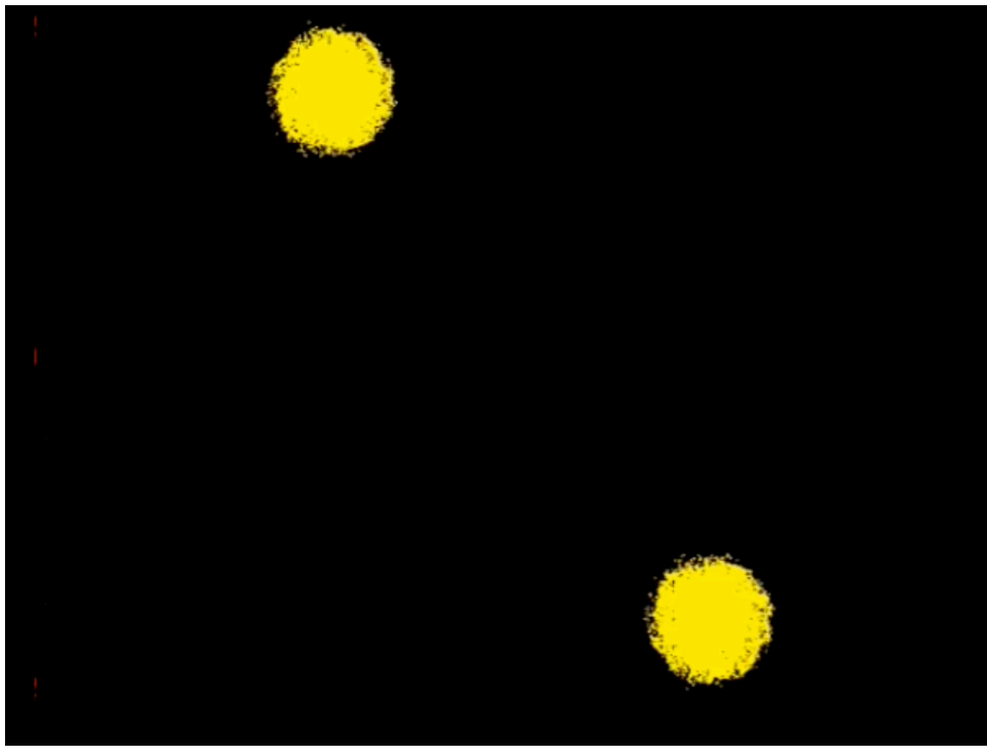
NagBody lectures: Introduction to numerical computation

Mario Alberto Rodríguez-Meza

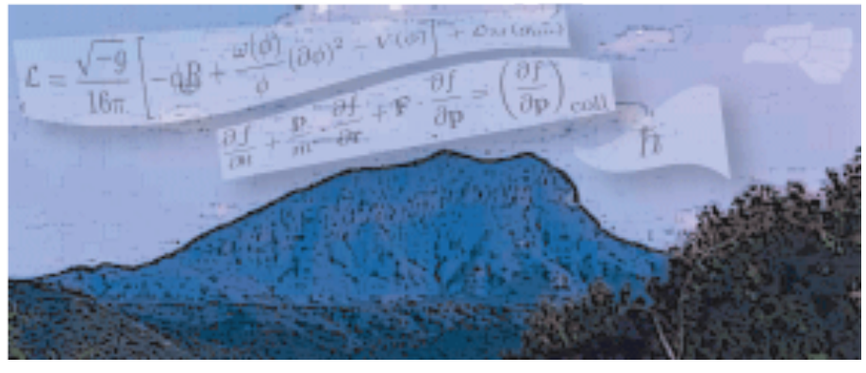
Instituto Nacional de Investigaciones Nucleares

Correo Electrónico: marioalberto.rodriguez@inin.gob.mx

http://bitbucket.org/rodriguezmeza



Seminario de investigación,
Departamento de Física,
Universidad de Guanajuato
3 de febrero al XX de junio de 2022
Sesiones virtuales (Zoom, Meet, etcétera)



References and material

- Cosmología numérica y estadística: NagBody kit (http://bitbucket.org/rodriguezmeza). Mario A. Rodríguez-Meza.

