/10
- real(kind=dp), parameter fr43 = 4._dp/3
- real(kind=dp), parameter fr53 = 5._dp/3
- real(kind=dp), parameter fr54 = 5._dp/4
- real(kind=dp), parameter fr83 = 8._dp/3
- real(kind=dp), parameter fr260_3 = 260._dp/3
- real(kind=dp) w0

  Spin-orbit strength W_0.
- real(kind=dp) t0
- real(kind=dp) x0
- real(kind=dp) t1
- real(kind=dp) x1
- real(kind=dp) t2
- real(kind=dp) x2
- real(kind=dp) t3
- real(kind=dp) x3
- real(kind=dp) sigma
- real(kind=dp), dimension(0:1) hbar2_2m_q

  $\frac{\hbar^2}{2m}$ *with isospin dependence, as required by BSk forces*
- logical j2_terms

  Whether functional uses $\boldsymbol{J}^2$ *terms.*
- real(kind=dp) b1
- real(kind=dp) b2
- real(kind=dp) b3
- real(kind=dp) b4
- real(kind=dp) b5
- real(kind=dp) b6
- real(kind=dp) b7
- real(kind=dp) b8
- real(kind=dp) b9
- real(kind=dp) b10
- real(kind=dp) b11
- real(kind=dp) b12
- real(kind=dp) b13
- real(kind=dp) alpha
- real(kind=dp) beta
- real(kind=dp) gamma
- real(kind=dp) t4
- real(kind=dp) x4
- real(kind=dp) t5
- real(kind=dp) x5
- real(kind=dp) fn_pos
- real(kind=dp) fn_neg
- real(kind=dp) fp_pos
- real(kind=dp) fp_neg
- real(kind=dp) epsilon_lambda
- real(kind=dp), dimension(:), allocatable r

  Mesh for r.
- real(kind=dp), dimension(:,:), allocatable rho_q
- real(kind=dp), dimension(:,:), allocatable del_rho_q
- real(kind=dp), dimension(:,:), allocatable del2_rho_q
- real(kind=dp), dimension(:), allocatable rho_t
- real(kind=dp), dimension(:), allocatable del_rho_t
- real(kind=dp), dimension(:), allocatable del2_rho_t

- real(kind=dp), dimension(:,:), allocatable f_q
- real(kind=dp), dimension(:,:), allocatable del_f_q
- real(kind=dp), dimension(:,:), allocatable del2_f_q
- real(kind=dp), dimension(:,:), allocatable w_q
- real(kind=dp), dimension(:,:), allocatable div_w_q
- real(kind=dp), dimension(:,:), allocatable u_q
- real(kind=dp), dimension(:,:), allocatable j_2_q
- real(kind=dp), dimension(:,:), allocatable j_q
- real(kind=dp), dimension(:,:), allocatable del_j_q
- real(kind=dp), dimension(:,:), allocatable div_j_2_q
- real(kind=dp), dimension(:,:), allocatable div_j_q
- real(kind=dp), dimension(:,:), allocatable tau_tf_q
- real(kind=dp), dimension(:,:), allocatable tau_2_l_q
- real(kind=dp), dimension(:,:), allocatable tau_2_nl_q
- real(kind=dp), dimension(:,:), allocatable tau_etf_q
- real(kind=dp), dimension(:), allocatable j_t
- real(kind=dp), dimension(:), allocatable del_j_t
- real(kind=dp), dimension(:), allocatable div_j_t
- real(kind=dp), dimension(:), allocatable tau_etf_t
- real(kind=dp), dimension(:), allocatable e_density_field
- real(kind=dp), dimension(:), allocatable e_density_sky
- real(kind=dp), dimension(:), allocatable v_c_di
- real(kind=dp), dimension(:), allocatable v_c_ex
- real(kind=dp), dimension(:), allocatable e_density_c_di
- real(kind=dp), dimension(:), allocatable e_density_c_ex
- real(kind=dp), dimension(:), allocatable v_c_pe
- real(kind=dp), dimension(:,:,:), allocatable tau_2_cont_q
- real(kind=dp), dimension(:), allocatable rho_ch

  Charge density.
- real(kind=dp), dimension(:,:), allocatable d2_rho_q
- real(kind=dp), dimension(:,:), allocatable d3_rho_q
- real(kind=dp), dimension(:,:), allocatable d4_rho_q
- real(kind=dp), dimension(:,:), allocatable d2_f_q
- real(kind=dp), dimension(:,:), allocatable d3_f_q
- real(kind=dp), dimension(:,:), allocatable d4_f_q
- real(kind=dp), dimension(:,:), allocatable a_q
- real(kind=dp), dimension(:,:), allocatable d1_a_q
- real(kind=dp), dimension(:,:), allocatable d2_a_q
- real(kind=dp), dimension(:,:), allocatable d3_a_q
- real(kind=dp), dimension(:,:), allocatable d4_a_q
- real(kind=dp), dimension(:,:), allocatable tau_4_no_spin_q
- real(kind=dp), dimension(:,:), allocatable tau_4_so_q
- real(kind=dp), dimension(:,:), allocatable j_4_q
- real(kind=dp), dimension(:,:), allocatable div_j_4_q
- real(kind=dp), dimension(:,:,:), allocatable tau_4_cont_q
- real(kind=dp), dimension(0:1) n_q

  Number of neutrons and protons.
- real(kind=dp) n_t

  Total number of particles.
- real(kind=dp) e_field

  Field energy.
- real(kind=dp) e_skyrme

  Skyrme energy.
- real(kind=dp), dimension(0:1) e_kinetic_q

Kinetic energy for neutron and protons.
- real(kind=dp) e_kinetic_t

  Total kinetic energy.
- real(kind=dp) e_so

  Spin-orbit energy.
- real(kind=dp) e_coulomb_di

  Direct Coulomb energy.
- real(kind=dp) e_coulomb_ex

  Exhange Coulomb energy.
- real(kind=dp) e_coulomb

  Total Coulomb energy.
- real(kind=dp) e_total

  Total energy.
- real(kind=dp), dimension(0:1) mu_q

  Neutron and proton chemical potential.
- real(kind=dp) mu_e

  Electron chemical potential.
- real(kind=dp) mu_c

  Coulomb interaction contribution to electron chemical potential.
- real(kind=dp) delta_mu

  Overall chemical potential (beta-equilibrium condition)
- real(kind=dp) pressure_nucl

  Nuclear pressure.
- real(kind=dp) pressure_e

  Electron pressure.
- real(kind=dp) pressure_ex

  Coulomb exchange pressure.
- real(kind=dp) pressure_t

  Total pressure.
- integer run_mode

  Mode to run code in (normal, test)
- logical verbose

  Whether to print all extra messages about run.
- real(kind=dp) dr

  Mesh spacing of r (fm).
- logical profile_r_max

  Whether to take "r_max" from "r_ws".
- real(kind=dp) r_max

  Max value of r (fm).
- logical specify_n

  Whether to specify "n" instead of "dr".
- integer n

  Number of mesh points.
- integer force

  Force to use.
- integer etf_order

  Order at which to calculate kinetic energy densities.
- logical coulomb_on

  Use Coulomb interaction or not.
- logical electrons_on

  Add electrons.

- integer nmaxstate

  Number of states that can be stored.
- integer lmax

  Maximum angular momentum of states to find.
- logical calc_chem_pots

  Calculate chemical potentials.
- logical, dimension(0:1) strutinsky_on

  Use Strutinsky Integral (SI) correction for neutrons and protons.
- real(kind=dp) strut_r_max

  Max value of r to use for box for single particle states (fm).
- logical emax0_mod

  Whether to modify "emax0" to always = 0.
- integer neutron_pairing

  Type of pairing calculation to perform for neutrons.
- logical proton_bcs

  Whether to do BCS for protons.
- real(kind=dp) pair_qp_cut

  Cut-off for quasiparticle energy for solving gap equation.
- logical smooth_qp_cut

  Whether to use smooth cut-off on quasiparticle energy.
- real(kind=dp) pair_k_max

  Maximum momentum for integral in gap equation.
- real(kind=dp) pair_v0

  Interaction strength parameter.
- real(kind=dp) pair_eta

  Interaction parameter eta.
- real(kind=dp) pair_alpha

  Interaction parameter alpha.
- real(kind=dp) pair_tol

  Gap equation self-consistency tolerance.
- real(kind=dp) pair_mix

  Mix of previous iteration in gap equation self-consistency loop.
- real(kind=dp) pair_dk

  Step size in integral in gap equation.
- real(kind=dp) pair_del_init

  Initial guess for pairing gap.
- integer pair_max_iters

  Maximum iterations for gap equation self-consistency loop.
- real(kind=dp) pair_num_tol

  BCS number equation self-consistency tolerance.
- real(kind=dp), dimension(5) n_profile
- real(kind=dp), dimension(5) p_profile
- real(kind=dp) num_n
- integer num_p
- real(kind=dp) r_ws
- character(18), dimension(10) n_floats = (/'(1(es24.16e3,1x))','(2(es24.16e3,1x))','(3(es24.16e3,1x))', '(4(es24.16e3,1x))','(5(es24.16e3,1x))','(6(es24.16e3,1x))','(7(es24.16e3,1x))', '(8(es24.16e3,1x))','(9(es24.16e3,1x))','(10(es24.16e3,1x))'/)
- character(27) info_format = '(a27,1x,a1,1x,es24.16e3)'
- character(8) force_string
- character(80), parameter line_break = '###

Separating output.

- character(62), parameter table_string = '--------------------------+-----------------------'
- character(1), dimension(0:1), parameter iso_string = (/'n','p'/)

  Isospin labels.
- character(4), parameter space4 = ' '

  Whitespace of length 4.
- integer strut_n
- real(kind=dp), dimension(:,:), allocatable dhmen
- real(kind=dp), dimension(:,:), allocatable d2hmen
- real(kind=dp), dimension(:,:), allocatable hb2m
- real(kind=dp), dimension(:,:), allocatable vpot
- real(kind=dp), dimension(:,:), allocatable vso
- real(kind=dp), dimension(0:1) ecut

  Cutoff energies for neutrons and protons.
- real(kind=dp), dimension(:,:), allocatable ps

  Storage for single particle wavefunctions.
- integer nnst

  Number of states found within cutoff energy.
- integer, dimension(:), allocatable jjp

  Storage for J of states found.
- integer, dimension(:), allocatable lp

  Storage for L of states found.
- real(kind=dp), dimension(:), allocatable ep

  Storage for energy of states found.
- real(kind=dp), dimension(0:1) e_sc_q

  Storage for shell correction energies.
- real(kind=dp) e_sc_t

  Storage for total shell correction energy.
- real(kind=dp), dimension(:), allocatable pair_gap_n

  Neutron pairing gap.
- real(kind=dp), dimension(:), allocatable delta_n

  Neutron pairing field.
- real(kind=dp), dimension(:), allocatable pair_gap_p

  Proton pairing gap.
- real(kind=dp), dimension(:), allocatable delta_p

  Proton pairing field.
- real(kind=dp), dimension(:), allocatable rho_p_bcs

  Proton density (from wavefunctions)
- real(kind=dp), dimension(:), allocatable rho_anom_p_bcs

  Anomalous density.
- real(kind=dp), dimension(:), allocatable strength_bcs

  Interaction strength for protons.
- real(kind=dp), dimension(:), allocatable occ_v

  Particle occupation probabilities.
- real(kind=dp), dimension(:), allocatable occ_u

  Hole occupation probabilities.
- real(kind=dp), dimension(:), allocatable e_qp_p

  Quasiparticle energies.
- real(kind=dp) num_p_bcs

  Number of protons calculated from occupations.
- real(kind=dp) e_pair_bcs

BCS pairing energy.

- real(kind=dp), dimension(0:1) e_pair_q

  Storage for pairing condensation energies.
- real(kind=dp) e_pair_t

  Storage for total pairing condensation energy.
- real(kind=dp) rho_e

  Electron density.
- real(kind=dp) e_kinetic_e

  Total electron kinetic energy.
- real(kind=dp) e_coulomb_e

  Total electron-electron potential energy from Coulomb interaction.
- real(kind=dp) e_coulomb_pe

  Total proton-electron potential energy from Coulomb interaction.

5.2.1 Detailed Description

Module to hold global parameters and variables.

Author

M. Shelley

5.2.2 Function/Subroutine Documentation

5.2.2.1 force_initialise()

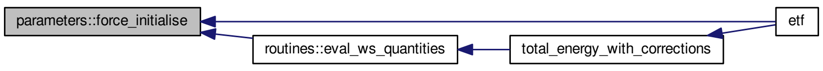
```
subroutine parameters::force_initialise ( )
```

Subroutine to initialise Skyrme force parameters with values for a given force specified in 'input.dat'.

Author

M. Shelley

Here is the caller graph for this function:


parameters::force_initialise
routines::eval_ws_quantities
total_energy_with_corrections
etf

5.2.3 Variable Documentation

5.2.3.1 a_q

```
real(kind=dp), dimension(:,:), allocatable parameters::a_q
```

5.2.3.2 d1_a_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d1_a_q
```

5.2.3.3 d2_a_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d2_a_q
```

5.2.3.4 d2_f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d2_f_q
```

5.2.3.5 d2_rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d2_rho_q
```

5.2.3.6 d3_a_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d3_a_q
```

5.2.3.7 d3_f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d3_f_q
```

5.2.3.8 d3_rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d3_rho_q
```

5.2.3.9 d4_a_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d4_a_q
```

5.2.3.10 d4_f_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d4_f_q
```

5.2.3.11 d4_rho_q

```
real(kind=dp), dimension(:,:), allocatable parameters::d4_rho_q
```

5.2.3.12 div_j_4_q

```
real(kind=dp), dimension(:,:), allocatable parameters::div_j_4_q
```

5.2.3.13 dp

```
integer, parameter parameters::dp = selected_real_kind(15, 300)
```

Precision.

5.2.3.14 j_4_q

```
real(kind=dp), dimension(:,:), allocatable parameters::j_4_q
```

5.2.3.15 tau_4_cont_q

```
real(kind=dp), dimension(:,:,:), allocatable parameters::tau_4_cont_q
```

5.2.3.16 tau_4_no_spin_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_4_no_spin_q
```

5.2.3.17 tau_4_so_q

```
real(kind=dp), dimension(:,:), allocatable parameters::tau_4_so_q
```

5.3 routines Module Reference

Module to hold main routines: densities, energies.

