iSALE基本操作

1. Input file(asteroid.inp)の読み方

2. Input file(material.inp)の読み方

黒澤 耕介
千葉工業大学 惑星探査研究センター 研究員

第3回iSALE講習会 於 国立天文台　2018 8/6

asteroid.inp & material.inp

iSALEの実行ファイルに食べさせる2つの入力ファイル

asteroid.inp (数値計算条件の設定)

- 座標系 (デカルト or 円柱座標)の選択.
- 計算領域, 格子サイズの設定.
- 計算時間, ファイル書き出し間隔設定.
- グローバル変数(重力加速度, 地表面温度など)の設定
- 衝突天体の設定(形状, サイズ, 速度, 温度構造)
- 標的天体の設定(形状, サイズ, 層数, 温度構造)
- 書き出し物理量選択
- トレーサ粒子設定

などなど

asteroid.inp & material.inp

iSALEの実行ファイルに食べさせる2つの入力ファイル

material.inp (物質モデルの設定)

- EOS(Tillotson or ANEOS)の選択
- 強度モデルの選択
  - -強度モデルの入力パラメータ(降伏応力など…)
- 空隙モデル(ε–α model)の設定

などなど…

困ったら....

1. iSALE-Manual: https://figshare.com/articles/iSALE-Dellen_manual/3473690

iSALE:
A multi-material, multi-rheology shock physics code for simulating impact phenomena in two and three dimensions.

Gareth S. Collins, Dirk Elbeshausen, Kai Wünnemann, Thomas M. Davison, Boris Ivanov, H. Jay Melosh

iSALE-Dellen release, July 8, 2016

2. parameters.db:各サンプルプログラムと同じフォルダ

```
<PARAM>
ABBREV : GRAD_TYPE : STR
DESC : Lithostatic gradient
<INFO>
Several different options are available to pre-compress the target/planet
as a consequence of the ambient gravitational field...

\begin{description}
\item[NONE] -- No gravity field; constant initial material properties

\item[DEFAULT] -- Spatially and temporally constant gravity field; initial material
            properties change with depth in target.

\item[CENTRAL] -- Spatially varying gravity field, but constant in time. For
            use in S\_TYPE == PLANET mode. Initial material properties change
            with distance from planet centre.

\item[SELF] -- Spatially and temporally varying gravity field, calculated
            from mutual gravitational attraction of all mass in domain.
            Initial material properties change according to gravity field.
            (Not currently available in iSALE-3D).
\end{description}
</INFO>
<CODE>
DIM : 2
OPTIONAL : YES
DEFVAL : DEFAULT
VALUES : DEFAULT : NONE : CENTRAL : SELF
</CODE>
```

変数名で検索すれば
丁寧な説明が書いてある.

asteroid.inpの読み方1

./examples/demo2D

```
#ISINP
-----------------------------------------------------------------------
--- this is the new input file used by iSALE versions of v7.0 and higher
-----------------------------------------------------------------------
--- lines beginning with '-' or '!' are treated as comments and not
--- further processed. The difference between the two comment lines
--- is, lines starting with '-' will appear also in the backup of this
--- input file and in the header of the jpeg-file, whereas lines
--- beginning with '!' are completely removed from these files.
-----------------------------------------------------------------------
--- First 8 columns are reserved for short parameter identification  ---
--- (available abbreviations are found in the documentation)         ---
---                                                                  ---
--- The next 20 columns are reserved for parameter description!      ---
---                                                                  ---
------------------- General Model Info ---------------------------------
VERSION                 __DO NOT MODIFY__              : 4.1
DIMENSION               dimension of input file        : 2
PATH                    Data file path                 : ./
MODEL                   Modelname                      : demo2D
```

asteroid.inpの読み方1

./examples/demo2D

```
#ISINP
-----------------------------------------------------------------------
--- this is the new inp                                  ions of v7.0 and higher
-----------------------------------------------------------------------
--- lines beginning with '-' or '!' are treated as comments and not
--- further processed. The difference between the two comment lines
--- is, lines starting with '-' will appear also in the backup of this
--- input file and in the header of the jpeg-file, whereas lines
--- beginning with '!' are completely removed from these files.
-----------------------------------------------------------------------
--- First 8 columns are reserved for short parameter identification  ---
--- (available abbreviations are found in the documentation)         ---
---                                                                  ---
--- The next 20 columns are reserved for parameter description!      ---
---                                                                  ---
------------------- General Model Info ---------------------------------
VERSION                 __DO NOT MODIFY__              : 4.1
DIMENSION               dimension of input file        : 2
PATH                    Data file path                 : ./
MODEL                   Modelname                      : demo2D
```