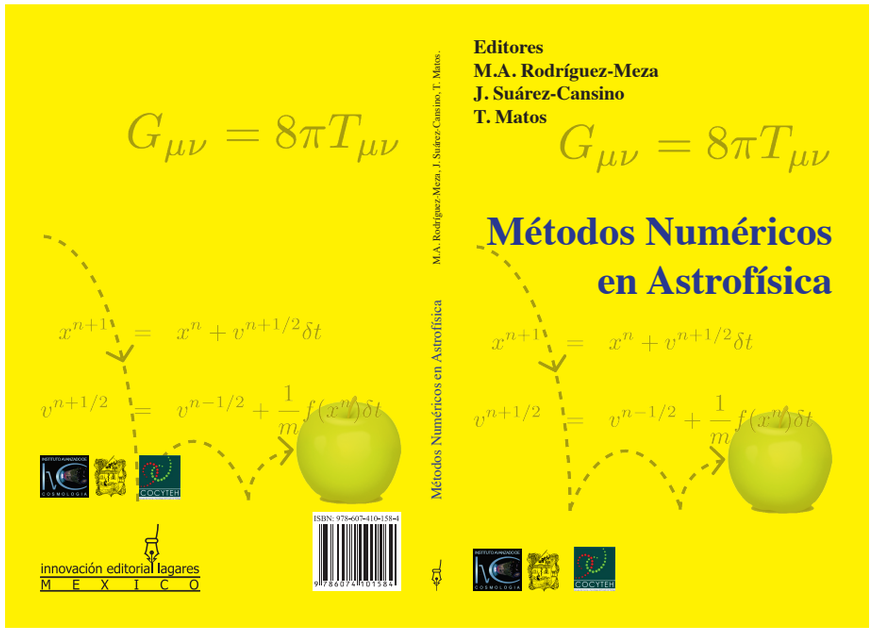
- Métodos numéricos en astrofísica, capítulo 1, Método de N-cuerpos en astrofísica. (https://www.researchgate.net/publication/316582859_Metodo_de_N-Cuerpos_en_Astrofisica)

- La estructura a gran escala del universo. Capítulo 22 en Travesuras cosmológicas de Einstein et al. https://www.researchgate.net/publication/316582400_La_estructura_a_gran_escala_del_universo_simulaciones_numericas

- https://www.researchgate.net/profile/Mario_Rodriguez-Meza

- https://www.researchgate.net/publication/314281416_Los_agujeros_negros_y_las_ondas_del_Dr_Einstein

- M.A. Rodriguez-Meza, Adv. Astron. 2012, 509682 (2012). arXiv: 1112.5201. (https://www.researchgate.net/publication/51967093_A_Scalar_Field_Dark_Matter_Model_and_Its_Role_in_the_Large-Scale_Structure_Formation_in_the_Universe)



Content: Introduction to numerical computation

- Basic algorithmic concepts
- Variables and constants
- Flow diagram

Algorithm concept

What is an algorithm?

Computer program

What is a computer program?

The three guys

Who are involved in an algorithm?

- The programer
- The one who execute the program
- The user

The three main stages

What are the three main stages in creating an algorithm?

The reserved words

What are the reserved word in the computer languages?

Errors in programming

What are the errors in the computer languages?

- Syntax errors
- Logic errors
- Runtime errors

Debugging in programming

How to debug a numerical code?