Functions/Subroutines

- integer function str2int (string)
- subroutine allocate_arrays ()

  Subroutine to allocate arrays for all densities and effective masses, and for their derivatives.
- subroutine initialise_uniform_mesh ()

  Subroutine to calculate number of mesh points for a uniform grid, allocate array for r, and then populate r with the mesh points.
- subroutine deallocate_mesh ()

  Subroutine to deallocate array for r.
- subroutine deallocate_arrays ()

  Subroutine to deallocate arrays for all densities and effective masses, and for their derivatives.
- real(kind=dp) function calc_rho_q (rhoqgas, rhoqliq, rq, aq, gammaq, r)

  Function to calculate the neutron or proton density at a given radius r, using supplied input parameters.
- subroutine calc_f_q (rhot, rhoq, q, fq)

  Subroutine to calculate the effective mass ratio $f_q = \frac{m}{m_q^*}$ for neutrons or protons, for standard Skyrme or for BSk forces.
- subroutine calc_w_q (delrho, delrhoq, Wq)

  *Function to calculate the spin-orbit field **W**$_q$ for neutrons or protons.*
- subroutine calc_tau_tf (rhoq, tauTF)

  Function to calculate the zeroth-order contribution to the kinetic energy density for neutrons or protons.
- subroutine calc_tau_2_l (rhoq, delrhoq, del2rhoq, tau2Lq, t2contq)

  Function to calculate the local second-order contribution to the kinetic energy density for neutrons or protons.
- subroutine calc_tau_2_nl (rhoq, delrhoq, fq, delfq, del2fq, Wq, q, tau2NLq, t2contq)

  Subroutine to calculate the non-local second-order contribution to the kinetic energy density for neutrons or protons.
- subroutine calc_tau_4_no_spin (rhoq, d1rhoq, d2rhoq, d3rhoq, d4rhoq, fq, d1fq, d2fq, d3fq, d4fq, tau4nospinq, t4contq)

  *Subroutine to calculate the fourth-order contributions to the kinetic energy density (without spin-orbit contributions) **tau**$_q$ for neutrons or protons.*
- subroutine calc_tau_4_so (rhoq, d1rhoq, fq, d1fq, d2fq, d1Aq, d2Aq, d3Aq, q, tau_4_so_q, t4contq)

  *Subroutine to calculate the fourth-order contributions to the kinetic energy density (spin-orbit contributions) **tau**$_q$ for neutrons or protons.*
- subroutine calc_j_2_q (rhoq, Wq, fq, q, J2q)

  *Subroutine to calculate the second-order contributions to the spin current density **J**$_q$ for neutrons or protons.*

- subroutine calc_j_4_q (rhoq, d1rhoq, fq, d1fq, d2fq, d1Aq, d2Aq, d3Aq, q, J4q)

  Subroutine to calculate the fourth-order contributions to the spin current density $\boldsymbol{J}_q$ for neutrons or protons.
- subroutine calc_div_j_2_q (rhoq, d1rhoq, fq, d1fq, d1Aq, d2Aq, q, divJ2q)

  Subroutine to calculate the second-order contributions to the divergence of the current density $\boldsymbol{J}_q$ for neutrons or protons.
- subroutine calc_div_j_4_q (rhoq, d1rhoq, d2rhoq, fq, d1fq, d2fq, d3fq, d1Aq, d2Aq, d3Aq, d4Aq, q, divJ4q)

  Subroutine to calculate the fourth-order contributions to the divergence of the current density $\boldsymbol{J}_q$ for neutrons or protons.
- real(kind=dp) function calc_u_q (rhot, rhon, rhop, delrhot, delrhon, delrhop, del2rhot, del2rhon, del2rhop, taut, taun, taup, divJt, divJq, q)

  Function to calculate the central potential U_q for neutrons or protons, for standard Skyrme or for BSk forces with extra terms.
- subroutine eval_fields ()

  Subroutine to evaluate matter density derivatives, and all fields: effective masses (and derivatives), spin-orbit fields, spin current densities (and derivatives)
- subroutine eval_tau_etf ()

  Subroutine to calculate the kinetic energy density τ_{ETF} with the (extended) Thomas-Fermi approximation at order specified by "etf_order".
- subroutine charge (rho, Neutr, Nprot, Ngrid1, del1, rhoch)

  Subroutine to calculate the charge density from the matter densities. Modified by M. Shelley.
- subroutine eval_coulomb (prot_dens, calc_exchange)

  Subroutine to evaluate the Coulomb potentials and energy densities, using either the proton or charge density.
- subroutine eval_electrons ()

  Subroutine to evaluate the proton-electron potential which contributes to U_q, all energy contributions, and the pressure, coming from a homogeneous electron gas. Also calculates the electron chemical potential.
- subroutine eval_u_q ()

  Subroutine to evaluate the central fields U_q.
- subroutine eval_skyrme_energy_density ()

  Subroutine to evaluate the Skyrme energy density, after first separately evaluating the field energy density.
- subroutine pressure ()

  Subroutine to calculate the nuclear contribution to the pressure, and then the total pressure.
- subroutine calc_particle_number ()

  Subroutine to calculate the number of particles in the Wigner-Seitz cell.
- subroutine eval_ws_quantities ()

  Subroutine to evaluate the various densities, fields, derivatives, energies, and particle numbers in the WS cell with densities rho_q.
- real(kind=dp) function calc_e_f_q (rhoq, fq, q)

  Subroutine to evaluate the Fermi energy at a given density and effective mass, for neutrons or protons.
- subroutine d1 (n, h, f, df)

  This subroutine computes the first derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.
- subroutine d2 (n, h, f, d2f)

  This subroutine computes the second derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.
- subroutine lap_sphe_symm (f, df_dr, d2f_dr2)

  Subroutine to carry out Laplacian in spherical symmetry.
- subroutine d3 (f, d3f_dr3)

  Subroutine to calculate third derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.
- subroutine d4 (f, d4f_dr4)

  Subroutine to calculate fourth derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.
- subroutine extrapolate_back_3 (grid)

Subroutine to extrapolate back 3 points on the r mesh, to faciliate the calculation of first and second derivatives using a 5-point stencil. Values in grid start at 4, extrapolated values are put in elements 3,2,1. Coefficients come from solving 4th-order polynomial, assuming that f'(0) = 0, and f(-h) = f(h).

- real(kind=dp) function ws_integral (quantity, n_max)

  Function to integrate a density or field over the whole W-S cell, using Simpson's rule (+ Simpson's 3/8 rule if odd number of points)
- subroutine write_densities ()

  Subroutine to write neutron and proton densities to files.
- subroutine write_fields ()

  Subroutine to write neutron and proton fields to files.
- subroutine write_sp_states_p ()

  Subroutine to write proton single particle energies to file, and extra details if BCS has been performed.

Variables

- integer file_unit_0
- integer file_unit_1

  Unit numbers for opening files.

5.3.1 Detailed Description

Module to hold main routines: densities, energies.

Author

M. Shelley

5.3.2 Function/Subroutine Documentation

5.3.2.1 allocate_arrays()

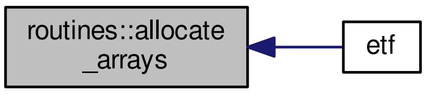
```
subroutine routines::allocate_arrays ( )
```

Subroutine to allocate arrays for all densities and effective masses, and for their derivatives.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.2 calc_div_j_2_q()

```
subroutine routines::calc_div_j_2_q (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) d1rhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) d1fq,
            real(kind=dp), dimension(1:n), intent(in) d1Aq,
            real(kind=dp), dimension(1:n), intent(in) d2Aq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) divJ2q )
```

Subroutine to calculate the second-order contributions to the divergence of the current density $\mathbf{J}_q$ for neutrons or protons.

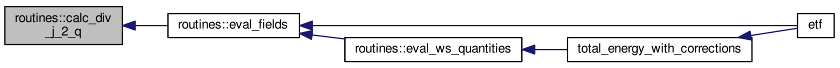
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*d1rhoq*	First derivative of neutron or proton density
in	*fq*	Effective mass for protons or neutrons
in	*d1fq*	First derivative of effective mass for neutrons or protons
in	*d1Aq*	First derivative of "composite" neutron or proton density A_q
in	*d2Aq*	Second derivative of "composite" neutron or proton density A_q
in	*q*	Isospin
in,out	*divJ2q*	Array for second-order contributions

Here is the caller graph for this function:



5.3.2.3 calc_div_j_4_q()

```
subroutine routines::calc_div_j_4_q (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) d1rhoq,
            real(kind=dp), dimension(1:n), intent(in) d2rhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) d1fq,
            real(kind=dp), dimension(1:n), intent(in) d2fq,
            real(kind=dp), dimension(1:n), intent(in) d3fq,
            real(kind=dp), dimension(1:n), intent(in) d1Aq,
            real(kind=dp), dimension(1:n), intent(in) d2Aq,
            real(kind=dp), dimension(1:n), intent(in) d3Aq,
            real(kind=dp), dimension(1:n), intent(in) d4Aq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) divJ4q )
```

Subroutine to calculate the fourth-order contributions to the divergence of the current density $\mathbf{J}_q$ for neutrons or protons.

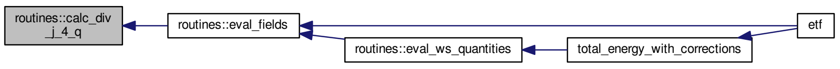
Author

M. Shelley

Parameters

`in`	*rhoq*	Neutron or proton density
`in`	*d1rhoq*	First derivative of neutron or proton density
`in`	*d2rhoq*	Second derivative of neutron or proton density
`in`	*fq*	Effective mass for protons or neutrons
`in`	*d1fq*	First derivative of effective mass for neutrons or protons
`in`	*d2fq*	Second derivative of effective mass for neutrons or protons
`in`	*d3fq*	Third derivative of effective mass for neutrons or protons
`in`	*d1Aq*	First derivative of "composite" neutron or proton density A_q
`in`	*d2Aq*	Second derivative of "composite" neutron or proton density A_q
`in`	*d3Aq*	Third derivative of "composite" neutron or proton density A_q
`in`	*d4Aq*	Fourth derivative of "composite" neutron or proton density A_q
`in`	*q*	Isospin
`in,out`	*divJ4q*	Array for fourth-order contributions

Here is the caller graph for this function:



5.3.2.4 calc_e_f_q()

```
real(kind=dp) function routines::calc_e_f_q (
              real(kind=dp), intent(in) rhoq,
              real(kind=dp), intent(in) fq,
              integer, intent(in) q )
```

Subroutine to evaluate the Fermi energy at a given density and effective mass, for neutrons or protons.

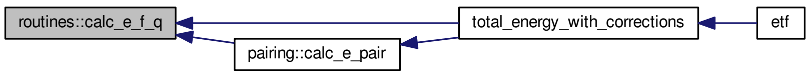
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*fn*	Neutron or proton effective mass

Here is the caller graph for this function:



5.3.2.5 calc_f_q()

```
subroutine routines::calc_f_q (
            real(kind=dp), dimension(:), intent(in) rhot,
            real(kind=dp), dimension(:), intent(in) rhoq,
            integer, intent(in) q,
            real(kind=dp), dimension(:), intent(inout) fq )
```

Subroutine to calculate the effective mass ratio $f_q = \frac{m}{m_q^*}$ for neutrons or protons, for standard Skyrme or for BSk forces.

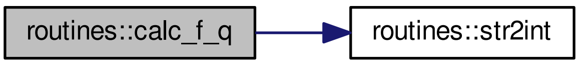
Author

M. Shelley

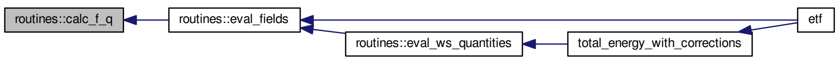
Parameters

in	*rhot*	Total density
in	*rhoq*	Neutron or proton density
in	*q*	Isospin
in,out	*fq*	Neutron or proton effective mass

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.6 calc_j_2_q()

```
subroutine routines::calc_j_2_q (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) Wq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) J2q )
```

Subroutine to calculate the second-order contributions to the spin current density $\mathbf{J}_q$ for neutrons or protons.

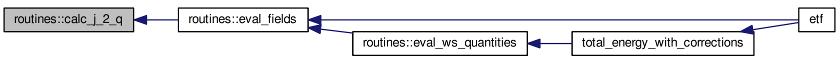
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*Wq*	Spin-orbit field
in	*fq*	Effective mass for neutrons or protons
in	*q*	Isospin [in,out] J2q Array for second-order contributions

Here is the caller graph for this function:



5.3.2.7 calc_j_4_q()

```
subroutine routines::calc_j_4_q (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) d1rhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) d1fq,
            real(kind=dp), dimension(1:n), intent(in) d2fq,
            real(kind=dp), dimension(1:n), intent(in) d1Aq,
            real(kind=dp), dimension(1:n), intent(in) d2Aq,
            real(kind=dp), dimension(1:n), intent(in) d3Aq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) J4q )
```

Subroutine to calculate the fourth-order contributions to the spin current density $\mathbf{J}_q$ for neutrons or protons.

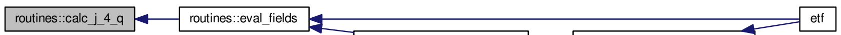
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*d1rhoq*	First derivative of neutron or proton density
in	*fq*	Effective mass for protons or neutrons
in	*d1fq*	First derivative of effective mass for neutrons or protons
in	*d2fq*	Second derivative of effective mass for neutrons or protons
in	*d1Aq*	First derivative of "composite" neutron or proton density A_q
in	*d2Aq*	Second derivative of "composite" neutron or proton density A_q
in	*d3Aq*	Third derivative of "composite" neutron or proton density A_q
in	*q*	Isospin
in,out	*J4q*	Array for fourth-order contributions

Here is the caller graph for this function:



5.3.2.8 calc_particle_number()

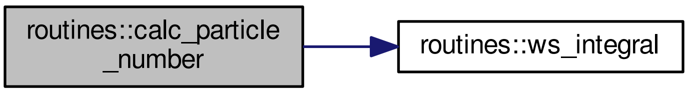
```
subroutine routines::calc_particle_number ( )
```

Subroutine to calculate the number of particles in the Wigner-Seitz cell.

