DD2356: Quantum SPH

Generated by Doxygen 1.8.17

1 DD2356_QuantumSPH	1
2 Namespace Index	3
2.1 Namespace List	3
3 File Index	5
3.1 File List	5
4 Namespace Documentation	7
4.1 CSVReader Namespace Reference	7
4.1.1 Function Documentation	7
4.1.1.1 read_and_plot()	7
4.2 quantumsph Namespace Reference	7
4.2.1 Function Documentation	8
4.2.1.1 acceleration()	8
4.2.1.2 density()	8
4.2.1.3 kernel()	9
4.2.1.4 main()	9
4.2.1.5 pressure()	9
4.2.1.6 probeDensity()	0
5 File Documentation 1	1
5.1 arithmeticCost.c File Reference	1
5.1.1 Macro Definition Documentation	1
5.1.1.1 N	2
5.1.2 Function Documentation	2
5.1.2.1 main()	2
5.2 CSVReader.py File Reference	2
5.3 quantumsph.py File Reference	2
5.4 quantumsph_Improved.c File Reference	3
5.4.1 Macro Definition Documentation	4
5.4.1.1 INV_SQRT_PI	4
5.4.2 Function Documentation	4
5.4.2.1 acceleration()	4
5.4.2.2 kernel_0()	4
5.4.2.3 kernel_1()	5
5.4.2.4 kernel_2()	5
5.4.2.5 main()	6
5.4.2.6 pressure()	6
5.4.2.7 probeDensity()	6
5.4.3 Variable Documentation	6
5.4.3.1 h_sq	7
5.4.3.2 inv_h	7
5.4.3.3 inv_h_5	7

5.4.3.4 inv_h_7	. 17
5.4.3.5 inv_h_cb	. 17
5.4.3.6 inv_h_sq	. 17
5.5 quantumsph_Initial.c File Reference	. 17
5.5.1 Macro Definition Documentation	18
5.5.1.1 PI	18
5.5.2 Function Documentation	18
5.5.2.1 acceleration()	. 18
5.5.2.2 density()	. 19
5.5.2.3 kernel()	. 19
5.5.2.4 main()	20
5.5.2.5 pressure()	20
5.5.2.6 probeDensity()	20
5.6 quantumsph_Memorize.c File Reference	21
5.6.1 Macro Definition Documentation	22
5.6.1.1 INV_SQRT_PI	22
5.6.2 Function Documentation	22
5.6.2.1 acceleration()	22
5.6.2.2 density()	23
5.6.2.3 FreeMatrix()	23
5.6.2.4 InitializeMatrix()	23
5.6.2.5 kernel_0()	24
5.6.2.6 kernel_0_mat()	24
5.6.2.7 kernel_1_mat()	25
5.6.2.8 kernel_2_mat()	25
5.6.2.9 main()	25
5.6.2.10 pressure()	26
5.6.2.11 probeDensity()	26
5.6.3 Variable Documentation	26
5.6.3.1 h_sq	. 27
5.6.3.2 inv_h	27
5.6.3.3 inv_h_5	27
5.6.3.4 inv_h_7	. 27
5.6.3.5 inv_h_cb	27
5.6.3.6 inv_h_sq	27
5.7 quantumsph_MPI.c File Reference	27
5.7.1 Macro Definition Documentation	28
5.7.1.1 INV_SQRT_PI	28
5.7.2 Function Documentation	29
5.7.2.1 acceleration()	29
5.7.2.2 FreeMatrix()	29
5.7.2.3 InitializeMatrix()	. 29

5.7.2.4 kernel_0()	. 30
5.7.2.5 kernel_1()	. 30
5.7.2.6 kernel_2()	. 31
5.7.2.7 main()	. 31
5.7.2.8 probeDensity()	. 31
5.7.2.9 relativePressure()	. 32
5.7.3 Variable Documentation	. 32
5.7.3.1 h_sq	. 32
5.7.3.2 inv_h	. 32
5.7.3.3 inv_h_5	. 32
5.7.3.4 inv_h_7	. 33
5.7.3.5 inv_h_cb	. 33
5.7.3.6 inv_h_sq	. 33
5.7.3.7 n	. 33
5.7.3.8 n_loc	. 33
5.7.3.9 rank	. 33
5.7.3.10 rem	. 33
5.7.3.11 size	. 33
5.8 quantumsph_OMP_Initial.c File Reference	. 34
5.8.1 Macro Definition Documentation	. 35
5.8.1.1 INV_SQRT_PI	. 35
5.8.2 Function Documentation	. 35
5.8.2.1 acceleration()	. 35
5.8.2.2 FreeMatrix()	. 36
5.8.2.3 InitializeMatrix()	. 36
5.8.2.4 kernel_0()	. 36
5.8.2.5 kernel_0_mat()	. 37
5.8.2.6 kernel_1_mat()	. 37
5.8.2.7 kernel_2_mat()	. 37
5.8.2.8 main()	. 38
5.8.2.9 probeDensity()	. 38
5.8.2.10 relativePressure()	. 38
5.8.3 Variable Documentation	. 39
5.8.3.1 h_sq	. 39
5.8.3.2 inv_h	. 39
5.8.3.3 inv_h_5	. 39
5.8.3.4 inv_h_7	. 39
5.8.3.5 inv_h_cb	. 40
5.8.3.6 inv_h_sq	. 40
5.9 quantumsph_OMP_Memorize16.c File Reference	. 40
5.9.1 Macro Definition Documentation	. 41
5.9.1.1 INV_SQRT_PI	. 41

5.9.2 Function Documentation	41
5.9.2.1 acceleration()	41
5.9.2.2 FreeMatrix()	42
5.9.2.3 InitializeMatrix()	42
5.9.2.4 kernel_0()	43
5.9.2.5 kernel_0_mat()	43
5.9.2.6 kernel_1_mat()	43
5.9.2.7 kernel_2_mat()	44
5.9.2.8 main()	44
5.9.2.9 probeDensity()	44
5.9.2.10 relativePressure()	45
5.9.3 Variable Documentation	45
5.9.3.1 h_sq	45
5.9.3.2 inv_h	45
5.9.3.3 inv_h_5	46
5.9.3.4 inv_h_7	46
5.9.3.5 inv_h_cb	46
5.9.3.6 inv_h_sq	46
5.10 quantumsph_OMP_Memorize32.c File Reference	46
5.10.1 Macro Definition Documentation	47
5.10.1.1 INV_SQRT_PI	47
5.10.2 Function Documentation	47
5.10.2.1 acceleration()	48
5.10.2.2 FreeMatrix()	48
5.10.2.3 InitializeMatrix()	48
5.10.2.4 kernel_0()	49
5.10.2.5 kernel_0_mat()	49
5.10.2.6 kernel_1_mat()	50
5.10.2.7 kernel_2_mat()	50
5.10.2.8 main()	50
5.10.2.9 probeDensity()	51
5.10.2.10 relativePressure()	51
5.10.3 Variable Documentation	51
5.10.3.1 h_sq	52
5.10.3.2 inv_h	52
5.10.3.3 inv_h_5	52
5.10.3.4 inv_h_7	52
5.10.3.5 inv_h_cb	52
5.10.3.6 inv_h_sq	52
5.11 quantumsph_OMP_Memorize64.c File Reference	52
5.11.1 Macro Definition Documentation	53
5.11.1.1 INV_SQRT_PI	53