Variables in programming

- What is a variable (and pointer concept). Types. Naming
- Declaring a variable

Commenting a code

How to comment a numerical code?

```
63  /*
64   * MAIN: toplevel routine for hierarchical N-body code.
65   */
66
67  int main(int argc, string argv[])
68  {
69    initparam(argv, defv);            /* initialize param access  */
70    headline = defv[0] + 1;           /* use default headline     */
71    startrun();                     /* get params & input data  */
72    startoutput();                  /* activate output code     */
73    if (nstep == 0) {               /* if data just initialized */
74      treeforce();                  /* calculate initial forces */
75      output();                     /* generate initial output  */
76    }
77    if (dtime != 0.0)               /* if time steps requested  */
78      while (tstop - tnow > 0.01 * dtime) {   /* while not past tstop     */
79        stepsystem();               /* advance step by step     */
80        output();                   /* output results each time */
81      }
82    return (0);                     /* end with proper status   */
83  }
```

Commenting a code

How to comment a numerical code?

```
214 /*
215  * STEPSYSTEM: advance N-body system using simple leap-frog.
216  */
217
218 local void stepsystem(void)
219 {
220   bodyptr p1, p2, p;
221
222   p1 = bodytab + MAX(nstatic, 0);       /* set dynamic body range   */
223   p2 = bodytab + nbody + MIN(nstatic, 0);
224   for (p = p1; p < p2; p++) {           /* loop over body range     */
225     ADDMULVS(Vel(p), Acc(p), 0.5 * dtime);  /* advance v by 1/2 step    */
226     ADDMULVS(Pos(p), Vel(p), dtime);        /* advance r by 1 step      */
227   }
228   treeforce();
229   for (p = p1; p < p2; p++) {           /* loop over body range     */
230     ADDMULVS(Vel(p), Acc(p), 0.5 * dtime);  /* advance v by 1/2 step    */
231   }
232   nstep++;                  /* count another time step  */
233   tnow = tnow + dtime;              /* finally, advance time    */
234 }
```


Commenting a code

How to comment a numerical code?

```
22
23  /* Output state variables. */
24
25  local bool forcehead;               /* force headers printed?   */
26  local real mtot;                        /* total mass of system     */
27  local real etot[3];             /* Etot, KE, PE of system   */
28  local matrix keten;             /* kinetic energy tensor    */
29  local matrix peten;             /* potential energy tensor  */
30  local vector cmpos;             /* center of mass position  */
31  local vector cmvel;             /* center of mass velocity  */
32  local vector amvec;             /* angular momentum vector  */
33
```


Commenting a code

How to comment a numerical code?

```
280  /* <A NAME="hackquad"></A>
281   * HACKQUAD: descend tree, evaluating quadrupole moments.  Note that this
282   * routine is coded so that the Subp() and Quad() components of a cell can
283   * share the same memory locations.
284   */
285
286  local void hackquad(cellptr p)
287  {
288    int ndesc, i;
289    nodeptr desc[NSUB], q;
290    vector dr;
291    real drsq;
292    matrix drdr, Idrsq, tmpm;
293
294    ndesc = 0;                          /* count occupied subnodes  */
295    for (i = 0; i < NSUB; i++)          /* loop over all subnodes   */
296      if (Subp(p)[i] != NULL)           /* if this one's occupied   */
297        desc[ndesc++] = Subp(p)[i];     /* copy it to safety        */
298    CLRM(Quad(p));                      /* init quadrupole moment   */
299    for (i = 0; i < ndesc; i++) {       /* loop over real subnodes  */
300      q = desc[i];                      /* access ech one in turn   */
301      if (Type(q) == CELL)              /* if it's also a cell      */
302        hackquad((cellptr) q);          /* then process it first    */
303      SUBV(dr, Pos(q), Pos(p));         /* find displacement vect.  */
304      OUTVP(drdr, dr, dr);              /* form outer prod. of dr   */
305      DOTVP(drsq, dr, dr);              /* and dot prod. dr * dr    */
306      SETMI(Idrsq);                     /* init unit matrix     */
307      MULMS(Idrsq, Idrsq, drsq);        /* and scale by dr * dr     */
308      MULMS(tmpm, drdr, 3.0);           /* scale drdr by 3      */
309      SUBM(tmpm, tmpm, Idrsq);          /* now form quad. moment    */
310      MULMS(tmpm, tmpm, Mass(q));       /* from cm of subnode       */
311      if (Type(q) == CELL)              /* if subnode is cell       */
312        ADDM(tmpm, tmpm, Quad(q));      /* then include its moment  */
313      ADDM(Quad(p), Quad(p), tmpm);     /* increment moment of cell */
314    }
315  }
```