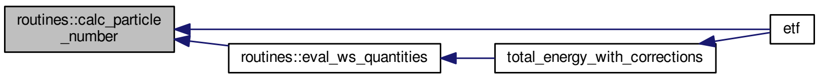
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:


routines::calc_particle_number
routines::eval_ws_quantities
total_energy_with_corrections
etf

5.3.2.9 calc_rho_q()

```
real(kind=dp) function routines::calc_rho_q (
            real(kind=dp), intent(in) rhoqgas,
            real(kind=dp), intent(in) rhoqliq,
            real(kind=dp), intent(in) rq,
            real(kind=dp), intent(in) aq,
            real(kind=dp), intent(in) gammaq,
            real(kind=dp), intent(in) r )
```

Function to calculate the neutron or proton density at a given radius r, using supplied input parameters.

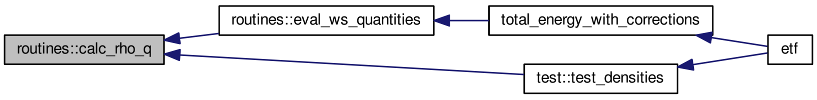
Author

M. Shelley

Parameters

in	*rhoqgas*	Asymptotic density in gas far from surface
in	*rhoqliq*	Asymptotic density in cluster far from surface
in	*rq*	Cluster radius
in	*aq*	Surface diffuseness
in	*gammaq*	Parameter allowing for "asymmetric surface"
in	*r*	Radius

Here is the caller graph for this function:



5.3.2.10 calc_tau_2_l()

```
subroutine routines::calc_tau_2_l (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) delrhoq,
            real(kind=dp), dimension(1:n), intent(in) del2rhoq,
            real(kind=dp), dimension(1:n), intent(inout) tau2Lq,
            real(kind=dp), dimension(1:n), intent(inout) t2contq )
```

Function to calculate the local second-order contribution to the kinetic energy density for neutrons or protons.

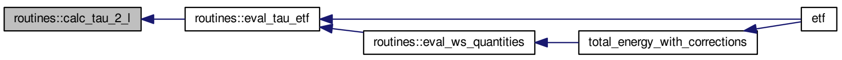
Author

M. Shelley

Parameters

`in`	*rhoq*	Neutron or proton density
`in`	*delrhoq*	Gradient of proton or neutron density
`in`	*del2rhoq*	Laplacian of proton or neutron density
`in,out`	*tau2Lq*	Array for local second-order contributions
`in,out`	*t2contq*	Array for individual second-order contributions

Here is the caller graph for this function:



5.3.2.11 calc_tau_2_nl()

```
subroutine routines::calc_tau_2_nl (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) delrhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) delfq,
            real(kind=dp), dimension(1:n), intent(in) del2fq,
            real(kind=dp), dimension(1:n), intent(in) Wq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) tau2NLq,
            real(kind=dp), dimension(1:n,2:4), intent(inout) t2contq )
```

Subroutine to calculate the non-local second-order contribution to the kinetic energy density for neutrons or protons.

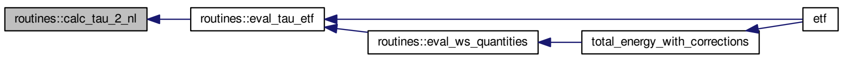
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*delrhoq*	Gradient of neutron or proton density
in	*fq*	Effective mass for neutrons or protons
in	*delfq*	Gradient of effective mass for neutrons or protons
in	*del2fq*	Laplacian of effective mass for neutrons or protons
in	*Wq*	Spin-orbit field
in	*q*	Isospin
in,out	*tau2NLq*	Array for non-local second-order contributions
in,out	*t2contq*	Array for individual second-order contributions

Here is the caller graph for this function:



5.3.2.12 calc_tau_4_no_spin()

```
subroutine routines::calc_tau_4_no_spin (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) d1rhoq,
            real(kind=dp), dimension(1:n), intent(in) d2rhoq,
            real(kind=dp), dimension(1:n), intent(in) d3rhoq,
            real(kind=dp), dimension(1:n), intent(in) d4rhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) d1fq,
            real(kind=dp), dimension(1:n), intent(in) d2fq,
            real(kind=dp), dimension(1:n), intent(in) d3fq,
            real(kind=dp), dimension(1:n), intent(in) d4fq,
            real(kind=dp), dimension(1:n), intent(inout) tau4nospinq,
            real(kind=dp), dimension(1:n,1:3), intent(inout) t4contq )
```

Subroutine to calculate the fourth-order contributions to the kinetic energy density (without spin-orbit contributions) **tau**$_q$ for neutrons or protons.

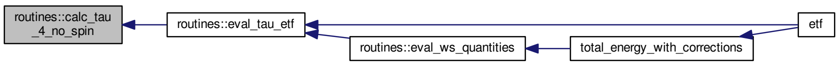
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*d1rhoq*	First derivative of neutron or proton density
in	*d2rhoq*	Second derivative of neutron or proton density
in	*d3rhoq*	Third derivative of neutron or proton density
in	*d4rhoq*	Fourth derivative of neutron or proton density
in	*fq*	Effective mass for neutrons or protons
in	*d1fq*	First derivative of effective mass for neutrons or protons
in	*d2fq*	Second derivative of effective mass for neutrons or protons
in	*d3fq*	Third derivative of effective mass for neutrons or protons
in	*d4fq*	Fourth derivative of effective mass for neutrons or protons
in,out	*tau4nospinq*	Array for fourth-order contributions (no spin-orbit)
in,out	*t4contq*	Array for individual fourth-order contributions

Here is the caller graph for this function:


routines::calc_tau_4_no_spin
routines::eval_tau_etf
etf
routines::eval_ws_quantities
total_energy_with_corrections

5.3.2.13 calc_tau_4_so()

```
subroutine routines::calc_tau_4_so (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(in) d1rhoq,
            real(kind=dp), dimension(1:n), intent(in) fq,
            real(kind=dp), dimension(1:n), intent(in) d1fq,
            real(kind=dp), dimension(1:n), intent(in) d2fq,
            real(kind=dp), dimension(1:n), intent(in) d1Aq,
            real(kind=dp), dimension(1:n), intent(in) d2Aq,
            real(kind=dp), dimension(1:n), intent(in) d3Aq,
            integer, intent(in) q,
            real(kind=dp), dimension(1:n), intent(inout) tau_4_so_q,
            real(kind=dp), dimension(1:n), intent(inout) t4contq )
```

Subroutine to calculate the fourth-order contributions to the kinetic energy density (spin-orbit contributions) **tau**$_q$ for neutrons or protons.

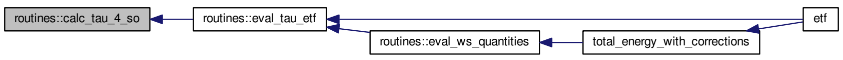
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in	*d1rhoq*	First derivative of neutron or proton density
in	*fq*	Effective mass for protons or neutrons
in	*d1fq*	First derivative of effective mass for neutrons or protons
in	*d2fq*	Second derivative of effective mass for neutrons or protons
in	*d1Aq*	First derivative of "composite" neutron or proton density A_q
in	*d2Aq*	Second derivative of "composite" neutron or proton density A_q
in	*d3Aq*	Third derivative of "composite" neutron or proton density A_q
in	*q*	Isospin
in,out	*tau_4_so↩ _q*	Array for fourth-order contributions (spin- orbit)
in,out	*t4contq*	Array for individual fourth-order contributions

Here is the caller graph for this function:



5.3.2.14 calc_tau_tf()

```
subroutine routines::calc_tau_tf (
            real(kind=dp), dimension(1:n), intent(in) rhoq,
            real(kind=dp), dimension(1:n), intent(inout) tauTF )
```

Function to calculate the zeroth-order contribution to the kinetic energy density for neutrons or protons.

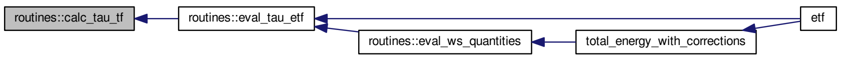
Author

M. Shelley

Parameters

in	*rhoq*	Neutron or proton density
in,out	*tauTF*	Array for zeroth-order contributions

Here is the caller graph for this function:



5.3.2.15 calc_u_q()

```
real(kind=dp) function routines::calc_u_q (
            real(kind=dp), intent(in) rhot,
            real(kind=dp), intent(in) rhon,
            real(kind=dp), intent(in) rhop,
            real(kind=dp), intent(in) delrhot,
            real(kind=dp), intent(in) delrhon,
            real(kind=dp), intent(in) delrhop,
            real(kind=dp), intent(in) del2rhot,
            real(kind=dp), intent(in) del2rhon,
            real(kind=dp), intent(in) del2rhop,
            real(kind=dp), intent(in) taut,
            real(kind=dp), intent(in) taun,
            real(kind=dp), intent(in) taup,
            real(kind=dp), intent(in) divJt,
            real(kind=dp), intent(in) divJq,
            integer, intent(in) q )
```

Function to calculate the central potential U_q for neutrons or protons, for standard Skyrme or for BSk forces with extra terms.

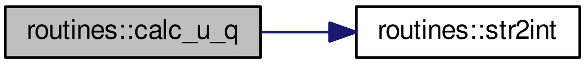
Author

M. Shelley

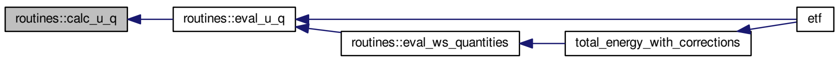
Parameters

in	*rhot*	Total density
in	*rhon*	Neutron density
in	*rhop*	Proton density
in	*delrhot*	First derivative of total density
in	*delrhon*	First derivative of neutron density
in	*delrhop*	First derivative of proton density
in	*del2rhot*	Laplacian of total density
in	*del2rhon*	Laplacian of neutron density
in	*del2rhop*	Laplacian of proton density
in	*taut*	Total kinetic density
in	*taun*	Neutron kinetic density
in	*taup*	Proton kinetic density
in	*divJt*	Divergence of total spin current density
in	*divJq*	Divergence of proton or neutron spin current density
in	*q*	Isospin

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.16 calc_w_q()

```
subroutine routines::calc_w_q (
            real(kind=dp), dimension(1:n), intent(in) delrho,
            real(kind=dp), dimension(1:n), intent(in) delrhoq,
            real(kind=dp), dimension(1:n), intent(inout) Wq )
```

Function to calculate the spin-orbit field $\mathbf{W}_q$ for neutrons or protons.

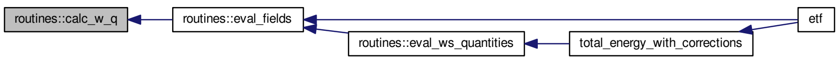
Author

M. Shelley

Parameters

`in`	*delrho*	Gradient of total density
`in`	*delrhoq*	Gradient of neutron or proton density
`in,out`	*Wq*	Array for spin-orbit field

Here is the caller graph for this function:



5.3.2.17 charge()

```
subroutine routines::charge (
            real(kind=dp), dimension(ngrid1,0:1), intent(in) rho,
            real(kind=dp), intent(in) Neutr,
            real(kind=dp), intent(in) Nprot,
            integer, intent(in) Ngrid1,
            real(kind=dp), intent(in) del1,
            real(kind=dp), dimension(ngrid1), intent(inout) rhoch )
```

Subroutine to calculate the charge density from the matter densities. Modified by M. Shelley.

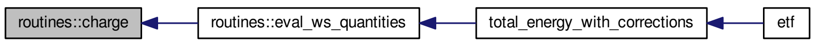
Author

A. Pastore, M. Shelley

Parameters

`in`	*rho*	Neutron and proton densities
`in`	*Neutr*	Number of neutrons
`in`	*Nprot*	Number of protons
`in`	*Ngrid1*	Number of mesh points
`in`	*del1*	Step size
`in,out`	*rhoch*	Array for charge density

Here is the caller graph for this function:



5.3.2.18 d1()

```
subroutine routines::d1 (
            integer, intent(in) n,
            real(kind=dp), intent(in) h,
            real(kind=dp), dimension(-1:n), intent(in) f,
            real(kind=dp), dimension(1:n), intent(inout) df )
```

This subroutine computes the first derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.

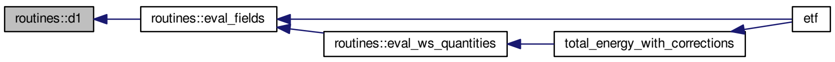
Author

A. Pastore, M. Shelley

Parameters

in	*n*	Number of meshpoints
in	*f*	Input function (1:n) with extrapolated values in -1,0
in	*h*	Step size
in,out	*df*	Array for first derivatives

Here is the caller graph for this function:



5.3.2.19 d2()

```
subroutine routines::d2 (
             integer, intent(in) n,
             real(kind=dp), intent(in) h,
             real(kind=dp), dimension(-1:n), intent(in) f,
             real(kind=dp), dimension(1:n), intent(inout) d2f )
```

This subroutine computes the second derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.

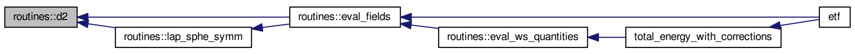
Author

A. Pastore, M. Shelley

Parameters

in	*n*	Number of meshpoints
in	*f*	Input function (1:n) with extrapolated values in -1,0
in	*h*	Step size
in,out	*d2f*	Array for second derivatives

Here is the caller graph for this function:



5.3.2.20 d3()

```
subroutine routines::d3 (
            real(kind=dp), dimension(-2:n), intent(in) f,
            real(kind=dp), dimension(1:n), intent(inout) d3f_dr3 )
```

Subroutine to calculate third derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.

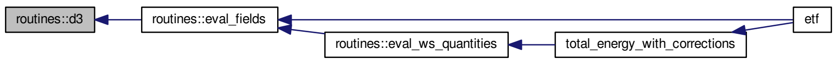
Author

M. Shelley

Parameters

in	*f*	Input function (1:n) with extrapolated values in -2,-1,0
in,out	*d3f_dr3*	Array for third derivative

Here is the caller graph for this function:



5.3.2.21 d4()

```
subroutine routines::d4 (
            real(kind=dp), dimension(-2:n), intent(in) f,
            real(kind=dp), dimension(1:n), intent(inout) d4f_dr4 )
```

Subroutine to calculate fourth derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.