5.11.2 Function Documentation	54
5.11.2.1 acceleration()	54
5.11.2.2 FreeMatrix()	54
5.11.2.3 InitializeMatrix()	54
5.11.2.4 kernel_0()	55
5.11.2.5 kernel_0_mat()	55
5.11.2.6 kernel_1_mat()	56
5.11.2.7 kernel_2_mat()	56
5.11.2.8 main()	56
5.11.2.9 probeDensity()	57
5.11.2.10 relativePressure()	57
5.11.3 Variable Documentation	57
5.11.3.1 h_sq	58
5.11.3.2 inv_h	58
5.11.3.3 inv_h_5	58
5.11.3.4 inv_h_7	58
5.11.3.5 inv_h_cb	58
5.11.3.6 inv_h_sq	58
5.12 quantumsph_OMP_NoMemory.c File Reference	58
5.12.1 Macro Definition Documentation	59
5.12.1.1 INV_SQRT_PI	59
5.12.2 Function Documentation	59
5.12.2.1 acceleration()	60
5.12.2.2 kernel_0()	60
5.12.2.3 kernel_1()	60
5.12.2.4 kernel_2()	61
5.12.2.5 main()	61
5.12.2.6 pressure()	61
5.12.2.7 probeDensity()	62
5.12.3 Variable Documentation	62
5.12.3.1 h_sq	62
5.12.3.2 inv_h	62
5.12.3.3 inv_h_5	62
5.12.3.4 inv_h_7	63
5.12.3.5 inv_h_cb	63
5.12.3.6 inv_h_sq	63
5.13 README.md File Reference	63
Index	65

Chapter 1

DD2356_QuantumSPH

DD2356_QuantumSPH

Chapter 2

Namespace Index

2.1 Namespace List

Here is a list of all namespaces with brief descriptions:

CSVReader	•
quantumsph	-

4 Namespace Index

Chapter 3

File Index

3.1 File List

Here is a list of all files with brief descriptions:

arithmeticCost.c
CSVReader.py
quantumsph.py
quantumsph_Improved.c
quantumsph_Initial.c
quantumsph_Memorize.c
quantumsph_MPI.c
quantumsph_OMP_Initial.c
quantumsph_OMP_Memorize16.c
quantumsph_OMP_Memorize32.c
quantumsph_OMP_Memorize64.c
quantumsph OMP NoMemory.c

6 File Index

Chapter 4

Namespace Documentation

4.1 CSVReader Namespace Reference

Functions

```
• def read_and_plot (file_name)
```

4.1.1 Function Documentation

4.1.1.1 read_and_plot()

4.2 quantumsph Namespace Reference

Functions

```
• def main ()
```

- def kernel (r, h, deriv)
- def density (x, m, h)
- def pressure (x, rho, m, h)
- def acceleration (x, u, m, rho, P, b, h)
- def probeDensity (x, m, h, xx)

4.2.1 Function Documentation

4.2.1.1 acceleration()

Returns

rho : np.array

Density vector.

```
def quantumsph.acceleration (
              X,
              m,
              rho,
              P,
              b,
Calculates acceleration of each particle due to quantum pressure, harmonic potential, velocity damping
  Parameters
  x : np.array
     Position vector.
  u : np.array
     Velocity vector.
  m : float
     SPH particle mass.
  rho : np.array
     Density vector.
  P : np.array
     Pressure vector.
  b : float
     Damping coefficient.
  h : float
      Scaling length.
  Returns
  a : np.array
     Acceleration vector.
4.2.1.2 density()
def quantumsph.density (
              х,
              m,
              h )
Compute density at each of the particle locations using smoothing kernel
  Parameters
  x : np.array
     Position vector.
  {\tt m} : float
     SPH particle mass.
  h : float
     Scaling length.
```

4.2.1.3 kernel()

4.2.1.4 main()

```
def quantumsph.main ( )
Main Loop.
Evolve the time-dependent SE and plot solutions (also saves it as results_py.csv file)
```

4.2.1.5 pressure()

```
def quantumsph.pressure (
              X,
              rho,
              m,
              h )
Compute ''pressure'' at each of the particles using smoothing kernel
   P = -(1/4) * (d^2 rho /dx^2 - (d rho / dx)^2/rho)
  Parameters
  x : np.array
     Position vector.
  rho : np.array
     Density vector.
  m : float
     SPH particle mass.
  h : float
     Scaling length.
  Returns
  P : np.array
     Pressure vector.
```

4.2.1.6 probeDensity()

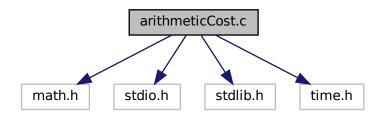
Chapter 5

File Documentation

5.1 arithmeticCost.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
```

Include dependency graph for arithmeticCost.c:



Macros

• #define N 1000000

The number of iterations.

Functions

• int main (int argc, char *argv[])

Timing kernel.

5.1.1 Macro Definition Documentation

5.1.1.1 N

```
#define N 1000000
```

The number of iterations.

5.1.2 Function Documentation

5.1.2.1 main()

```
int main (
          int argc,
          char * argv[] )
```

Timing kernel.

Compute the execution time of N integer addition, N double precision multiply add, and N calls to the math 'exp' function

5.2 CSVReader.py File Reference

Namespaces

CSVReader

Functions

• def CSVReader.read_and_plot (file_name)

5.3 quantumsph.py File Reference

Namespaces

• quantumsph

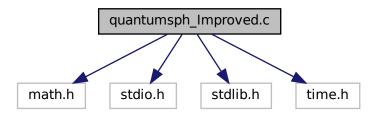
Functions

- def quantumsph.main ()
- def quantumsph.kernel (r, h, deriv)
- def quantumsph.density (x, m, h)
- def quantumsph.pressure (x, rho, m, h)
- def quantumsph.acceleration (x, u, m, rho, P, b, h)
- def quantumsph.probeDensity (x, m, h, xx)

5.4 quantumsph Improved.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
```

Include dependency graph for quantumsph_Improved.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

```
• double kernel_0 (double r)
```

SPH Gaussian smoothing kernel (1D).