Flow diagram

- main.c
  - mainloop.c

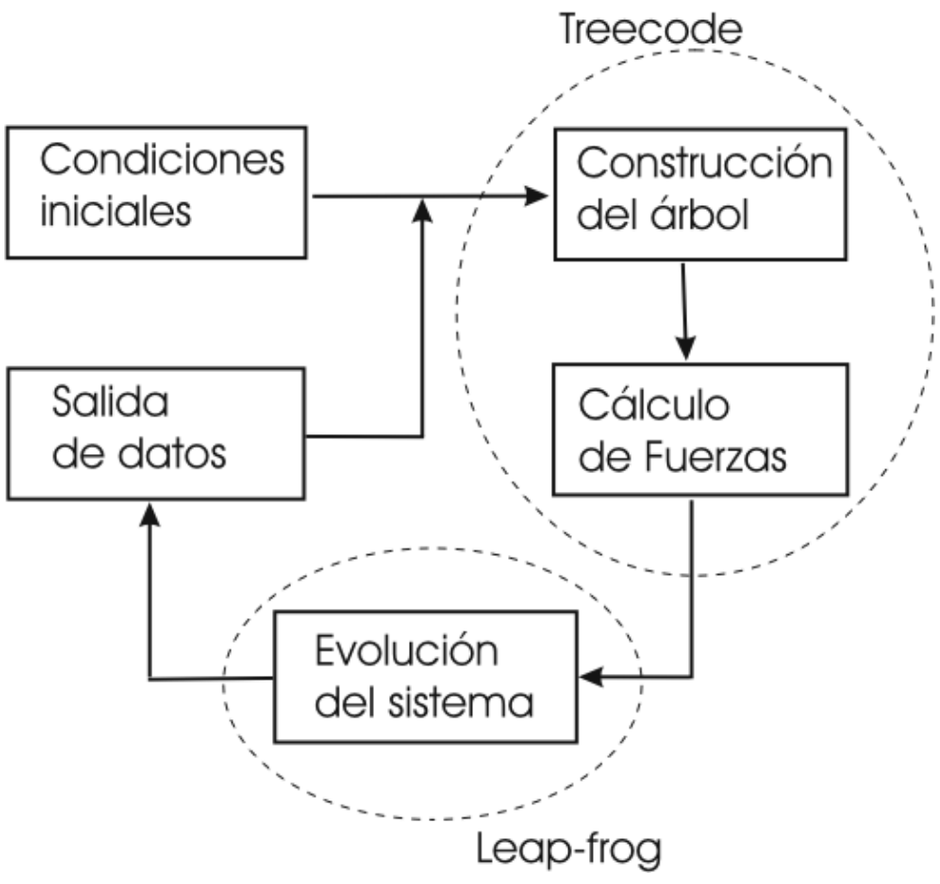
- cmdline_defs.h
- data_structure.h
- globaldefs.h
- protodefs.h