コメントアウトの方法

asteroid.inpの読み方1

./examples/demo2D

```
#ISINP
-----------------------------------------------------------------------
--- this is the new input file used by iSALE versions of v7.0 and higher
-----------------------------------------------------------------------
--- lines beginning with '-' or '!' are treated as comments and not
--- further processed. The difference between the two comment lines
--- is, lines starting with '-' will appear also in the backup of this
--- input file and in the header of the jpeg-file, whereas lines
--- beginning with '!' are completely removed from these files.
-----------------------------------------------------------------------
--- First 8 columns are reserved for short parameter identification  ---
--- (available abbreviations are found in the documentation)         ---
---                                                                  ---
--- The next 20 columns are reserved for parameter description!      ---
---                                                                  ---
------------------- General Model Info ---------------------------------
```

計算データが格納されるディレクトリのパスと名前の指定

```
PATH                    Data file path                  : ./
MODEL                   Modelname                       : demo2D
```

asteroid.inpの読み方2

計算格子設定

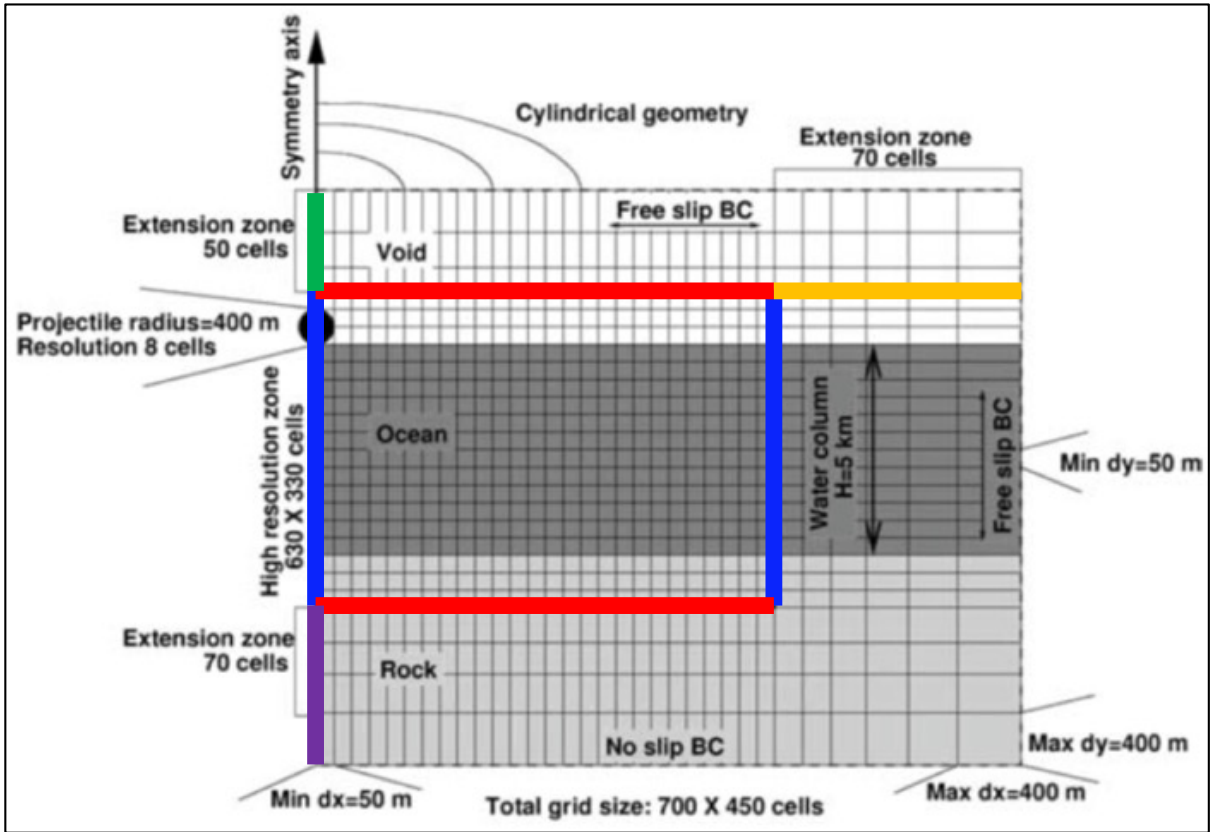
```
------------------- Mesh Geometry Parameters -----------------------
GRIDH          horizontal cells     : 0        : 80       : 32
GRIDV          vertical cells       : 35       : 90       : 15

GRIDEXT        ext. factor          : 1.03d0
GRIDSPC        grid spacing         : 100.D0
GRIDSPCM       max. grid spacing    : -20.D0
```