• double kernel_1 (double r)

SPH Gaussian smoothing kernel (1D), first derivative.

• double kernel_2 (double r)

SPH Gaussian smoothing kernel (1D), second derivative.

• void pressure (double *rP, double *x, int n)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

• void acceleration (double *a, double *x, double *u, double *rP, int n, double b)

Calculates acceleration of each particle.

void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

int main (int argc, char *argv[])

Main loop.

Variables

- double h_sq
- · double inv h
- double inv_h_sq
- double inv_h_cb
- double inv_h_5
- double inv_h_7

5.4.1 Macro Definition Documentation

5.4.1.1 INV_SQRT_PI

```
#define INV_SQRT_PI 0.56418958354775627928
```

Constant equal to 1.0/sqrt(pi)

5.4.2 Function Documentation

5.4.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
X	positions of the particles
и	velocity vector
rP	relative pressure vector
n	number of particles
b	damping coefficient

5.4.2.2 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.4.2.3 kernel_1()

```
double kernel_1 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D), first derivative.

This function returns the weight associated with the first derivative of the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.4.2.4 kernel_2()

```
double kernel_2 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D), second derivative.

This function returns the weight associated with the second derivative of the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.4.2.5 main()

```
int main (
          int argc,
          char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.4.2.6 pressure()

```
void pressure ( \label{eq:condition} \operatorname{double} \ * \ rP, \\ \operatorname{double} \ * \ x, \\ \operatorname{int} \ n \ )
```

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)
X	positions of the particles
n	number of particles

5.4.2.7 probeDensity()

```
void probeDensity (
          double * rr,
          double * x,
          int n,
          double * xx,
          int nxx )
```

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.4.3 Variable Documentation

5.4.3.1 h_sq

double h_sq

5.4.3.2 inv_h

double inv_h

5.4.3.3 inv_h_5

double inv_h_5

5.4.3.4 inv_h_7

double inv_h_7

5.4.3.5 inv_h_cb

double inv_h_cb

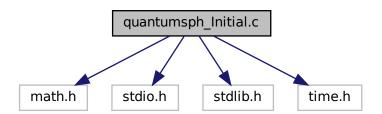
5.4.3.6 inv_h_sq

double inv_h_sq

5.5 quantumsph_Initial.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
```

Include dependency graph for quantumsph_Initial.c:



Macros

#define PI 3.14159265358979323846
 The pi constant.

Functions

• double kernel (double r, double h, int deriv)

```
SPH Gaussian smoothing kernel (1D).
```

• void density (double *rho, double *x, int n, double m, double h)

Compute density at each of the particle locations using smoothing kernel.

• void pressure (double *P, double *x, double *rho, int n, double m, double h)

Compute "pressure" at each of the particle locations using smoothing kernel.

void acceleration (double *a, double *x, double *u, double *rho, double *P, int n, double m, double b, double h)

Calculates acceleration of each particle.

• void probeDensity (double *rr, double *x, int n, double m, double h, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

5.5.1 Macro Definition Documentation

5.5.1.1 PI

```
#define PI 3.14159265358979323846
```

The pi constant.

5.5.2 Function Documentation

5.5.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
Х	positions of the particles
и	velocity vector
rho	density vector
Р	pressure vector
n	number of particles
m	SPH particle mass
b	damping coefficient
h	scaling length

5.5.2.2 density()

Compute density at each of the particle locations using smoothing kernel.

Parameters

rho	density vector to be updated
X	positions of the particles
n	number of particles
m SPH particle mass	
h	scaling length

5.5.2.3 kernel()

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel, for the specified derivative order.

Parameters

r	distance between particles
h	analina lanath
11	scaling length
Generated	by Doxygen .
deriv	by Doxygen derivative order

Returns

weight

5.5.2.4 main()

```
int main (
          int argc,
          char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.5.2.5 pressure()

Compute "pressure" at each of the particle locations using smoothing kernel.

Parameters

P	pressure vector to be updated, P = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)
X	positions of the particles
rho	density vector
n	number of particles
m	SPH particle mass
h	scaling length

5.5.2.6 probeDensity()

Probe the density at specified locations.

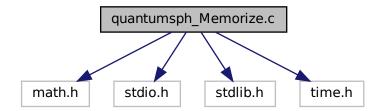
Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
m	SPH particle mass
h	scaling length
XX	probe locations
nxx	number of probe locations

5.6 quantumsph_Memorize.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
```

Include dependency graph for quantumsph_Memorize.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

• double ** InitializeMatrix (int n_row, int n_col)

Allocate memory space for a matrix.

void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

void kernel_0_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), for a set of particles.

void kernel 1 mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

void kernel_2_mat (double **ker, double *x, int n)

```
SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.
```

• double kernel_0 (double r)

SPH Gaussian smoothing kernel (1D).

void density (double *rho, double **ker_0, int n)

Compute density at each of the particle locations using smoothing kernel.

• void pressure (double *rP, double *rho, double **ker_0, double **ker_1, double **ker_2, int n)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

- void acceleration (double *a, double *x, double *u, double *rP, double **ker_1, int n, double b)

 Calculates acceleration of each particle.
- void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

```
 double h_sq
```

- · double inv h
- double inv_h_sq
- double inv_h_cb
- double inv h 5
- double inv_h_7

5.6.1 Macro Definition Documentation

5.6.1.1 INV SQRT PI

```
#define INV_SQRT_PI 0.56418958354775627928
```

Constant equal to 1.0/sqrt(pi)

5.6.2 Function Documentation

5.6.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
Х	positions of the particles
и	velocity vector
rP	relative pressure vector
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
n	number of particles
b	damping coefficient

5.6.2.2 density()

Compute density at each of the particle locations using smoothing kernel.

Parameters

rho	density vector to be updated
ker⊷	pre-computed smoothing kernel - interactions between particles
_0	
n	number of particles

5.6.2.3 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.6.2.4 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.6.2.5 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

r	distance between particles
h	scaling length

Returns

weight

5.6.2.6 kernel_0_mat()

SPH Gaussian smoothing kernel (1D), for a set of particles.