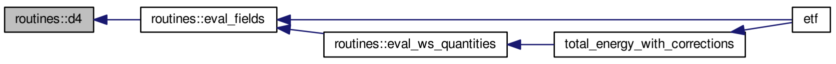
Author

M. Shelley

Parameters

in	*f*	Input function (1:n) with extrapolated values in -2,-1,0
in,out	*d4f_dr4*	Array for fourth derivative

Here is the caller graph for this function:



5.3.2.22 deallocate_arrays()

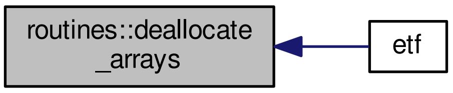
`subroutine routines::deallocate_arrays ( )`

Subroutine to deallocate arrays for all densities and effective masses, and for their derivatives.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.23 deallocate_mesh()

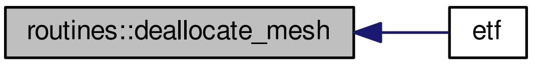
`subroutine routines::deallocate_mesh ( )`

Subroutine to deallocate array for r.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.24 eval_coulomb()

```
subroutine routines::eval_coulomb (
             real(kind=dp), dimension(1:n), intent(in) prot_dens,
             logical, intent(in) calc_exchange )
```

Subroutine to evaluate the Coulomb potentials and energy densities, using either the proton or charge density.

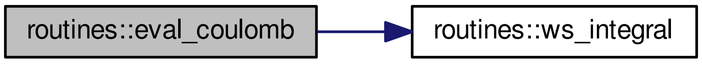
Author

M. Shelley

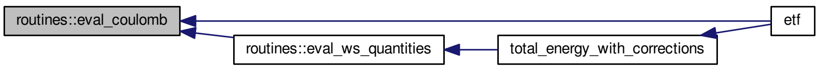
Parameters

in	*prot_dens*	Density to use (proton or charge)
in	*calc_exchange*	Whether to calculate exchange potential

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.25 eval_electrons()

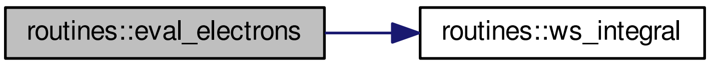
```
subroutine routines::eval_electrons ( )
```

Subroutine to evaluate the proton-electron potential which contributes to U_q, all energy contributions, and the pressure, coming from a homogeneous electron gas. Also calculates the electron chemical potential.

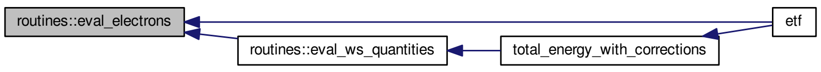
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.26 eval_fields()

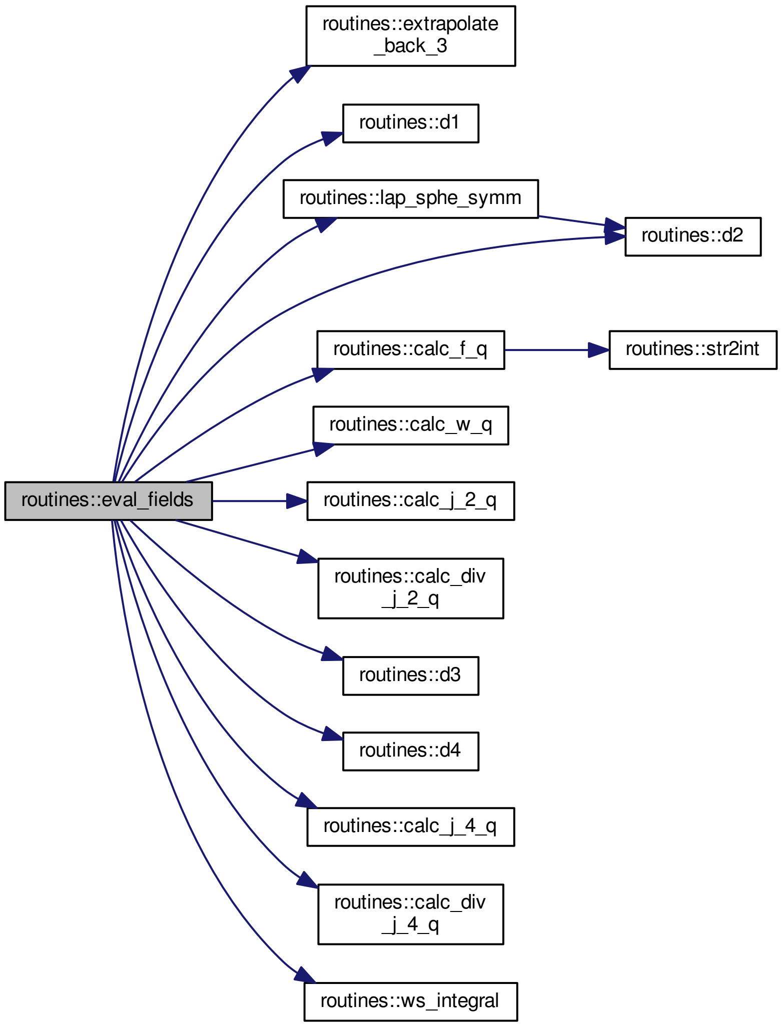
```
subroutine routines::eval_fields ( )
```

Subroutine to evaluate matter density derivatives, and all fields: effective masses (and derivatives), spin-orbit fields, spin current densities (and derivatives)

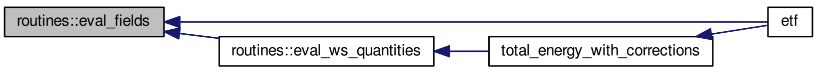
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.27 eval_skyrme_energy_density()

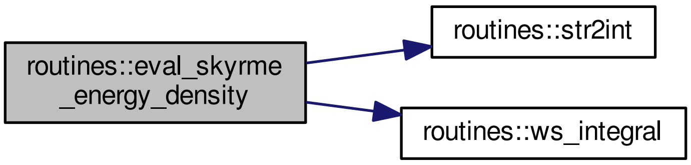
```
subroutine routines::eval_skyrme_energy_density ( )
```

Subroutine to evaluate the Skyrme energy density, after first separately evaluating the field energy density.

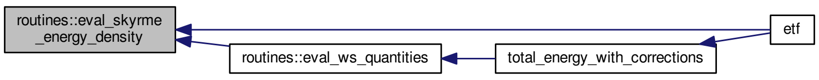
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:


routines::eval_skyrme _energy_density
etf
routines::eval_ws_quantities
total_energy_with_corrections

5.3.2.28 eval_tau_etf()

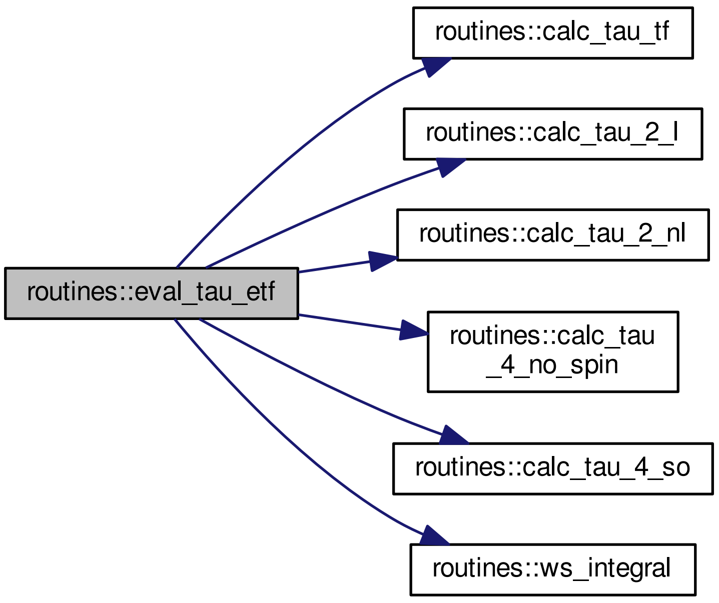
```
subroutine routines::eval_tau_etf ( )
```

Subroutine to calculate the kinetic energy density τ_{ETF} with the (extended) Thomas-Fermi approximation at order specified by "etf_order".

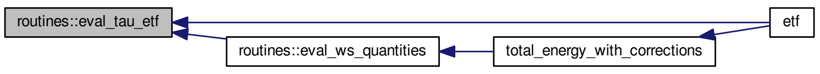
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.29 eval_u_q()

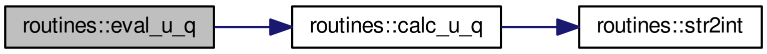
```
subroutine routines::eval_u_q ( )
```

Subroutine to evaluate the central fields U_q.

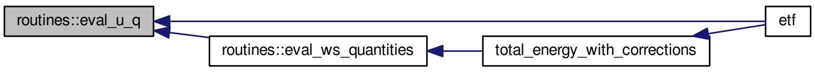
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.30 eval_ws_quantities()

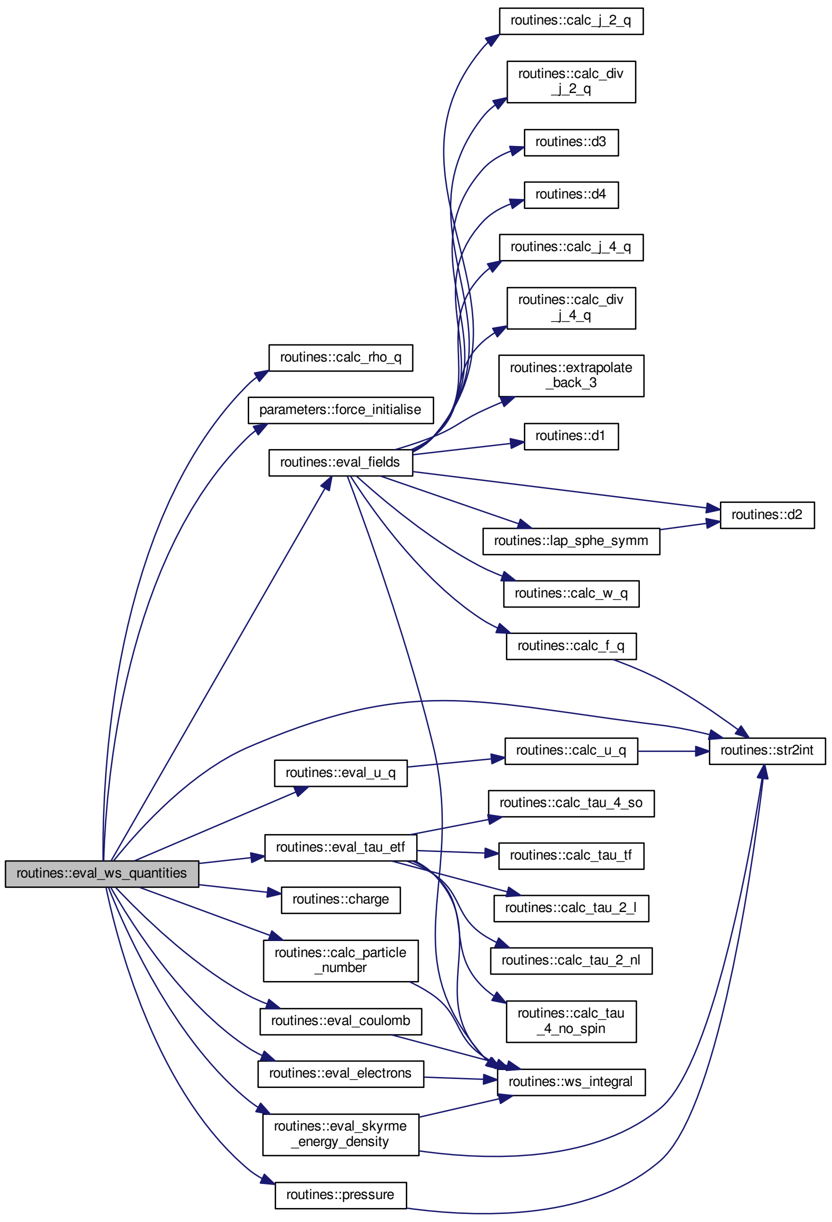
```
subroutine routines::eval_ws_quantities ( )
```

Subroutine to evaluate the various densities, fields, derivatives, energies, and particle numbers in the WS cell with densities rho_q.

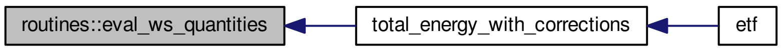
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.31 extrapolate_back_3()

```
subroutine routines::extrapolate_back_3 (
            real(kind=dp), dimension(:), intent(inout) grid )
```

Subroutine to extrapolate back 3 points on the r mesh, to faciliate the calculation of first and second derivatives using a 5-point stencil. Values in grid start at 4, extrapolated values are put in elements 3,2,1. Coefficients come from solving 4th-order polynomial, assuming that f'(0) = 0, and f(-h) = f(h).

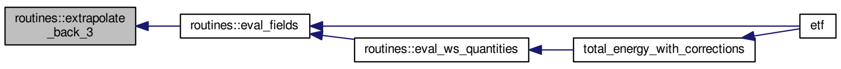
Author

M. Shelley

Parameters

`in,out`	*grid*	Array of quantity evaluated on r mesh, with 3 elements before r = dr

Here is the caller graph for this function:


routines::extrapolate_back_3
routines::eval_fields
routines::eval_ws_quantities
total_energy_with_corrections
etf

5.3.2.32 initialise_uniform_mesh()

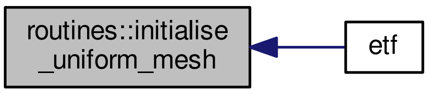
```
subroutine routines::initialise_uniform_mesh ( )
```

Subroutine to calculate number of mesh points for a uniform grid, allocate array for r, and then populate r with the mesh points.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.33 lap_sphe_symm()

```
subroutine routines::lap_sphe_symm (
            real(kind=dp), dimension(-2:n), intent(in) f,
            real(kind=dp), dimension(1:n), intent(in) df_dr,
            real(kind=dp), dimension(1:n), intent(inout) d2f_dr2 )
```

Subroutine to carry out Laplacian in spherical symmetry.