asteroid.inpの読み方2

計算格子設定

計算領域(確保する格子)の指定

GRIDH	horizontal cells	: 0	: 80	: 32
GRIDV	vertical cells	: 35	: 90	: 15



High-resolution zone
は真ん中

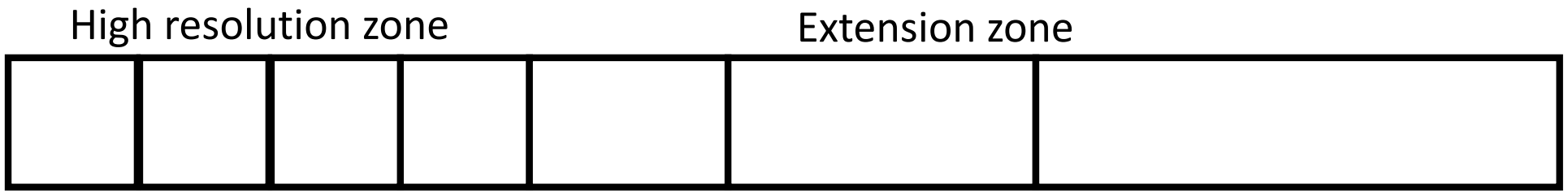
※円柱座標系では動径方向セルの
内側方向のExtension zoneは
設定できない. -> 常に0

asteroid.inpの読み方2

計算格子設定

GRIDEXT	ext. factor	: 1.03d0
GRIDSPC	grid spacing	: 100.D0 1 gridの実空間での距離
GRIDSPCM	max. grid spacing	: -20.D0

CRIDEXTとGRIDSPCMはExtension cellのサイズを指定.



Extension zoneのCell sizeは

・公比GRIDEXTの等比数列.

・ただし, 上限Cell sizeはGRIDSPCM

GRIDSPCMの値の前に"マイナス"を付けると,自動的にGRIDSPCで規格化したCell sizeに設定.

asteroid.inpの読み方3

```
------------------- Global Setup Parameters -------------
S_TYPE          setup type              : DEFAULT
ALE_MODE        ALE modus               : EULER
T_SURF          Surface temp            : 293.D0
DTDZSURF        Temp. grad. surf.       : 10.D-3
D_LITH          Lithosp. thickness      : 80.D3
R_PLANET        Planet radius           : 6370.D0
GRAV_V          gravity                 : -9.81D0
GRAD_TYPE       gradient type           : DEFAULT
GRAD_DIM        gradient dimension      : 2
```

asteroid.inpの読み方3

```
------------------- Global Setup Parameters -------------
S_TYPE                setup type                    : DEFAULT
```

計算目的によって使いわける.

VALUES : DEFAULT : PLANET : LANDSLIDE : MESO_PORE
: MESO_PART : MESO_BMP : DEFORM
: ROTATE : SHEARFLOW

例. 自己重力入りの計算を行いたいときはPLANETを選択.

今日の講習は「DEFAULT」を使います.

asteroid.inpの読み方3

T_SURF	Surface temp	: 293.D0
DTDZSURF	Temp. grad. surf.	: 10.D-3
D_LITH	Lithosp. thickness	: 80.D3
R_PLANET	Planet radius	: 6370.D0

衝突天体と標的の地表面温度,温度構造を決めるパラメータ.

VALUES : CONST : COND : CONDCONV : CONDCONVCAP : USER

一様温度の場合, 必要なのはT_SURFのみ.

asteroid.inpの読み方3

GRAV_V　　gravity　　: -9.81D0

重力加速度(m/s^2)

GRAD_TYPE　　gradient type　　: DEFAULT

VALUES : DEFAULT : NONE : CENTRAL : SELF

時空間一定　　時間一定　　自己重力

GRAD_DIM　　gradient dimension　　: 2

GRAD_DIM = 0 - No gradient calculated.
GRAD_DIM = 1 - One-dimensional gradient in the target (vertical direction only)
GRAD_DIM = 2 - Two-dimensional gradient in the target (vertical and X-direction only)
GRAD_DIM = 3 - Three-dimensional gradient in the target (all directions)