This function computes the weight associated with the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights	
_X	positions of the particles	
n	number of particles	Generated by Doxygen

5.6.2.7 kernel_1_mat()

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

This function computes the weight associated with the first derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
Х	positions of the particles
n	number of particles

5.6.2.8 kernel_2_mat()

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

This function computes the weight associated with the second derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.6.2.9 main()

```
int main (
          int argc,
          char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.6.2.10 pressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)
rho	density vector
<i>ker</i> ← _0	pre-computed smoothing kernel - interactions between particles
ker⊷ _1	pre-computed first derivative of smoothing kernel - interactions between particles
ker⊷ _2	pre-computed second derivative of smoothing kernel - interactions between particles
n	number of particles

5.6.2.11 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.6.3 Variable Documentation

5.6.3.1 h_sq

double h_sq

5.6.3.2 inv_h

double inv_h

5.6.3.3 inv_h_5

double inv_h_5

5.6.3.4 inv_h_7

double inv_h_7

5.6.3.5 inv_h_cb

double inv_h_cb

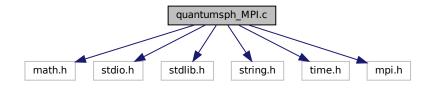
5.6.3.6 inv_h_sq

double inv_h_sq

5.7 quantumsph_MPI.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <time.h>
#include <mpi.h>
```

Include dependency graph for quantumsph_MPI.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

```
• double ** InitializeMatrix (int n_row, int n_col)
```

Allocate memory space for a matrix.

void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

• double kernel_0 (double r)

SPH Gaussian smoothing kernel (1D).

• double kernel_1 (double r)

SPH Gaussian smoothing kernel (1D), first derivative.

• double kernel_2 (double r)

SPH Gaussian smoothing kernel (1D), second derivative.

void relativePressure (double *rP, double **ker_0, double **ker_1, double *x, double *x_ext)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

• void acceleration (double *a, double *x, double *u, double *rP, double *rP_ext, double **ker_1, double b)

Calculates acceleration of each particle.

• void probeDensity (double *rr, double *x, double *x_ext, double *xx, int nxx_loc)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

- int n
- · int rank
- int size
- int n_loc
- int rem
- double h_sq
- double inv_h
- double inv h sq
- double inv_h_cb
- double inv_h_5
- double inv_h_7

5.7.1 Macro Definition Documentation

5.7.1.1 INV_SQRT_PI

#define INV_SQRT_PI 0.56418958354775627928

Constant equal to 1.0/sqrt(pi)

5.7.2 Function Documentation

5.7.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
X	positions of the particles
и	velocity vector
rP	relative pressure vector
rP_ext	allocated memory space for receiving other process's relative pressure vectors
ker←	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
b	damping coefficient

5.7.2.2 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.7.2.3 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.7.2.4 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

r	distance between particles
h	scaling length

Returns

weight

5.7.2.5 kernel_1()

```
double kernel_1 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D), first derivative.

This function returns the weight associated with the first derivative of the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.7.2.6 kernel_2()

```
\begin{array}{c} \texttt{double kernel\_2 (} \\ & \texttt{double } r \ ) \end{array}
```

SPH Gaussian smoothing kernel (1D), second derivative.

This function returns the weight associated with the second derivative of the SPH Gaussian smoothing kernel.

Parameters

```
r distance between particles
```

Returns

weight

5.7.2.7 main()

```
int main (
          int argc,
          char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.7.2.8 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated	
х	positions of the particles	
x ext	allocated memory space for receiving positions of other processes's particles	
Geynyerated	Generated by programment ocations	
nxx	number of probe locations	

5.7.2.9 relativePressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Computes "relative pressure" at each of the particle locations using smoothing kernel. Also stores interactions relative to the smoothing kernel and it's first derivative in ker_0 and ker_1.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho /dx 2 - (d rho / dx) 2 /rho)/(rho 2)
ker⊷	smoothing kernel to be computed - interactions between particles
_0	
ker⊷	first derivative of smoothing kernel to be computed - interactions between particles
_1	
Х	positions of the particles
x_ext	allocated memory space for receiving positions of other processes's particles

5.7.3 Variable Documentation

5.7.3.1 h_sq

double h_sq

5.7.3.2 inv_h

double inv_h

5.7.3.3 inv_h_5

double inv_h_5

5.7.3.4 inv_h_7

double inv_h_7

5.7.3.5 inv_h_cb

double inv_h_cb

5.7.3.6 inv_h_sq

 $\verb"double inv_h_sq"$

5.7.3.7 n

int n

5.7.3.8 n_loc

int n_loc

5.7.3.9 rank

int rank

5.7.3.10 rem

int rem

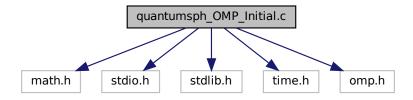
5.7.3.11 size

int size

5.8 quantumsph_OMP_Initial.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <omp.h>
```

Include dependency graph for quantumsph_OMP_Initial.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

- double ** InitializeMatrix (int n_row, int n_col)
 - Allocate memory space for a matrix.
- void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

- void kernel_0_mat (double **ker, double *x, int n)
 - SPH Gaussian smoothing kernel (1D), for a set of particles.
- void kernel_1_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

- void kernel_2_mat (double **ker, double *x, int n)
 - SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.
- double kernel_0 (double r)

SPH Gaussian smoothing kernel (1D).

- void relativePressure (double *rP, double *x, double **ker_0, double **ker_1, double **ker_2, int n)
 - Compute "relative pressure" at each of the particle locations using smoothing kernel.
- $\bullet \ \ void\ acceleration\ (double\ *a,\ double\ *x,\ double\ *u,\ double\ *rP,\ double\ **ker_1,\ int\ n,\ double\ b)$

Calculates acceleration of each particle.

void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

```
double h_sq
double inv_h
double inv_h_sq
double inv_h_cb
double inv_h_5
double inv_h_7
```

5.8.1 Macro Definition Documentation

5.8.1.1 INV_SQRT_PI

```
#define INV_SQRT_PI 0.56418958354775627928
```

Constant equal to 1.0/sqrt(pi)

5.8.2 Function Documentation

5.8.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
Х	positions of the particles
и	velocity vector
rP	relative pressure vector
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
n	number of particles
b	damping coefficient

5.8.2.2 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.8.2.3 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.8.2.4 kernel_0()

```
double kernel_0 ( \label{eq:condition} \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.8.2.5 kernel_0_mat()

SPH Gaussian smoothing kernel (1D), for a set of particles.