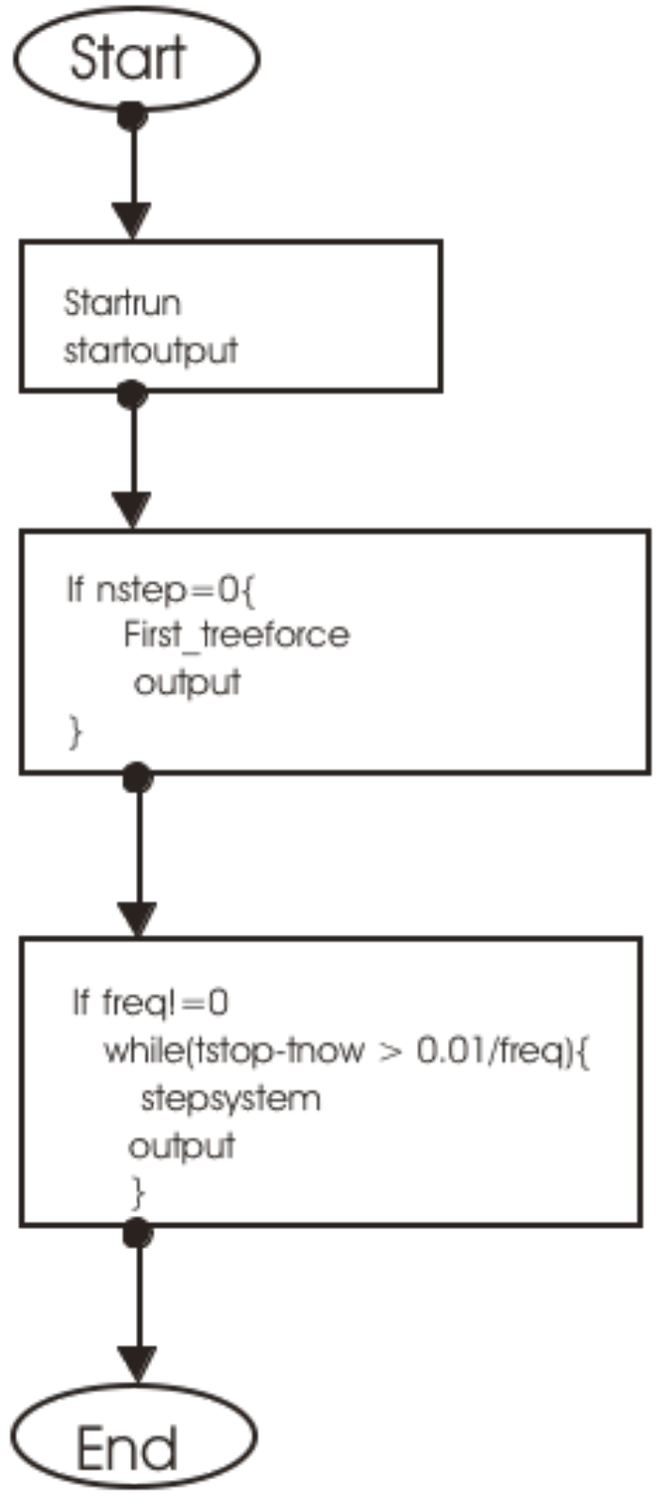
- template.c
- template_io.c
- startrun.c