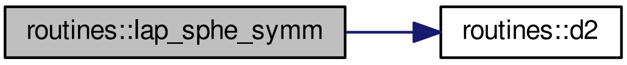
Author

M. Shelley

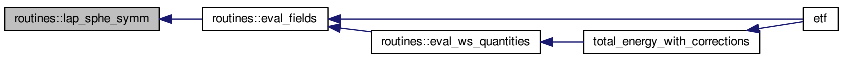
Parameters

`in`	*f*	Input function (1:n) with extrapolated values in -2,-1,0
`in`	*df_dr*	First derivative array
`in,out`	*d2f_dr2*	Array for Laplacian

Here is the call graph for this function:



Here is the caller graph for this function:



5.3.2.34 pressure()

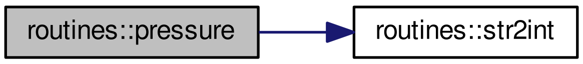
```
subroutine routines::pressure ( )
```

Subroutine to calculate the nuclear contribution to the pressure, and then the total pressure.

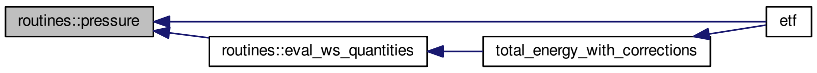
Author

M. Shelley

Here is the call graph for this function:



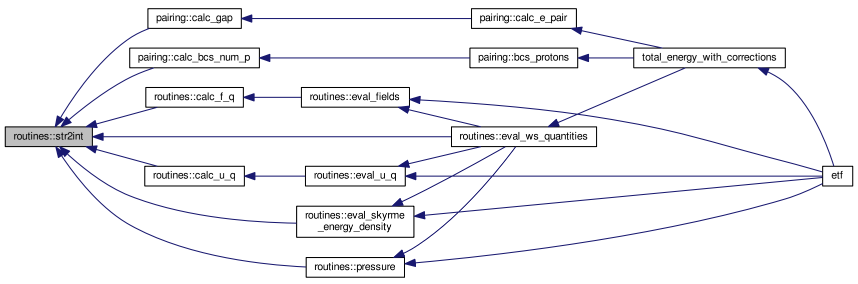
Here is the caller graph for this function:



5.3.2.35 str2int()

```
integer function routines::str2int (
            character(len=*), intent(in) string )
```

Here is the caller graph for this function:



5.3.2.36 write_densities()

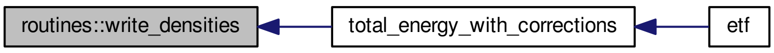
```
subroutine routines::write_densities ( )
```

Subroutine to write neutron and proton densities to files.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.37 write_fields()

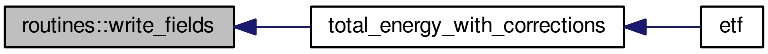
```
subroutine routines::write_fields ( )
```

Subroutine to write neutron and proton fields to files.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.38 write_sp_states_p()

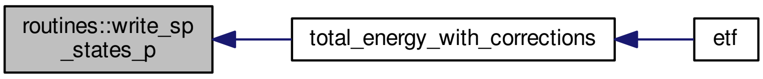
```
subroutine routines::write_sp_states_p ( )
```

Subroutine to write proton single particle energies to file, and extra details if BCS has been performed.

Author

M. Shelley

Here is the caller graph for this function:



5.3.2.39 ws_integral()

```
real(kind=dp) function routines::ws_integral (
            real(kind=dp), dimension(:), intent(in) quantity,
            integer, intent(in) n_max )
```

Function to integrate a density or field over the whole W-S cell, using Simpson's rule (+ Simpson's 3/8 rule if odd number of points)

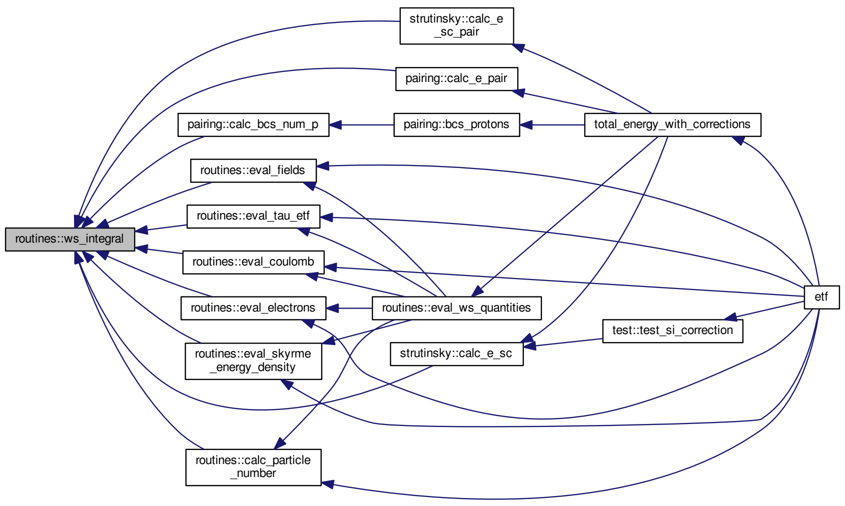
Author

M. Shelley

Parameters

in	*quantity*	Array of quantity, evaluated on r mesh, to be integrated
in	*n_max*	Maximum mesh point in array for integration

Here is the caller graph for this function:



5.3.3 Variable Documentation

5.3.3.1 file_unit_0

```
integer routines::file_unit_0
```

5.3.3.2 file_unit_1

```
integer routines::file_unit_1
```

Unit numbers for opening files.

5.4 rspace Module Reference

Module to hold routines for calculating single particle energies. Written by A. Pastore, some variables and use statements modified by M. Shelley for integration into etf code.

Functions/Subroutines

- subroutine boundary (h, Lmax, Ecut, Nmaxt, PS, NNST, JJP, LP, EP, isospin)
- subroutine numerov (h, Nrmax, Emax0, N, L, J, EFINAL, U, V, VSO, HME, GI, GIprimo, no)

5.4.1 Detailed Description

Module to hold routines for calculating single particle energies. Written by A. Pastore, some variables and use statements modified by M. Shelley for integration into etf code.

Author

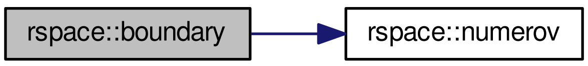
A. Pastore, M. Shelley

5.4.2 Function/Subroutine Documentation

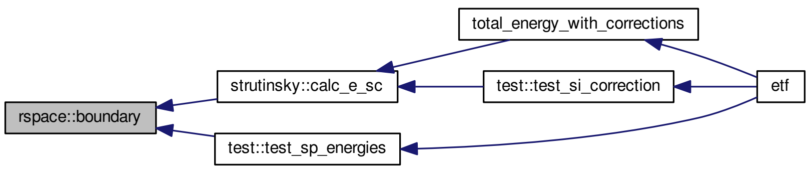
5.4.2.1 boundary()

```
subroutine rspace::boundary (
             double precision h,
             integer Lmax,
             double precision Ecut,
             integer Nmaxt,
             double precision, dimension(nmaxstate,nmaxt) PS,
             integer NNST,
             integer, dimension(nmaxstate) JJP,
             integer, dimension(nmaxstate) LP,
             double precision, dimension(nmaxstate) EP,
             integer isospin )
```

Here is the call graph for this function:



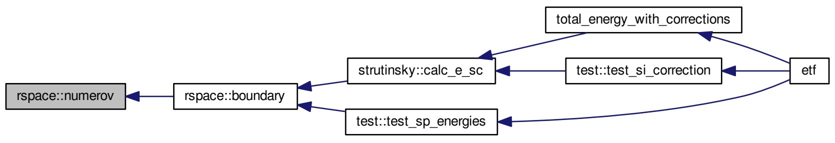
Here is the caller graph for this function:



5.4.2.2 numerov()

```
subroutine rspace::numerov (
            double precision h,
            integer Nrmax,
            double precision Emax0,
            integer N,
            integer L,
            integer J,
            double precision EFINAL,
            double precision, dimension(nrmax) U,
            double precision, dimension(nrmax) V,
            double precision, dimension(nrmax) VSO,
            double precision, dimension(nrmax) HME,
            double precision, dimension(nrmax) GI,
            double precision, dimension(nrmax) GIprimo,
            integer no )
```

Here is the caller graph for this function:



5.5 strutinsky Module Reference

Module to hold routines for carrying out Strutinsky correction.

Functions/Subroutines

- subroutine sp_states_setup ()

  Subroutine to allocate + initialise variables needed in 'boundary' routine, and allocate arrays needed for BCS.
- subroutine sp_states_deallocate ()

  Subroutine to deallocate arrays needed in 'boundary' routine, and deallocate arrays needed for BCS.
- subroutine state_sort (sp_J, sp_L, sp_E, sp_wfns)

  Subroutine to sort single particle states by their energies. Use bubble sort.
- subroutine calc_e_sc (q)

  Subroutine to calculate the Strutinsky shell correction energy for isospin q. First, sum over occupied states of s.p. energies. Second, integrate over W-S cell of smoothed ETF densities and fields.
- subroutine calc_e_sc_pair ()

  Subroutine to calculate the Strutinsky shell correction energy for protons, using BCS occupation probabilities.

5.5.1 Detailed Description

Module to hold routines for carrying out Strutinsky correction.

Author

M. Shelley

5.5.2 Function/Subroutine Documentation

5.5.2.1 calc_e_sc()

```
subroutine strutinsky::calc_e_sc (
            integer, intent(in) q )
```

Subroutine to calculate the Strutinsky shell correction energy for isospin q. First, sum over occupied states of s.p. energies. Second, integrate over W-S cell of smoothed ETF densities and fields.

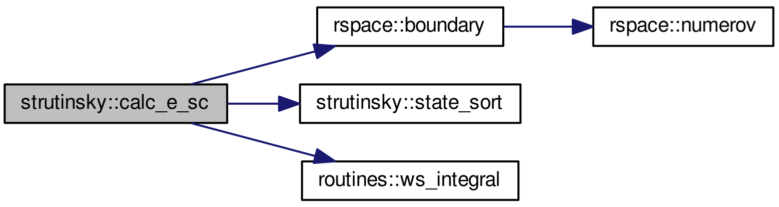
Author

M. Shelley

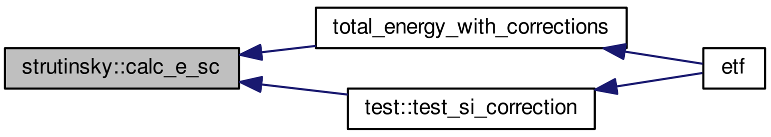
Parameters

in	*q*	Isospin
in	*q*	Isospin

Here is the call graph for this function:



Here is the caller graph for this function:



5.5.2.2 calc_e_sc_pair()

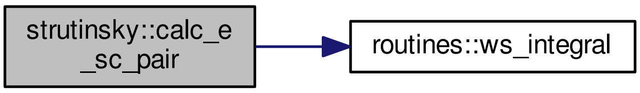
`subroutine strutinsky::calc_e_sc_pair ( )`

Subroutine to calculate the Strutinsky shell correction energy for protons, using BCS occupation probabilities.

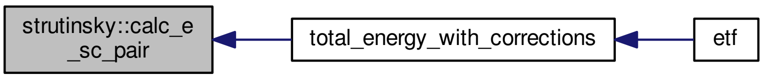
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.5.2.3 sp_states_deallocate()

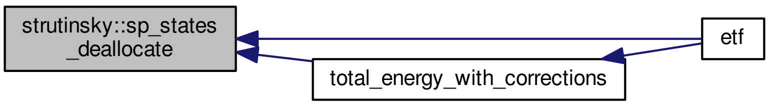
`subroutine strutinsky::sp_states_deallocate ( )`

Subroutine to deallocate arrays needed in 'boundary' routine, and deallocate arrays needed for BCS.

Author

M. Shelley

Here is the caller graph for this function:


strutinsky::sp_states_deallocate
etf
total_energy_with_corrections

5.5.2.4 sp_states_setup()

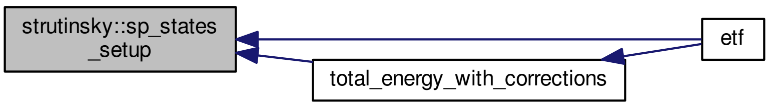
```
subroutine strutinsky::sp_states_setup ( )
```

Subroutine to allocate + initialise variables needed in 'boundary' routine, and allocate arrays needed for BCS.

Author

M. Shelley

Here is the caller graph for this function:



5.5.2.5 state_sort()

```
subroutine strutinsky::state_sort (
            integer, dimension(:), intent(inout) sp_J,
            integer, dimension(:), intent(inout) sp_L,
            real(kind=dp), dimension(:), intent(inout) sp_E,
            real(kind=dp), dimension(:,:), intent(inout) sp_wfns )
```

Subroutine to sort single particle states by their energies. Use bubble sort.

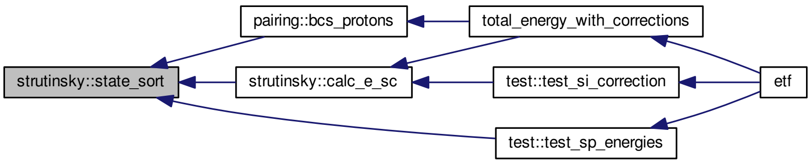
Author

M. Shelley

Parameters

in,out	*sp_J*	Array for (2)J's of single particle states
in,out	*sp_L*	Array for L's of single particle states
in,out	*sp_E*	Array for energies of single particle states
in,out	*sp_wfns*	Array for wavefunctions of single particle states

Here is the caller graph for this function:



5.6 test Module Reference

Module to hold test routines.

Functions/Subroutines

- subroutine read_test_params ()

  Subroutine to read from "test_input.in" parameters used for test routines.
- subroutine test_densities ()

  Subroutine to calculate the density profiles using sample parameters.
- subroutine test_density_derivs ()

  Subroutine to test some derivatives of the total and individual densities.
- subroutine test_eff_mass ()

  Subroutine to test effective masses fm^{-3}.
- subroutine test_kinetic_densities ()

  Subroutine to test kinetic energy densities.
- subroutine test_spin_current_densities ()

  Subroutine to write spin current densities and spin-orbit fields to file.
- subroutine orders_kinetic_densities ()

  Subroutine to write order-by-order comparison of kinetic densities to file.
- subroutine test_central_potentials ()

  Subroutine to write spin central potentials to file.
- subroutine write_ws_cell_array_quantity (quantity)

  Utility subroutine that can be called anywhere at any time, for writing a quantity (evaluated over WS cell) to file.
- subroutine test_calc_particle_number ()

  Subroutine to test calculation of neutron and proton particle numbers.
- subroutine test_calc_coulomb_energy ()

  Subroutine to test calculation of Coulomb energy.
- subroutine test_calc_skyrme_energy ()

  Subroutine to test calculation of Skyrme energy.
- subroutine test_sp_energies ()

  Subroutine to test calculation of single particle energies.
- subroutine test_si_correction ()

  Subroutine to test the Strutinsky integral correction.
- subroutine bartel_bencheikh_benchmark ()

  Subroutine to check different contributions to τ_{ETF} at 2nd order, for comparison with results in Bartel and Bencheikh (2002)

Variables

- integer file_unit
- integer file_unit_2

  Unit numbers for opening files.
- integer sample_profile

  Test density profile to use.