This function computes the weight associated with the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
Χ	positions of the particles
n	number of particles

5.8.2.6 kernel_1_mat()

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

This function computes the weight associated with the first derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.8.2.7 kernel 2 mat()

```
double * x, int n)
```

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

This function computes the weight associated with the second derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
Х	positions of the particles
n	number of particles

5.8.2.8 main()

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.8.2.9 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.8.2.10 relativePressure()

```
void relativePressure (
```

```
double * rP,
double * x,
double ** ker_0,
double ** ker_1,
double ** ker_2,
int n )
```

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)
Х	positions of the particles
ker← _0	pre-computed smoothing kernel - interactions between particles
ker⊷ _1	pre-computed first derivative of smoothing kernel - interactions between particles
ker⊷ _2	pre-computed second derivative of smoothing kernel - interactions between particles
n	number of particles

5.8.3 Variable Documentation

5.8.3.1 h_sq

double h_sq

5.8.3.2 inv_h

double inv_h

5.8.3.3 inv_h_5

double inv_h_5

5.8.3.4 inv_h_7

double inv_h_7

5.8.3.5 inv_h_cb

double inv_h_cb

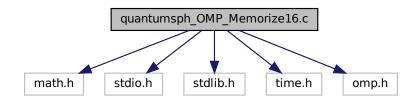
5.8.3.6 inv_h_sq

double inv_h_sq

5.9 quantumsph_OMP_Memorize16.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <omp.h>
```

Include dependency graph for quantumsph_OMP_Memorize16.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

• double ** InitializeMatrix (int n_row, int n_col)

Allocate memory space for a matrix.

void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

void kernel_0_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), for a set of particles.

void kernel_1_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

void kernel_2_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

```
    double kernel_0 (double r)
        SPH Gaussian smoothing kernel (1D).
    void relativePressure (double *rP, double *x, double **ker_0, double **ker_1, double **ker_2, int n)
        Compute "relative pressure" at each of the particle locations using smoothing kernel.
    void acceleration (double *a, double *x, double *u, double *rP, double **ker_1, int n, double b)
        Calculates acceleration of each particle.
    void probeDensity (double *rr, double *x, int n, double *xx, int nxx)
        Probe the density at specified locations.
    int main (int argc, char *argv[])
        Main loop.
```

Variables

```
double h_sq
double inv_h
double inv_h_cb
double inv_h_5
double inv_h_7
```

5.9.1 Macro Definition Documentation

```
5.9.1.1 INV_SQRT_PI

#define INV_SQRT_PI 0.56418958354775627928

Constant equal to 1.0/sqrt(pi)
```

5.9.2 Function Documentation

5.9.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
Х	positions of the particles
и	velocity vector
rP	relative pressure vector
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
n	number of particles
b	damping coefficient

5.9.2.2 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.9.2.3 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.9.2.4 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

```
r distance between particles
```

Returns

weight

5.9.2.5 kernel_0_mat()

SPH Gaussian smoothing kernel (1D), for a set of particles.

This function computes the weight associated with the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

	ker	matrix to be updated with the computed weights
	Χ	positions of the particles
Ī	n	number of particles

5.9.2.6 kernel_1_mat()

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

This function computes the weight associated with the first derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.9.2.7 kernel_2_mat()

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

This function computes the weight associated with the second derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.9.2.8 main()

```
int main (
                int argc,
                 char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.9.2.9 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.9.2.10 relativePressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)
Х	positions of the particles
ker⊷	pre-computed smoothing kernel - interactions between particles
_0	
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
ker⊷	pre-computed second derivative of smoothing kernel - interactions between particles
_2	
n	number of particles

5.9.3 Variable Documentation

5.9.3.1 h_sq

double h_sq

5.9.3.2 inv_h

double inv_h

5.9.3.3 inv_h_5

double inv_h_5

5.9.3.4 inv h 7

double inv_h_7

5.9.3.5 inv_h_cb

double inv_h_cb

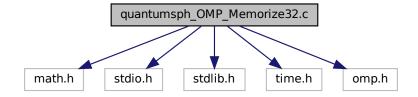
5.9.3.6 inv_h_sq

double inv_h_sq

5.10 quantumsph_OMP_Memorize32.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <omp.h>
```

Include dependency graph for quantumsph_OMP_Memorize32.c:



Macros

#define INV_SQRT_PI 0.56418958354775627928
 Constant equal to 1.0/sqrt(pi)

Functions

```
• double ** InitializeMatrix (int n_row, int n_col)
```

Allocate memory space for a matrix.

void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

void kernel_0_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), for a set of particles.

void kernel_1_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

• void kernel_2_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

• double kernel_0 (double r)

SPH Gaussian smoothing kernel (1D).

void relativePressure (double *rP, double *x, double **ker 0, double **ker 1, double **ker 2, int n)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

• void acceleration (double *a, double *x, double *u, double *rP, double **ker_1, int n, double b)

Calculates acceleration of each particle.

void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

- double h sq
- · double inv_h
- double inv_h_sq
- double inv h cb
- double inv_h_5
- double inv_h_7

5.10.1 Macro Definition Documentation

5.10.1.1 INV_SQRT_PI

#define INV_SQRT_PI 0.56418958354775627928

Constant equal to 1.0/sqrt(pi)

5.10.2 Function Documentation

5.10.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
X	positions of the particles
и	velocity vector
rP	relative pressure vector
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
n	number of particles
b	damping coefficient

5.10.2.2 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.10.2.3 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.10.2.4 kernel_0()

```
double kernel_0 ( \label{eq:condition} \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

```
r distance between particles
```

Returns

weight

5.10.2.5 kernel_0_mat()

```
void kernel_0_mat ( \label{eq:condition} \operatorname{double} \ ** \ ker, \operatorname{double} \ * \ x, \operatorname{int} \ n \ )
```

SPH Gaussian smoothing kernel (1D), for a set of particles.