- models.c
- models.h

- Data structures
- Routines and functions

Flow diagram



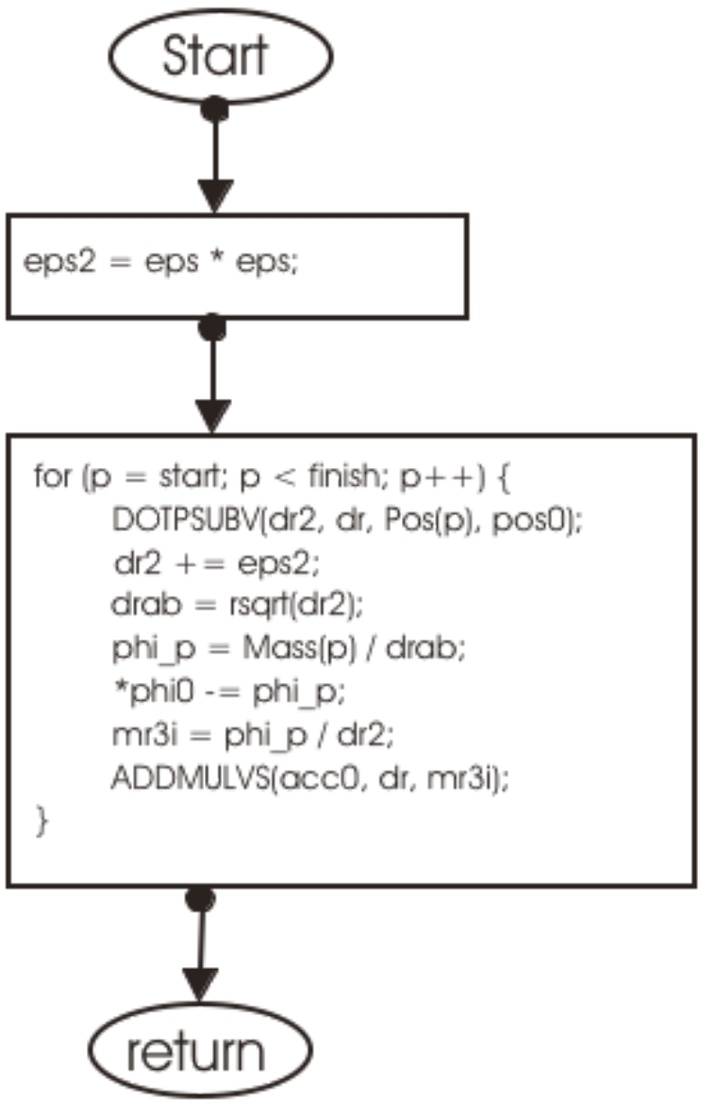


Flow diagram

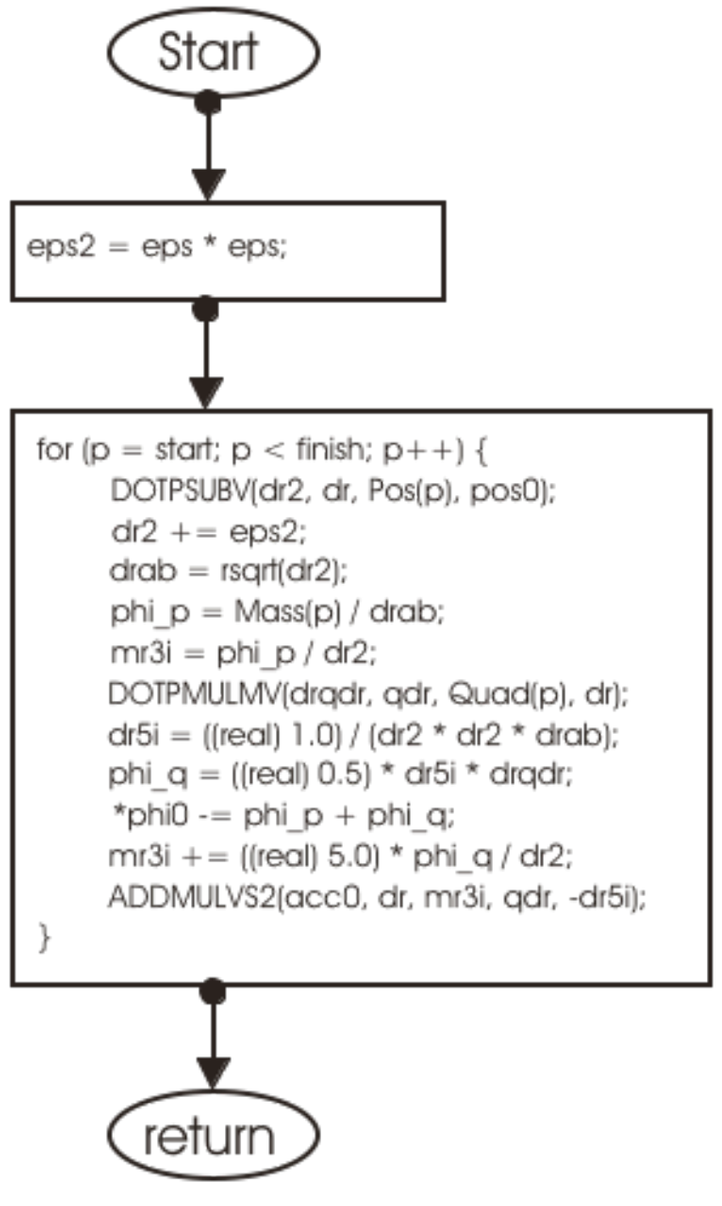
$$\psi(\mathbf{r}) = \frac{m}{r} + \frac{1}{2}\sum_{i,j} Q_{ij}\frac{x_i x_j}{r^5} + \ldots$$