5.6.1 Detailed Description

Module to hold test routines.

Author

M. Shelley

5.6.2 Function/Subroutine Documentation

5.6.2.1 bartel_bencheikh_benchmark()

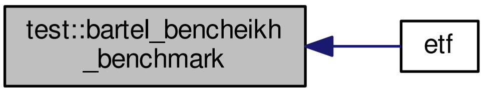
```
subroutine test::bartel_bencheikh_benchmark ( )
```

Subroutine to check different contributions to τ_{ETF} at 2nd order, for comparison with results in Bartel and Bencheikh (2002)

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.2 orders_kinetic_densities()

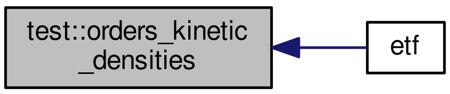
```
subroutine test::orders_kinetic_densities ( )
```

Subroutine to write order-by-order comparison of kinetic densities to file.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.3 read_test_params()

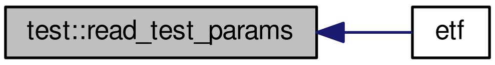
```
subroutine test::read_test_params ( )
```

Subroutine to read from "test_input.in" parameters used for test routines.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.4 test_calc_coulomb_energy()

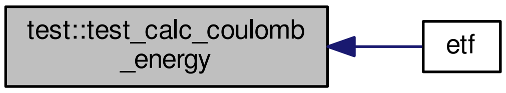
```
subroutine test::test_calc_coulomb_energy ( )
```

Subroutine to test calculation of Coulomb energy.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.5 test_calc_particle_number()

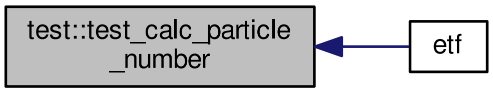
```
subroutine test::test_calc_particle_number ( )
```

Subroutine to test calculation of neutron and proton particle numbers.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.6 test_calc_skyrme_energy()

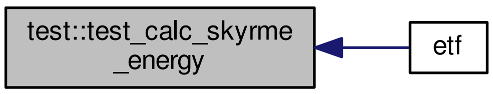
```
subroutine test::test_calc_skyrme_energy ( )
```

Subroutine to test calculation of Skyrme energy.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.7 test_central_potentials()

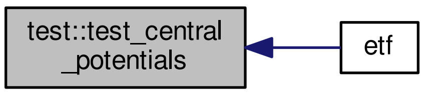
```
subroutine test::test_central_potentials ( )
```

Subroutine to write spin central potentials to file.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.8 test_densities()

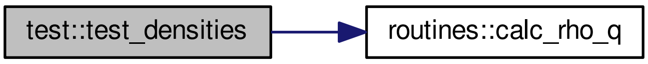
```
subroutine test::test_densities ( )
```

Subroutine to calculate the density profiles using sample parameters.

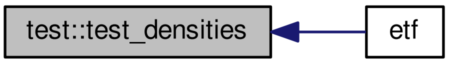
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.6.2.9 test_density_derivs()

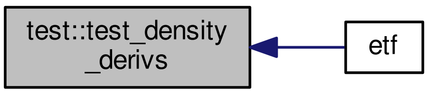
```
subroutine test::test_density_derivs ( )
```

Subroutine to test some derivatives of the total and individual densities.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.10 test_eff_mass()

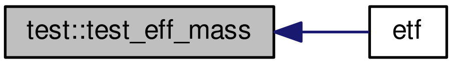
```
subroutine test::test_eff_mass ( )
```

Subroutine to test effective masses fm^{-3}.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.11 test_kinetic_densities()

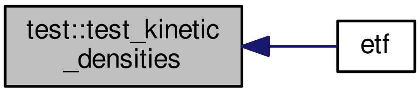
```
subroutine test::test_kinetic_densities ( )
```

Subroutine to test kinetic energy densities.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.12 test_si_correction()

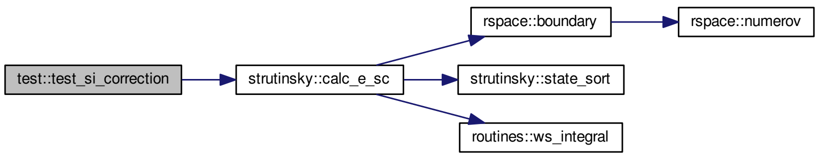
```
subroutine test::test_si_correction ( )
```

Subroutine to test the Strutinsky integral correction.

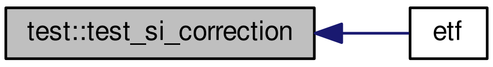
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.6.2.13 test_sp_energies()

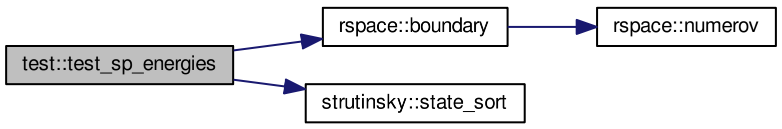
```
subroutine test::test_sp_energies ( )
```

Subroutine to test calculation of single particle energies.

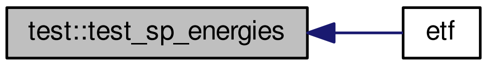
Author

M. Shelley

Here is the call graph for this function:



Here is the caller graph for this function:



5.6.2.14 test_spin_current_densities()

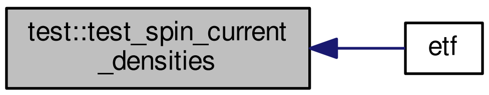
```
subroutine test::test_spin_current_densities ( )
```

Subroutine to write spin current densities and spin-orbit fields to file.

Author

M. Shelley

Here is the caller graph for this function:



5.6.2.15 write_ws_cell_array_quantity()

```
subroutine test::write_ws_cell_array_quantity (
            real(kind=dp), dimension(1:n), intent(in) quantity )
```

Utility subroutine that can be called anywhere at any time, for writing a quantity (evaluated over WS cell) to file.

Author

M. Shelley

Parameters

in	*quantity*	Array to be written to file (1:n)

5.6.3 Variable Documentation

5.6.3.1 file_unit

```
integer test::file_unit
```

5.6.3.2 file_unit_2

```
integer test::file_unit_2
```

Unit numbers for opening files.

5.6.3.3 sample_profile

```
integer test::sample_profile
```

Test density profile to use.

Chapter 6

File Documentation

6.1 srcs/boundary.f90 File Reference

Modules

- module rspace

  Module to hold routines for calculating single particle energies. Written by A. Pastore, some variables and use statements modified by M. Shelley for integration into etf code.

Functions/Subroutines

- subroutine rspace::boundary (h, Lmax, Ecut, Nmaxt, PS, NNST, JJP, LP, EP, isospin)
- subroutine rspace::numerov (h, Nrmax, Emax0, N, L, J, EFINAL, U, V, VSO, HME, GI, GIprimo, no)

6.2 srcs/etf.f90 File Reference

Functions/Subroutines

- program etf

  Program to calculate the equation of state in the inner crust with the extended Thomas-Fermi (ETF) approach.
- subroutine total_energy_with_corrections (write_files_print_info)

  Subroutine to evaluate all WS quantities using supplied profile parameters, and calculate total energy, with pairing and shell corrections included. Write densities and fields to files, and all info to screen, if specified.

6.2.1 Function/Subroutine Documentation

6.2.1.1 etf()

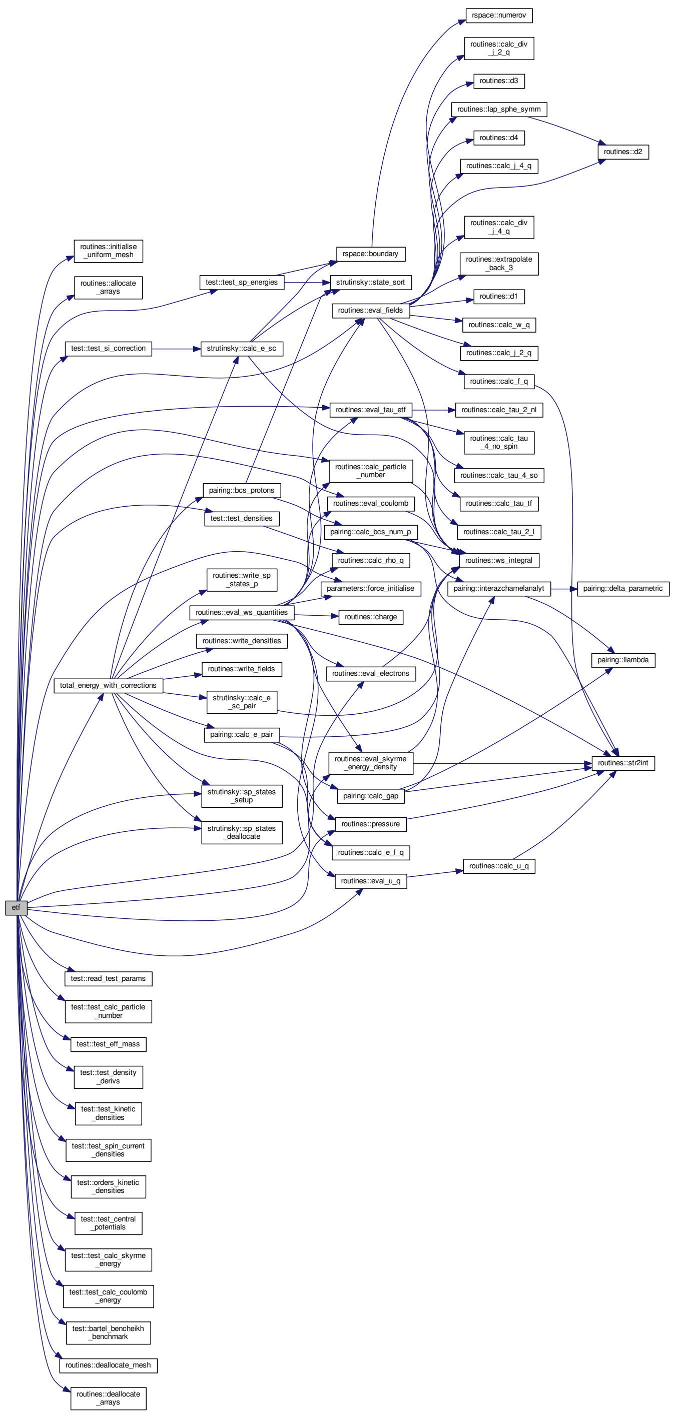
```
program etf ( )
```

Program to calculate the equation of state in the inner crust with the extended Thomas-Fermi (ETF) approach.

Author

M. Shelley

Here is the call graph for this function:



6.2.1.2 total_energy_with_corrections()

```
subroutine etf::total_energy_with_corrections (
            logical, intent(in) write_files_print_info )
```

Subroutine to evaluate all WS quantities using supplied profile parameters, and calculate total energy, with pairing and shell corrections included. Write densities and fields to files, and all info to screen, if specified.

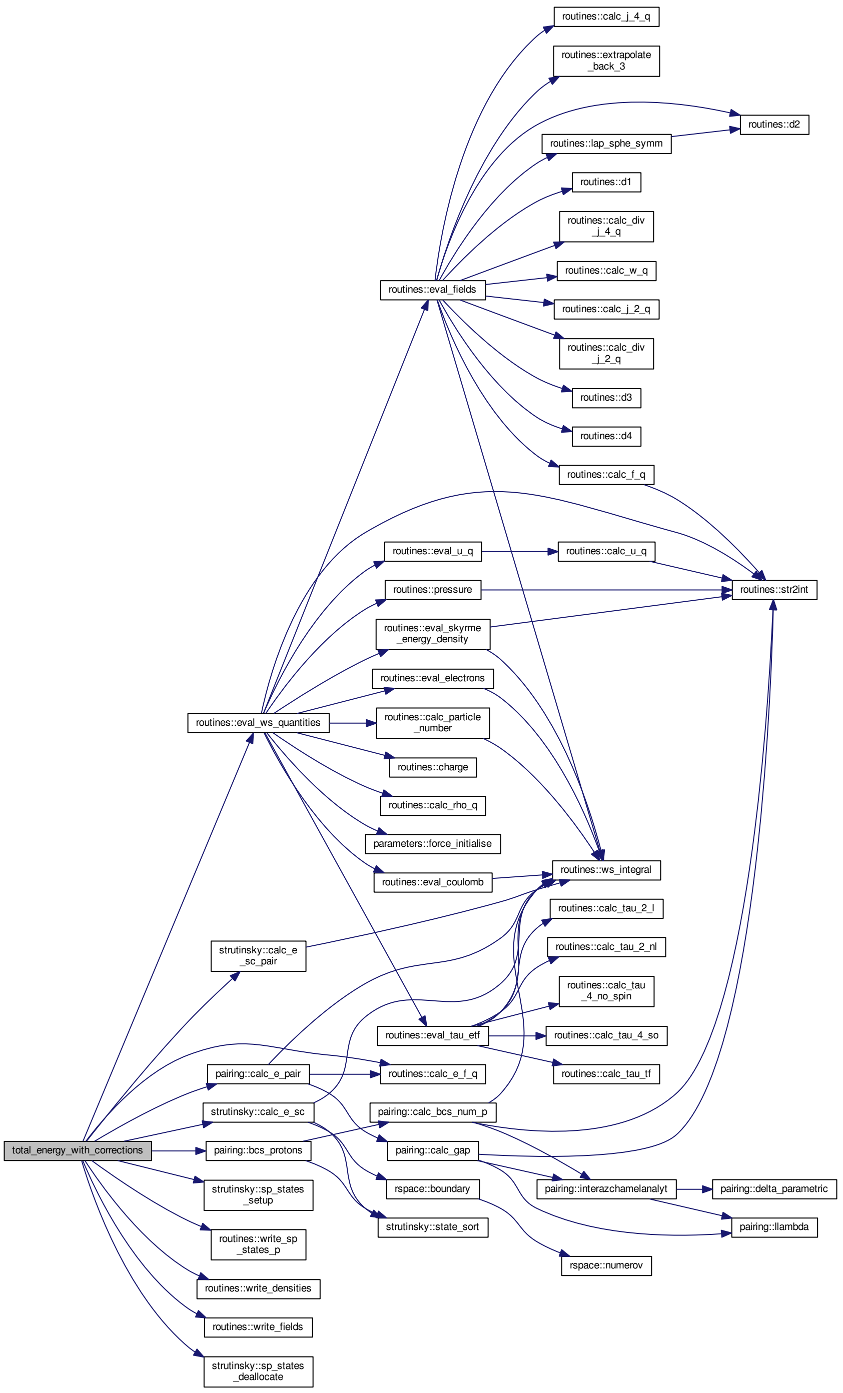
Author

M. Shelley

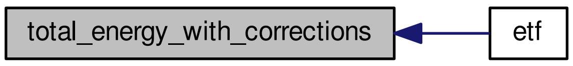
Parameters

in	*write_files_print_info*	Whether to write to files and screen

Here is the call graph for this function:



Here is the caller graph for this function:



6.3 srcs/pairing.f90 File Reference

Modules

- module pairing

  Module to hold routines for carrying out Strutinsky correction.