This function computes the weight associated with the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
Х	positions of the particles
n	number of particles

5.10.2.6 kernel_1_mat()

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

This function computes the weight associated with the first derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.10.2.7 kernel_2_mat()

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

This function computes the weight associated with the second derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.10.2.8 main()

```
int main (
                int argc,
                 char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.10.2.9 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
Х	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.10.2.10 relativePressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx)^2/rho)/(rho^2)
Х	positions of the particles
ker⊷	pre-computed smoothing kernel - interactions between particles
_0	
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
ker←	pre-computed second derivative of smoothing kernel - interactions between particles
_2	
n	number of particles

5.10.3 Variable Documentation

5.10.3.1 h_sq

double h_sq

5.10.3.2 inv_h

double inv_h

5.10.3.3 inv_h_5

double inv_h_5

5.10.3.4 inv_h_7

double inv_h_7

5.10.3.5 inv_h_cb

double inv_h_cb

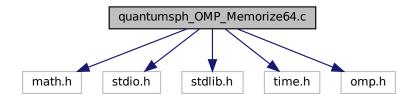
5.10.3.6 inv_h_sq

double inv_h_sq

5.11 quantumsph_OMP_Memorize64.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <omp.h>
```

Include dependency graph for quantumsph_OMP_Memorize64.c:



Macros

```
    #define INV_SQRT_PI 0.56418958354775627928
    Constant equal to 1.0/sqrt(pi)
```

Functions

```
    double ** InitializeMatrix (int n_row, int n_col)
    Allocate memory space for a matrix.
```

void FreeMatrix (double **A)

Frees memory space allocated for a matrix.

void kernel_0_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), for a set of particles.

void kernel_1_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

void kernel_2_mat (double **ker, double *x, int n)

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

• double kernel_0 (double r)

SPH Gaussian smoothing kernel (1D).

• void relativePressure (double *rP, double *x, double **ker_0, double **ker_1, double **ker_2, int n)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

void acceleration (double *a, double *x, double *rP, double **ker_1, int n, double b)

Calculates acceleration of each particle.

void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

- double h_sq
- · double inv h
- double inv_h_sq
- · double inv_h_cb
- double inv_h_5
- double inv_h_7

5.11.1 Macro Definition Documentation

5.11.1.1 INV_SQRT_PI

```
#define INV_SQRT_PI 0.56418958354775627928
```

Constant equal to 1.0/sqrt(pi)

5.11.2 Function Documentation

5.11.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
X	positions of the particles
и	velocity vector
rP	relative pressure vector
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
n	number of particles
b	damping coefficient

5.11.2.2 FreeMatrix()

Frees memory space allocated for a matrix.

Parameters

A matrix, pointer to memory space to be freed

5.11.2.3 InitializeMatrix()

Allocate memory space for a matrix.

This function allocates memory space for a matrix with n_row rows and n_col columns

Parameters

n_row	number of rows
n_col	number of columns

Returns

pointer to space allocated

5.11.2.4 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

```
r distance between particles
```

Returns

weight

5.11.2.5 kernel_0_mat()

SPH Gaussian smoothing kernel (1D), for a set of particles.

This function computes the weight associated with the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights	
X	positions of the particles	
n	number of particles	

Generated by Doxygen

5.11.2.6 kernel_1_mat()

SPH Gaussian smoothing kernel (1D), first derivative, for a set of particles.

This function computes the weight associated with the first derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.11.2.7 kernel_2_mat()

SPH Gaussian smoothing kernel (1D), second derivative, for a set of particles.

This function computes the weight associated with the second derivative of the SPH Gaussian smoothing kernel, for all pairwise interactions of the particles in x. It stores them in ker.

Parameters

ker	matrix to be updated with the computed weights
X	positions of the particles
n	number of particles

5.11.2.8 main()

```
int main (
          int argc,
          char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.11.2.9 probeDensity()

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.11.2.10 relativePressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rP	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)
X	positions of the particles
ker⊷	pre-computed smoothing kernel - interactions between particles
_0	
ker⊷	pre-computed first derivative of smoothing kernel - interactions between particles
_1	
ker⊷	pre-computed second derivative of smoothing kernel - interactions between particles
_2	
n	number of particles

5.11.3 Variable Documentation

5.11.3.1 h_sq

double h_sq

5.11.3.2 inv_h

double inv_h

5.11.3.3 inv_h_5

double inv_h_5

5.11.3.4 inv_h_7

double inv_h_7

5.11.3.5 inv_h_cb

double inv_h_cb

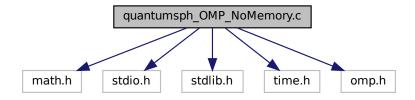
5.11.3.6 inv_h_sq

double inv_h_sq

5.12 quantumsph_OMP_NoMemory.c File Reference

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#include <omp.h>
```

Include dependency graph for quantumsph_OMP_NoMemory.c:



Macros

```
    #define INV_SQRT_PI 0.56418958354775627928
    Constant equal to 1.0/sqrt(pi)
```

Functions

```
    double kernel_0 (double r)
    SPH Gaussian smoothing kernel (1D).
```

• double kernel_1 (double r)

SPH Gaussian smoothing kernel (1D), first derivative.

• double kernel_2 (double r)

SPH Gaussian smoothing kernel (1D), second derivative.

• void pressure (double *rP, double *x, int n)

Compute "relative pressure" at each of the particle locations using smoothing kernel.

• void acceleration (double *a, double *x, double *u, double *rP, int n, double b)

Calculates acceleration of each particle.

• void probeDensity (double *rr, double *x, int n, double *xx, int nxx)

Probe the density at specified locations.

• int main (int argc, char *argv[])

Main loop.

Variables

- double h sq
- double inv_h
- double inv_h_sq
- double inv h cb
- double inv_h_5
- double inv_h_7

5.12.1 Macro Definition Documentation

5.12.1.1 INV_SQRT_PI

```
#define INV_SQRT_PI 0.56418958354775627928
```

Constant equal to 1.0/sqrt(pi)

5.12.2 Function Documentation

5.12.2.1 acceleration()

Calculates acceleration of each particle.

Calculates acceleration of each particle due to quantum pressure, harmonic potential, and velocity damping.