Sum nodes and cells

local void sumnode(cellptr start, cellptr finish,
vector pos0, real *phi0, vector acc0)



local void sumcell(cellptr start, cellptr finish,
vector pos0, real *phi0, vector acc0)



Conclusions: Introduction to numerical computation

We have seen:

- What is an algorithm
- What is a computer program
- The three guys involved in an algorithm
- The three main stages involved in creating an algorithm
- Reserved words
- Syntax error, logic error and runtime error
- Debbuging
- Commenting a numerical code

Conclusions: Introduction to numerical computation

We have also seen:

- What is a variable (and pointer concept). Types. Naming
- Declaring a variable
- Flow diagrams

References and material

- Cosmología numérica y estadística: NagBody kit (http://bitbucket.org/rodriguezmeza). Mario A. Rodríguez-Meza.

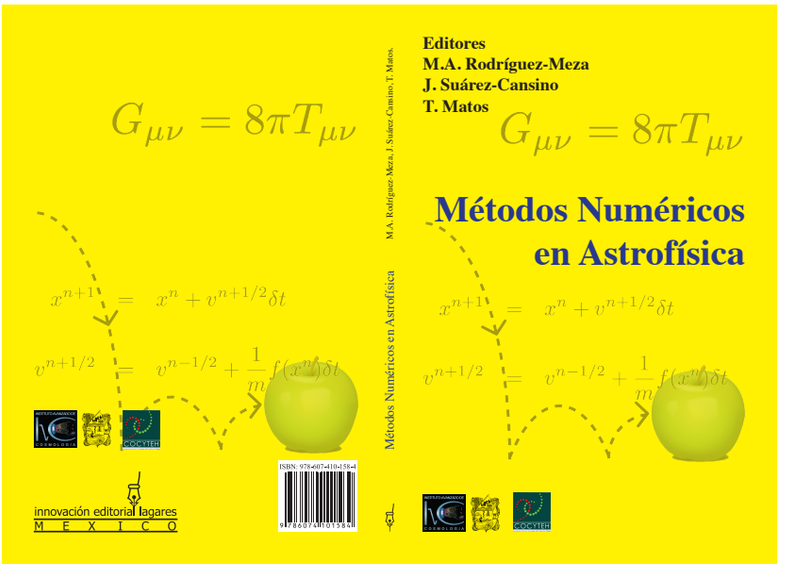
- Métodos numéricos en astrofísica, capítulo 1, Método de N-cuerpos en astrofísica. (https://www.researchgate.net/publication/316582859_Metodo_de_N-Cuerpos_en_Astrofisica)

- La estructura a gran escala del universo. Capítulo 22 en Travesuras cosmológicas de Einstein et al. https://www.researchgate.net/publication/316582400_La_estructura_a_gran_escala_del_universo_simulaciones_numericas

- https://www.researchgate.net/profile/Mario_Rodriguez-Meza

- https://www.researchgate.net/publication/314281416_Los_agujeros_negros_y_las_ondas_del_Dr_Einstein

- M.A. Rodriguez-Meza, Adv. Astron. 2012, 509682 (2012). arXiv: 1112.5201. (https://www.researchgate.net/publication/51967093_A_Scalar_Field_Dark_Matter_Model_and_Its_Role_in_the_Large-Scale_Structure_Formation_in_the_Universe)



See you!