Functions/Subroutines

- subroutine pairing::calc_e_pair ()

  Subroutine to calculate the pairing energy for the WS cell, using the method specified in "input.in".
- real(kind=dp) function pairing::calc_gap (r, rhon, rhop, fq, mu)

  Function to calculate the pairing gap in infinite neutron matter, for specified density and effective mass.
- subroutine pairing::bcs_protons ()

  Subroutine to perform BCS for protons.
- real(kind=dp) function pairing::calc_bcs_num_p (mu_p)

  Function to solve gap equation at given chemical potential "mu_p", returning the (BCS) number of protons.
- real(kind=dp) function pairing::interazchamelanalyt (rhon, rhop, hbm, itz)

  Function to calculate the interaction strength for the effective contact pairing force. Modified by M. Shelley.
- real(kind=dp) function pairing::llambda (x)

  Function to calculate the pairing cutoff for the effective contact pairing force.
- real(kind=dp) function pairing::delta_parametric (kf, YY, itz, xk0)

  Function to calculate the pairing gap using the analytical BSk expression. Modified by M. Shelley.

6.4 srcs/parameters.f90 File Reference

Modules

- module parameters

  Module to hold global parameters and variables.

Functions/Subroutines

- subroutine parameters::force_initialise ()

  Subroutine to initialise Skyrme force parameters with values for a given force specified in 'input.dat'.

Variables

- integer, parameter parameters::dp = selected_real_kind(15, 300)

  Precision.
- real(kind=dp), parameter parameters::pi = 3.1415926535897932_dp

  π
- real(kind=dp), parameter parameters::hbar2_2m = 20.73553_dp

  $\frac{\hbar^2}{2m}$ *for SLy forces*
- real(kind=dp), parameter parameters::rho0 = 0.16_dp

  ρ_0*, nuclear saturation density* $[fm^{-3}]$
- real(kind=dp), parameter parameters::e2 = 1.439978408596513_dp

  e^2*, electric charge squared* $[MeV \cdot fm]$
- real(kind=dp), parameter parameters::mec2 = 0.51099895_dp

  Electron rest mass $[MeV/c^2]$.
- real(kind=dp), parameter parameters::mnc2 = 939.56542052_dp
- real(kind=dp), parameter parameters::mpc2 = 938.27208816_dp
- real(kind=dp), parameter parameters::hbarc = 197.3269804_dp

  $\hbar * c$
- real(kind=dp), parameter parameters::mamuc2 = 931.49386_dp

  Atomic mass unit u.
- real(kind=dp), parameter parameters::xmh = 7.28896940_dp
- real(kind=dp), parameter parameters::rydb = 13.6056981e-6_dp

  Rydberg constant.
- real(kind=dp), parameter parameters::xmp = xmh - mec2 + rydb
- real(kind=dp), parameter parameters::xmn = 8.07132281_dp
- real(kind=dp), parameter parameters::fr12 = 1._dp/2
- real(kind=dp), parameter parameters::fr14 = 1._dp/4
- real(kind=dp), parameter parameters::fr18 = 1._dp/8
- real(kind=dp), parameter parameters::fr1_16 = 1._dp/16
- real(kind=dp), parameter parameters::fr1_32 = 1._dp/32
- real(kind=dp), parameter parameters::fr13 = 1._dp/3
- real(kind=dp), parameter parameters::fr16 = 1._dp/6
- real(kind=dp), parameter parameters::fr1_12 = 1._dp/12
- real(kind=dp), parameter parameters::fr1_24 = 1._dp/24
- real(kind=dp), parameter parameters::fr1_36 = 1._dp/36
- real(kind=dp), parameter parameters::fr23 = 2._dp/3
- real(kind=dp), parameter parameters::fr29 = 2._dp/9
- real(kind=dp), parameter parameters::fr32 = 3._dp/2
- real(kind=dp), parameter parameters::fr34 = 3._dp/4
- real(kind=dp), parameter parameters::fr35 = 3._dp/5
- real(kind=dp), parameter parameters::fr38 = 3._dp/8
- real(kind=dp), parameter parameters::fr3_10 = 3._dp/10
- real(kind=dp), parameter parameters::fr43 = 4._dp/3
- real(kind=dp), parameter parameters::fr53 = 5._dp/3
- real(kind=dp), parameter parameters::fr54 = 5._dp/4
- real(kind=dp), parameter parameters::fr83 = 8._dp/3
- real(kind=dp), parameter parameters::fr260_3 = 260._dp/3
- real(kind=dp) parameters::w0

  Spin-orbit strength W_0.
- real(kind=dp) parameters::t0
- real(kind=dp) parameters::x0
- real(kind=dp) parameters::t1
- real(kind=dp) parameters::x1

- real(kind=dp) parameters::t2
- real(kind=dp) parameters::x2
- real(kind=dp) parameters::t3
- real(kind=dp) parameters::x3
- real(kind=dp) parameters::sigma
- real(kind=dp), dimension(0:1) parameters::hbar2_2m_q

  $\frac{\hbar^2}{2m}$ *with isospin dependence, as required by BSk forces*
- logical parameters::j2_terms

  Whether functional uses $\boldsymbol{J}^2$ *terms.*
- real(kind=dp) parameters::b1
- real(kind=dp) parameters::b2
- real(kind=dp) parameters::b3
- real(kind=dp) parameters::b4
- real(kind=dp) parameters::b5
- real(kind=dp) parameters::b6
- real(kind=dp) parameters::b7
- real(kind=dp) parameters::b8
- real(kind=dp) parameters::b9
- real(kind=dp) parameters::b10
- real(kind=dp) parameters::b11
- real(kind=dp) parameters::b12
- real(kind=dp) parameters::b13
- real(kind=dp) parameters::alpha
- real(kind=dp) parameters::beta
- real(kind=dp) parameters::gamma
- real(kind=dp) parameters::t4
- real(kind=dp) parameters::x4
- real(kind=dp) parameters::t5
- real(kind=dp) parameters::x5
- real(kind=dp) parameters::fn_pos
- real(kind=dp) parameters::fn_neg
- real(kind=dp) parameters::fp_pos
- real(kind=dp) parameters::fp_neg
- real(kind=dp) parameters::epsilon_lambda
- real(kind=dp), dimension(:), allocatable parameters::r

  Mesh for r.
- real(kind=dp), dimension(:,:), allocatable parameters::rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::del2_rho_q
- real(kind=dp), dimension(:), allocatable parameters::rho_t
- real(kind=dp), dimension(:), allocatable parameters::del_rho_t
- real(kind=dp), dimension(:), allocatable parameters::del2_rho_t
- real(kind=dp), dimension(:,:), allocatable parameters::f_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::del2_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::w_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_w_q
- real(kind=dp), dimension(:,:), allocatable parameters::u_q
- real(kind=dp), dimension(:,:), allocatable parameters::j_2_q
- real(kind=dp), dimension(:,:), allocatable parameters::j_q
- real(kind=dp), dimension(:,:), allocatable parameters::del_j_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_j_2_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_j_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_tf_q

- real(kind=dp), dimension(:,:), allocatable parameters::tau_2_l_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_2_nl_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_etf_q
- real(kind=dp), dimension(:), allocatable parameters::j_t
- real(kind=dp), dimension(:), allocatable parameters::del_j_t
- real(kind=dp), dimension(:), allocatable parameters::div_j_t
- real(kind=dp), dimension(:), allocatable parameters::tau_etf_t
- real(kind=dp), dimension(:), allocatable parameters::e_density_field
- real(kind=dp), dimension(:), allocatable parameters::e_density_sky
- real(kind=dp), dimension(:), allocatable parameters::v_c_di
- real(kind=dp), dimension(:), allocatable parameters::v_c_ex
- real(kind=dp), dimension(:), allocatable parameters::e_density_c_di
- real(kind=dp), dimension(:), allocatable parameters::e_density_c_ex
- real(kind=dp), dimension(:), allocatable parameters::v_c_pe
- real(kind=dp), dimension(:,:,:), allocatable parameters::tau_2_cont_q
- real(kind=dp), dimension(:), allocatable parameters::rho_ch

  Charge density.
- real(kind=dp), dimension(:,:), allocatable parameters::d2_rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::d3_rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::d4_rho_q
- real(kind=dp), dimension(:,:), allocatable parameters::d2_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::d3_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::d4_f_q
- real(kind=dp), dimension(:,:), allocatable parameters::a_q
- real(kind=dp), dimension(:,:), allocatable parameters::d1_a_q
- real(kind=dp), dimension(:,:), allocatable parameters::d2_a_q
- real(kind=dp), dimension(:,:), allocatable parameters::d3_a_q
- real(kind=dp), dimension(:,:), allocatable parameters::d4_a_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_4_no_spin_q
- real(kind=dp), dimension(:,:), allocatable parameters::tau_4_so_q
- real(kind=dp), dimension(:,:), allocatable parameters::j_4_q
- real(kind=dp), dimension(:,:), allocatable parameters::div_j_4_q
- real(kind=dp), dimension(:,:,:), allocatable parameters::tau_4_cont_q
- real(kind=dp), dimension(0:1) parameters::n_q

  Number of neutrons and protons.
- real(kind=dp) parameters::n_t

  Total number of particles.
- real(kind=dp) parameters::e_field

  Field energy.
- real(kind=dp) parameters::e_skyrme

  Skyrme energy.
- real(kind=dp), dimension(0:1) parameters::e_kinetic_q

  Kinetic energy for neutron and protons.
- real(kind=dp) parameters::e_kinetic_t

  Total kinetic energy.
- real(kind=dp) parameters::e_so

  Spin-orbit energy.
- real(kind=dp) parameters::e_coulomb_di

  Direct Coulomb energy.
- real(kind=dp) parameters::e_coulomb_ex

  Exhange Coulomb energy.
- real(kind=dp) parameters::e_coulomb

  Total Coulomb energy.

- real(kind=dp) parameters::e_total

  Total energy.
- real(kind=dp), dimension(0:1) parameters::mu_q

  Neutron and proton chemical potential.
- real(kind=dp) parameters::mu_e

  Electron chemical potential.
- real(kind=dp) parameters::mu_c

  Coulomb interaction contribution to electron chemical potential.
- real(kind=dp) parameters::delta_mu

  Overall chemical potential (beta-equilibrium condition)
- real(kind=dp) parameters::pressure_nucl

  Nuclear pressure.
- real(kind=dp) parameters::pressure_e

  Electron pressure.
- real(kind=dp) parameters::pressure_ex

  Coulomb exchange pressure.
- real(kind=dp) parameters::pressure_t

  Total pressure.
- integer parameters::run_mode

  Mode to run code in (normal, test)
- logical parameters::verbose

  Whether to print all extra messages about run.
- real(kind=dp) parameters::dr

  Mesh spacing of r (fm).
- logical parameters::profile_r_max

  Whether to take "r_max" from "r_ws".
- real(kind=dp) parameters::r_max

  Max value of r (fm).
- logical parameters::specify_n

  Whether to specify "n" instead of "dr".
- integer parameters::n

  Number of mesh points.
- integer parameters::force

  Force to use.
- integer parameters::etf_order

  Order at which to calculate kinetic energy densities.
- logical parameters::coulomb_on

  Use Coulomb interaction or not.
- logical parameters::electrons_on

  Add electrons.
- integer parameters::nmaxstate

  Number of states that can be stored.
- integer parameters::lmax

  Maximum angular momentum of states to find.
- logical parameters::calc_chem_pots

  Calculate chemical potentials.
- logical, dimension(0:1) parameters::strutinsky_on

  Use Strutinsky Integral (SI) correction for neutrons and protons.
- real(kind=dp) parameters::strut_r_max

  Max value of r to use for box for single particle states (fm).
- logical parameters::emax0_mod

Whether to modify "emax0" to always = 0.
- integer parameters::neutron_pairing

  Type of pairing calculation to perform for neutrons.
- logical parameters::proton_bcs

  Whether to do BCS for protons.
- real(kind=dp) parameters::pair_qp_cut

  Cut-off for quasiparticle energy for solving gap equation.
- logical parameters::smooth_qp_cut

  Whether to use smooth cut-off on quasiparticle energy.
- real(kind=dp) parameters::pair_k_max

  Maximum momentum for integral in gap equation.
- real(kind=dp) parameters::pair_v0

  Interaction strength parameter.
- real(kind=dp) parameters::pair_eta

  Interaction parameter eta.
- real(kind=dp) parameters::pair_alpha

  Interaction parameter alpha.
- real(kind=dp) parameters::pair_tol

  Gap equation self-consistency tolerance.
- real(kind=dp) parameters::pair_mix

  Mix of previous iteration in gap equation self-consistency loop.
- real(kind=dp) parameters::pair_dk

  Step size in integral in gap equation.
- real(kind=dp) parameters::pair_del_init

  Initial guess for pairing gap.
- integer parameters::pair_max_iters

  Maximum iterations for gap equation self-consistency loop.
- real(kind=dp) parameters::pair_num_tol