Parameters

а	acceleration vector to be updated
X	positions of the particles
и	velocity vector
rP	relative pressure vector
n	number of particles
b	damping coefficient

5.12.2.2 kernel_0()

```
double kernel_0 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D).

This function returns the weight associated with the SPH Gaussian smoothing kernel.

Parameters

r	distance between particles
h	scaling length

Returns

weight

5.12.2.3 kernel_1()

```
\begin{array}{c} \mbox{double kernel\_1 (} \\ \mbox{double } r \mbox{)} \end{array}
```

SPH Gaussian smoothing kernel (1D), first derivative.

This function returns the weight associated with the first derivative of the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.12.2.4 kernel_2()

```
double kernel_2 ( \label{eq:double r } \mbox{double } r \mbox{ )}
```

SPH Gaussian smoothing kernel (1D), second derivative.

This function returns the weight associated with the second derivative of the SPH Gaussian smoothing kernel.

Parameters

r distance between particles

Returns

weight

5.12.2.5 main()

```
int main (
                int argc,
                 char * argv[] )
```

Main loop.

Evolve the time-dependant Schrödinger equation, and save the solution in "results.csv"

5.12.2.6 pressure()

Compute "relative pressure" at each of the particle locations using smoothing kernel.

Parameters

rF	pressure vector to be updated, rP = -(1/4)*(d^2 rho / dx^2 - (d rho / dx) 2 /rho)/(rho 2)	
X	positions of the particles	
n	number of particles	

5.12.2.7 probeDensity()

```
void probeDensity (
          double * rr,
          double * x,
          int n,
          double * xx,
          int nxx )
```

Probe the density at specified locations.

Parameters

rr	density at specified locations, vector to be updated
X	positions of the particles
n	number of particles
XX	probe locations
nxx	number of probe locations

5.12.3 Variable Documentation

5.12.3.1 h_sq

double h_sq

5.12.3.2 inv_h

double inv_h

5.12.3.3 inv_h_5

double inv_h_5

5.12.3.4 inv_h_7

double inv_h_7

5.12.3.5 inv_h_cb

double inv_h_cb

5.12.3.6 inv_h_sq

double inv_h_sq

5.13 README.md File Reference

Index

acceleration	quantumsph_Memorize.c, 27
quantumsph, 8	quantumsph_MPI.c, 32
quantumsph_Improved.c, 14	quantumsph_OMP_Initial.c, 39
quantumsph_Initial.c, 18	quantumsph_OMP_Memorize16.c, 45
quantumsph_Memorize.c, 22	quantumsph_OMP_Memorize32.c, 52
quantumsph_MPI.c, 29	quantumsph_OMP_Memorize64.c, 58
quantumsph_OMP_Initial.c, 35	quantumsph_OMP_NoMemory.c, 62
quantumsph_OMP_Memorize16.c, 41	inv_h_5
quantumsph_OMP_Memorize32.c, 47	quantumsph_Improved.c, 17
quantumsph_OMP_Memorize64.c, 54	quantumsph_Memorize.c, 27
quantumsph_OMP_NoMemory.c, 59	quantumsph_MPI.c, 32
arithmeticCost.c, 11	quantumsph_OMP_Initial.c, 39
main, 12	quantumsph_OMP_Memorize16.c, 45
N, 11	quantumsph_OMP_Memorize32.c, 52
00\/D	quantumsph_OMP_Memorize64.c, 58
CSVReader, 7	quantumsph_OMP_NoMemory.c, 62
read_and_plot, 7	inv_h_7
CSVReader.py, 12	quantumsph_Improved.c, 17
density	quantumsph_Memorize.c, 27
quantumsph, 8	quantumsph MPI.c, 32
quantumsph_Initial.c, 19	quantumsph_OMP_Initial.c, 39
quantumsph_Memorize.c, 23	quantumsph_OMP_Memorize16.c, 46
quantamopn_moments.o, 20	quantumsph_OMP_Memorize32.c, 52
FreeMatrix	quantumsph_OMP_Memorize64.c, 58
quantumsph_Memorize.c, 23	quantumsph_OMP_NoMemory.c, 62
quantumsph_MPI.c, 29	inv_h_cb
quantumsph_OMP_Initial.c, 36	quantumsph_Improved.c, 17
quantumsph_OMP_Memorize16.c, 42	quantumsph_Memorize.c, 27
quantumsph_OMP_Memorize32.c, 48	quantumsph_MPI.c, 33
quantumsph_OMP_Memorize64.c, 54	quantumsph_OMP_Initial.c, 39
	quantumsph_OMP_Memorize16.c, 46
h_sq	quantumsph_OMP_Memorize32.c, 52
quantumsph_Improved.c, 16	quantumsph_OMP_Memorize64.c, 58
quantumsph_Memorize.c, 26	quantumsph_OMP_NoMemory.c, 63
quantumsph_MPI.c, 32	inv_h_sq
quantumsph_OMP_Initial.c, 39	quantumsph Improved.c, 17
quantumsph_OMP_Memorize16.c, 45	quantumsph_Memorize.c, 27
quantumsph_OMP_Memorize32.c, 51	quantumsph_MPI.c, 33
quantumsph_OMP_Memorize64.c, 57	quantumsph_OMP_Initial.c, 40
quantumsph_OMP_NoMemory.c, 62	quantumsph_OMP_Memorize16.c, 46
InitializeMatrix	quantumsph_OMP_Memorize32.c, 52
quantumsph_Memorize.c, 23	quantumsph_OMP_Memorize64.c, 58
quantumsph_MPI.c, 29	quantumsph_OMP_NoMemory.c, 63
quantumsph OMP Initial.c, 36	INV SQRT PI
quantumsph_OMP_Memorize16.c, 42	quantumsph_Improved.c, 14
quantumsph_OMP_Memorize32.c, 48	quantumsph_Memorize.c, 22
quantumsph OMP Memorize64.c, 54	quantumsph_MPI.c, 28
inv h	quantumsph_OMP_Initial.c, 35
quantumsph_Improved.c, 17	quantumsph_OMP_Memorize16.c, 41
quantumoph_mproved.c, 17	quantumspri_Own _wemonze10.6, 41

66 INDEX

quantumsph_OMP_Memorize32.c, 47 quantumsph_OMP_Memorize64.c, 53	quantumsph_MPI.c, 33 n_loc
quantumsph_OMP_NoMemory.c, 59	quantumsph_MPI.c, 33
kornal	PI
kernel quantumsph, 8	quantumsph_Initial.c, 18
quantumsph_Initial.c, 19	pressure
kernel 0	quantumsph, 9
quantumsph_Improved.c, 14	quantumsph_Improved.c, 16
quantumsph_Memorize.c, 24	quantumsph_Initial.c, 20
quantumsph MPI.c, 30	quantumsph_Memorize.c, 25
quantumsph_OMP_Initial.c, 36	quantumsph_OMP_NoMemory.c, 61
quantumsph_OMP_Memorize16.c, 42	probeDensity
quantumsph_OMP_Memorize32.c, 49	quantumsph, 9
quantumsph_OMP_Memorize64.c, 55	quantumsph_Improved.c, 16
quantumsph_OMP_NoMemory.c, 60	quantumsph_Initial.c, 20
kernel_0_mat	quantumsph_Memorize.c, 26
quantumsph_Memorize.c, 24	quantumsph_MPI.c, 31
quantumsph_OMP_Initial.c, 37	quantumsph_OMP_Initial.c, 38
quantumsph_OMP_Memorize16.c, 43	quantumsph OMP Memorize16.c, 44
quantumsph_OMP_Memorize32.c, 49	quantumsph_OMP_Memorize32.c, 50
quantumsph_OMP_Memorize64.c, 55	quantumsph_OMP_Memorize64.c, 56
kernel 1	quantumsph_OMP_NoMemory.c, 62
quantumsph_Improved.c, 15	quantumoph_own _nowemory.o, oz
quantumsph_MPI.c, 30	quantumsph, 7
quantumsph_OMP_NoMemory.c, 60	acceleration, 8
kernel_1_mat	density, 8
quantumsph_Memorize.c, 25	kernel, 8
quantumsph_OMP_Initial.c, 37	main, 9
quantumsph_OMP_Memorize16.c, 43	pressure, 9
quantumsph_OMP_Memorize32.c, 50	probeDensity, 9
quantumsph_OMP_Memorize64.c, 56	quantumsph.py, 12
kernel 2	quantumsph_Improved.c, 13
quantumsph_Improved.c, 15	acceleration, 14
quantumsph_MPI.c, 31	h sq, 16
quantumsph_OMP_NoMemory.c, 61	inv_h, 17
kernel_2_mat	inv_h_5, 17
quantumsph_Memorize.c, 25	inv_h_7, 17
quantumsph_Memorize.c, 25 quantumsph_OMP_Initial.c, 37	inv_h_cb, 17
quantumsph_OMP_Memorize16.c, 44	inv h sq, 17
quantumsph_OMP_Memorize32.c, 50	INV_SQRT_PI, 14
quantumsph_OMP_Memorize64.c, 56	kernel_0, 14
quantumspri_Own _wemonzeo4.c, 30	kernel 1, 15
main	kernel 2, 15
arithmeticCost.c, 12	main, 15
quantumsph, 9	pressure, 16
quantumsph_Improved.c, 15	probeDensity, 16
quantumsph_Initial.c, 20	quantumsph_Initial.c, 17
quantumsph_Memorize.c, 25	acceleration, 18
quantumsph_MPI.c, 31	density, 19
quantumsph_OMP_Initial.c, 38	kernel, 19
quantumsph_OMP_Memorize16.c, 44	main, 20
quantumsph_OMP_Memorize32.c, 50	PI, 18
quantumsph_OMP_Memorize64.c, 56	pressure, 20
quantumsph_OMP_NoMemory.c, 61	probeDensity, 20
	quantumsph_Memorize.c, 21
N	acceleration, 22
arithmeticCost.c, 11	density, 23
n	FreeMatrix, 23

INDEX 67

h_sq, 26	h_sq, 45
InitializeMatrix, 23	InitializeMatrix, 42
inv_h, 27	inv_h, 45
inv_h_5, 27	inv_h_5, 45
inv_h_7, 27	inv_h_7, 46
inv_h_cb, 27	inv_h_cb, 46
inv_h_sq, 27	inv_h_sq, 46
INV_SQRT_PI, 22	INV_SQRT_PI, 41
kernel 0, 24	kernel_0, 42
kernel_0_mat, 24	kernel_0_mat, 43
kernel_1_mat, 25	kernel_1_mat, 43
kernel_2_mat, 25	kernel 2 mat, 44
main, 25	main, 44
pressure, 25	probeDensity, 44
probeDensity, 26	relativePressure, 45
quantumsph_MPI.c, 27	quantumsph_OMP_Memorize32.c, 46
acceleration, 29	. – –
	acceleration, 47
FreeMatrix, 29	FreeMatrix, 48
h_sq, 32	h_sq, 51
InitializeMatrix, 29	InitializeMatrix, 48
inv_h, 32	inv_h, 52
inv_h_5, 32	inv_h_5, 52
inv_h_7, 32	inv_h_7, 52
inv_h_cb, 33	inv_h_cb, 52
inv_h_sq, 33	inv_h_sq, 52
INV_SQRT_PI, 28	INV_SQRT_PI, 47
kernel_0, 30	kernel_0, 49
kernel_1, 30	kernel_0_mat, 49
kernel_2, 31	kernel_1_mat, 50
main, 31	kernel_2_mat, 50
n, 33	main, 50
n_loc, <mark>33</mark>	probeDensity, 50
probeDensity, 31	relativePressure, 51
rank, 33	quantumsph_OMP_Memorize64.c, 52
relativePressure, 32	acceleration, 54
rem, 33	FreeMatrix, 54
size, 33	h_sq, 57
quantumsph_OMP_Initial.c, 34	InitializeMatrix, 54
acceleration, 35	inv_h, 58
FreeMatrix, 36	inv_h_5, <mark>58</mark>
h_sq, 39	inv_h_7, <mark>58</mark>
InitializeMatrix, 36	inv_h_cb, 58
inv_h, 39	inv_h_sq, 58
inv_h_5, 39	INV SQRT PI, 53
inv_h_7, 39	kernel_0, 55
inv_h_cb, 39	kernel_0_mat, 55
inv_h_sq, 40	kernel_1_mat, 56
INV_SQRT_PI, 35	kernel_2_mat, 56
kernel_0, 36	main, 56
kernel_0_mat, 37	probeDensity, 56
kernel_1_mat, 37	relativePressure, 57
kernel_2_mat, 37	quantumsph_OMP_NoMemory.c, 58
main, 38	acceleration, 59
probeDensity, 38	h_sq, 62
relativePressure, 38	inv_h, 62
quantumsph_OMP_Memorize16.c, 40	inv_h_5, 62
acceleration, 41	inv_h_7, 62
FreeMatrix, 42	inv_h_cb, 63
i iddividuit, 72	111V_11_60, 00

68 INDEX

```
inv_h_sq, 63
    INV_SQRT_PI, 59
    kernel_0, 60
    kernel_1, 60
    kernel_2, 61
    main, 61
    pressure, 61
    probeDensity, 62
rank
    quantumsph_MPI.c, 33
read_and_plot
    CSVReader, 7
README.md, 63
relativePressure
    quantumsph_MPI.c, 32
    quantumsph_OMP_Initial.c, 38
    quantumsph_OMP_Memorize16.c, 45
    quantumsph_OMP_Memorize32.c, 51
    quantumsph_OMP_Memorize64.c, 57
rem
    quantumsph_MPI.c, 33
size
    quantumsph_MPI.c, 33
```