  BCS number equation self-consistency tolerance.
- real(kind=dp), dimension(5) parameters::n_profile
- real(kind=dp), dimension(5) parameters::p_profile
- real(kind=dp) parameters::num_n
- integer parameters::num_p
- real(kind=dp) parameters::r_ws
- character(18), dimension(10) parameters::n_floats = (/'(1(es24.16e3,1x))','(2(es24.16e3,1x))','(3(es24.↩16e3,1x))', '(4(es24.16e3,1x))','(5(es24.16e3,1x))','(6(es24.16e3,1x))','(7(es24.16e3,1x))', '(8(es24.↩16e3,1x))','(9(es24.16e3,1x))','(10(es24.16e3,1x))'/)
- character(27) parameters::info_format = '(a27,1x,a1,1x,es24.16e3)'
- character(8) parameters::force_string
- character(80), parameter parameters::line_break = '###

  Separating output.
- character(62), parameter parameters::table_string = '---------------------------+------------------------'
- character(1), dimension(0:1), parameter parameters::iso_string = (/'n','p'/)

  Isospin labels.
- character(4), parameter parameters::space4 = ' '

  Whitespace of length 4.
- integer parameters::strut_n
- real(kind=dp), dimension(:,:), allocatable parameters::dhmen
- real(kind=dp), dimension(:,:), allocatable parameters::d2hmen
- real(kind=dp), dimension(:,:), allocatable parameters::hb2m
- real(kind=dp), dimension(:,:), allocatable parameters::vpot
- real(kind=dp), dimension(:,:), allocatable parameters::vso

- real(kind=dp), dimension(0:1) parameters::ecut

    Cutoff energies for neutrons and protons.
- real(kind=dp), dimension(:,:), allocatable parameters::ps

    Storage for single particle wavefunctions.
- integer parameters::nnst

    Number of states found within cutoff energy.
- integer, dimension(:), allocatable parameters::jjp

    Storage for J of states found.
- integer, dimension(:), allocatable parameters::lp

    Storage for L of states found.
- real(kind=dp), dimension(:), allocatable parameters::ep

    Storage for energy of states found.
- real(kind=dp), dimension(0:1) parameters::e_sc_q

    Storage for shell correction energies.
- real(kind=dp) parameters::e_sc_t

    Storage for total shell correction energy.
- real(kind=dp), dimension(:), allocatable parameters::pair_gap_n

    Neutron pairing gap.
- real(kind=dp), dimension(:), allocatable parameters::delta_n

    Neutron pairing field.
- real(kind=dp), dimension(:), allocatable parameters::pair_gap_p

    Proton pairing gap.
- real(kind=dp), dimension(:), allocatable parameters::delta_p

    Proton pairing field.
- real(kind=dp), dimension(:), allocatable parameters::rho_p_bcs

    Proton density (from wavefunctions)
- real(kind=dp), dimension(:), allocatable parameters::rho_anom_p_bcs

    Anomalous density.
- real(kind=dp), dimension(:), allocatable parameters::strength_bcs

    Interaction strength for protons.
- real(kind=dp), dimension(:), allocatable parameters::occ_v

    Particle occupation probabilities.
- real(kind=dp), dimension(:), allocatable parameters::occ_u

    Hole occupation probabilities.
- real(kind=dp), dimension(:), allocatable parameters::e_qp_p

    Quasiparticle energies.
- real(kind=dp) parameters::num_p_bcs

    Number of protons calculated from occupations.
- real(kind=dp) parameters::e_pair_bcs

    BCS pairing energy.
- real(kind=dp), dimension(0:1) parameters::e_pair_q

    Storage for pairing condensation energies.
- real(kind=dp) parameters::e_pair_t

    Storage for total pairing condensation energy.
- real(kind=dp) parameters::rho_e

    Electron density.
- real(kind=dp) parameters::e_kinetic_e

    Total electron kinetic energy.
- real(kind=dp) parameters::e_coulomb_e

    Total electron-electron potential energy from Coulomb interaction.
- real(kind=dp) parameters::e_coulomb_pe

    Total proton-electron potential energy from Coulomb interaction.

6.5 srcs/routines.f90 File Reference

Modules

- module routines

  Module to hold main routines: densities, energies.

Functions/Subroutines

- integer function routines::str2int (string)
- subroutine routines::allocate_arrays ()

  Subroutine to allocate arrays for all densities and effective masses, and for their derivatives.
- subroutine routines::initialise_uniform_mesh ()

  Subroutine to calculate number of mesh points for a uniform grid, allocate array for r, and then populate r with the mesh points.
- subroutine routines::deallocate_mesh ()

  Subroutine to deallocate array for r.
- subroutine routines::deallocate_arrays ()

  Subroutine to deallocate arrays for all densities and effective masses, and for their derivatives.
- real(kind=dp) function routines::calc_rho_q (rhoqgas, rhoqliq, rq, aq, gammaq, r)

  Function to calculate the neutron or proton density at a given radius r, using supplied input parameters.
- subroutine routines::calc_f_q (rhot, rhoq, q, fq)

  Subroutine to calculate the effective mass ratio $f_q = \frac{m}{m^*_q}$ for neutrons or protons, for standard Skyrme or for BSk forces.
- subroutine routines::calc_w_q (delrho, delrhoq, Wq)

  Function to calculate the spin-orbit field $\boldsymbol{W}_q$ for neutrons or protons.
- subroutine routines::calc_tau_tf (rhoq, tauTF)

  Function to calculate the zeroth-order contribution to the kinetic energy density for neutrons or protons.
- subroutine routines::calc_tau_2_l (rhoq, delrhoq, del2rhoq, tau2Lq, t2contq)

  Function to calculate the local second-order contribution to the kinetic energy density for neutrons or protons.
- subroutine routines::calc_tau_2_nl (rhoq, delrhoq, fq, delfq, del2fq, Wq, q, tau2NLq, t2contq)

  Subroutine to calculate the non-local second-order contribution to the kinetic energy density for neutrons or protons.
- subroutine routines::calc_tau_4_no_spin (rhoq, d1rhoq, d2rhoq, d3rhoq, d4rhoq, fq, d1fq, d2fq, d3fq, d4fq, tau4nospinq, t4contq)

  Subroutine to calculate the fourth-order contributions to the kinetic energy density (without spin-orbit contributions) $\boldsymbol{tau}_q$ for neutrons or protons.
- subroutine routines::calc_tau_4_so (rhoq, d1rhoq, fq, d1fq, d2fq, d1Aq, d2Aq, d3Aq, q, tau_4_so_q, t4contq)

  Subroutine to calculate the fourth-order contributions to the kinetic energy density (spin-orbit contributions) $\boldsymbol{tau}_q$ for neutrons or protons.
- subroutine routines::calc_j_2_q (rhoq, Wq, fq, q, J2q)

  Subroutine to calculate the second-order contributions to the spin current density $\boldsymbol{J}_q$ for neutrons or protons.
- subroutine routines::calc_j_4_q (rhoq, d1rhoq, fq, d1fq, d2fq, d1Aq, d2Aq, d3Aq, q, J4q)

  Subroutine to calculate the fourth-order contributions to the spin current density $\boldsymbol{J}_q$ for neutrons or protons.
- subroutine routines::calc_div_j_2_q (rhoq, d1rhoq, fq, d1fq, d1Aq, d2Aq, q, divJ2q)

  Subroutine to calculate the second-order contributions to the divergence of the current density $\boldsymbol{J}_q$ for neutrons or protons.
- subroutine routines::calc_div_j_4_q (rhoq, d1rhoq, d2rhoq, fq, d1fq, d2fq, d3fq, d1Aq, d2Aq, d3Aq, d4Aq, q, divJ4q)

  Subroutine to calculate the fourth-order contributions to the divergence of the current density $\boldsymbol{J}_q$ for neutrons or protons.

- real(kind=dp) function routines::calc_u_q (rhot, rhon, rhop, delrhot, delrhon, delrhop, del2rhot, del2rhon, del2rhop, taut, taun, taup, divJt, divJq, q)

    Function to calculate the central potential U_q for neutrons or protons, for standard Skyrme or for BSk forces with extra terms.
- subroutine routines::eval_fields ()

    Subroutine to evaluate matter density derivatives, and all fields: effective masses (and derivatives), spin-orbit fields, spin current densities (and derivatives)
- subroutine routines::eval_tau_etf ()

    Subroutine to calculate the kinetic energy density τ_{ETF} with the (extended) Thomas-Fermi approximation at order specified by "etf_order".
- subroutine routines::charge (rho, Neutr, Nprot, Ngrid1, del1, rhoch)

    Subroutine to calculate the charge density from the matter densities. Modified by M. Shelley.
- subroutine routines::eval_coulomb (prot_dens, calc_exchange)

    Subroutine to evaluate the Coulomb potentials and energy densities, using either the proton or charge density.
- subroutine routines::eval_electrons ()

    Subroutine to evaluate the proton-electron potential which contributes to U_q, all energy contributions, and the pressure, coming from a homogeneous electron gas. Also calculates the electron chemical potential.
- subroutine routines::eval_u_q ()

    Subroutine to evaluate the central fields U_q.
- subroutine routines::eval_skyrme_energy_density ()

    Subroutine to evaluate the Skyrme energy density, after first separately evaluating the field energy density.
- subroutine routines::pressure ()

    Subroutine to calculate the nuclear contribution to the pressure, and then the total pressure.
- subroutine routines::calc_particle_number ()

    Subroutine to calculate the number of particles in the Wigner-Seitz cell.
- subroutine routines::eval_ws_quantities ()

    Subroutine to evaluate the various densities, fields, derivatives, energies, and particle numbers in the WS cell with densities rho_q.
- real(kind=dp) function routines::calc_e_f_q (rhoq, fq, q)

    Subroutine to evaluate the Fermi energy at a given density and effective mass, for neutrons or protons.
- subroutine routines::d1 (n, h, f, df)

    This subroutine computes the first derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.
- subroutine routines::d2 (n, h, f, d2f)

    This subroutine computes the second derivative of function evaluated on the meshpoints 1,...,npt. The input is the function f with extrapolated values in -1, 0. Modified by M. Shelley.
- subroutine routines::lap_sphe_symm (f, df_dr, d2f_dr2)

    Subroutine to carry out Laplacian in spherical symmetry.
- subroutine routines::d3 (f, d3f_dr3)

    Subroutine to calculate third derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.
- subroutine routines::d4 (f, d4f_dr4)

    Subroutine to calculate fourth derivative of function f evaluated on evenly-spaced meshpoints from 1 to n. Works with extrapolated values in -2,-1,0. Uses 7-point stencil.
- subroutine routines::extrapolate_back_3 (grid)

    Subroutine to extrapolate back 3 points on the r mesh, to faciliate the calculation of first and second derivatives using a 5-point stencil. Values in grid start at 4, extrapolated values are put in elements 3,2,1. Coefficients come from solving 4th-order polynomial, assuming that f'(0) = 0, and f(-h) = f(h).
- real(kind=dp) function routines::ws_integral (quantity, n_max)

    Function to integrate a density or field over the whole W-S cell, using Simpson's rule (+ Simpson's 3/8 rule if odd number of points)
- subroutine routines::write_densities ()

    Subroutine to write neutron and proton densities to files.

- subroutine routines::write_fields ()

  Subroutine to write neutron and proton fields to files.
- subroutine routines::write_sp_states_p ()

  Subroutine to write proton single particle energies to file, and extra details if BCS has been performed.

Variables

- integer routines::file_unit_0
- integer routines::file_unit_1

  Unit numbers for opening files.

6.6 srcs/strutinsky.f90 File Reference

Modules

- module strutinsky

  Module to hold routines for carrying out Strutinsky correction.

Functions/Subroutines

- subroutine strutinsky::sp_states_setup ()

  Subroutine to allocate + initialise variables needed in 'boundary' routine, and allocate arrays needed for BCS.
- subroutine strutinsky::sp_states_deallocate ()

  Subroutine to deallocate arrays needed in 'boundary' routine, and deallocate arrays needed for BCS.
- subroutine strutinsky::state_sort (sp_J, sp_L, sp_E, sp_wfns)

  Subroutine to sort single particle states by their energies. Use bubble sort.
- subroutine strutinsky::calc_e_sc (q)

  Subroutine to calculate the Strutinsky shell correction energy for isospin q. First, sum over occupied states of s.p. energies. Second, integrate over W-S cell of smoothed ETF densities and fields.
- subroutine strutinsky::calc_e_sc_pair ()

  Subroutine to calculate the Strutinsky shell correction energy for protons, using BCS occupation probabilities.

6.7 srcs/test.f90 File Reference

Modules

- module test

  Module to hold test routines.

Functions/Subroutines

- subroutine test::read_test_params ()

  Subroutine to read from "test_input.in" parameters used for test routines.
- subroutine test::test_densities ()

  Subroutine to calculate the density profiles using sample parameters.
- subroutine test::test_density_derivs ()

  Subroutine to test some derivatives of the total and individual densities.
- subroutine test::test_eff_mass ()

  Subroutine to test effective masses fm^{-3}.
- subroutine test::test_kinetic_densities ()

  Subroutine to test kinetic energy densities.
- subroutine test::test_spin_current_densities ()

  Subroutine to write spin current densities and spin-orbit fields to file.
- subroutine test::orders_kinetic_densities ()

  Subroutine to write order-by-order comparison of kinetic densities to file.
- subroutine test::test_central_potentials ()

  Subroutine to write spin central potentials to file.
- subroutine test::write_ws_cell_array_quantity (quantity)

  Utility subroutine that can be called anywhere at any time, for writing a quantity (evaluated over WS cell) to file.
- subroutine test::test_calc_particle_number ()

  Subroutine to test calculation of neutron and proton particle numbers.
- subroutine test::test_calc_coulomb_energy ()

  Subroutine to test calculation of Coulomb energy.
- subroutine test::test_calc_skyrme_energy ()

  Subroutine to test calculation of Skyrme energy.
- subroutine test::test_sp_energies ()

  Subroutine to test calculation of single particle energies.
- subroutine test::test_si_correction ()

  Subroutine to test the Strutinsky integral correction.
- subroutine test::bartel_bencheikh_benchmark ()

  Subroutine to check different contributions to τ_{ETF} at 2nd order, for comparison with results in Bartel and Bencheikh (2002)

Variables

- integer test::file_unit
- integer test::file_unit_2

  Unit numbers for opening files.
- integer test::sample_profile

  Test density profile to use.

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