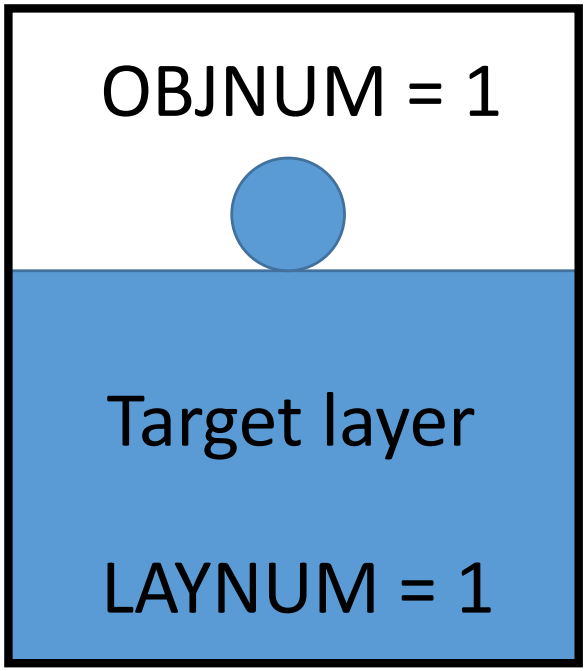
asteroid.inpの読み方4

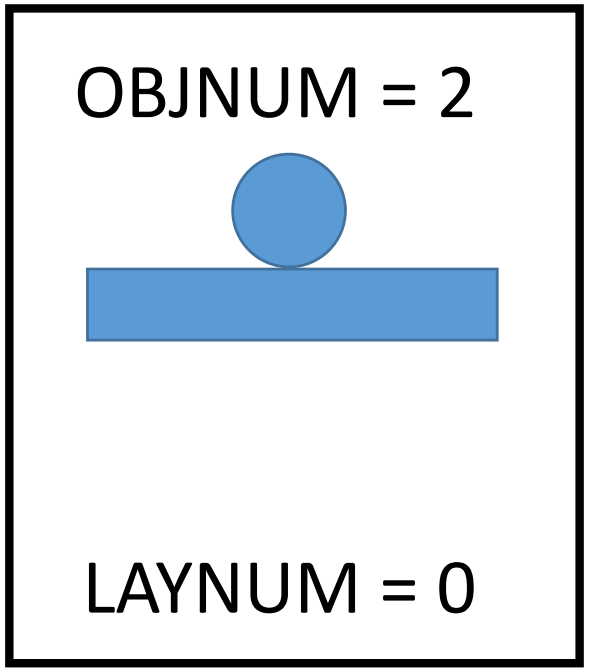
```
-------------------- Projectile Parameters ------------
OBJNUM    number of proj.        : 1
OBJRESH   CPPR horizontal        : 8
OBJVEL    object velocity        : -6.5D3
OBJMAT    object material        : mygrani
OBJTYPE   object type            : SPHEROID
OBJTPROF  object temp prof       : CONST
```

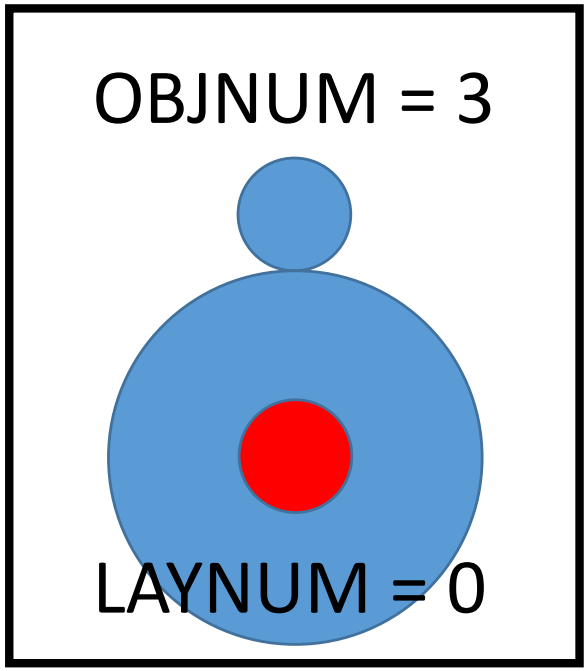
asteroid.inpの読み方4

```
------------Projectile Parameters -------------------
OBJNUM                number of proj.          : 1
```

“Projectile”の数







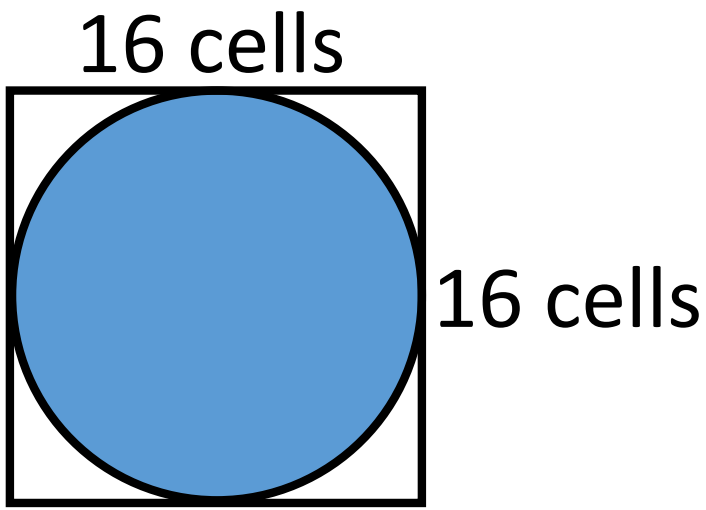
asteroid.inpの読み方4

OBJRESH	CPPR horizontal	: 8

CPPR: Cells Per Projectile Radius

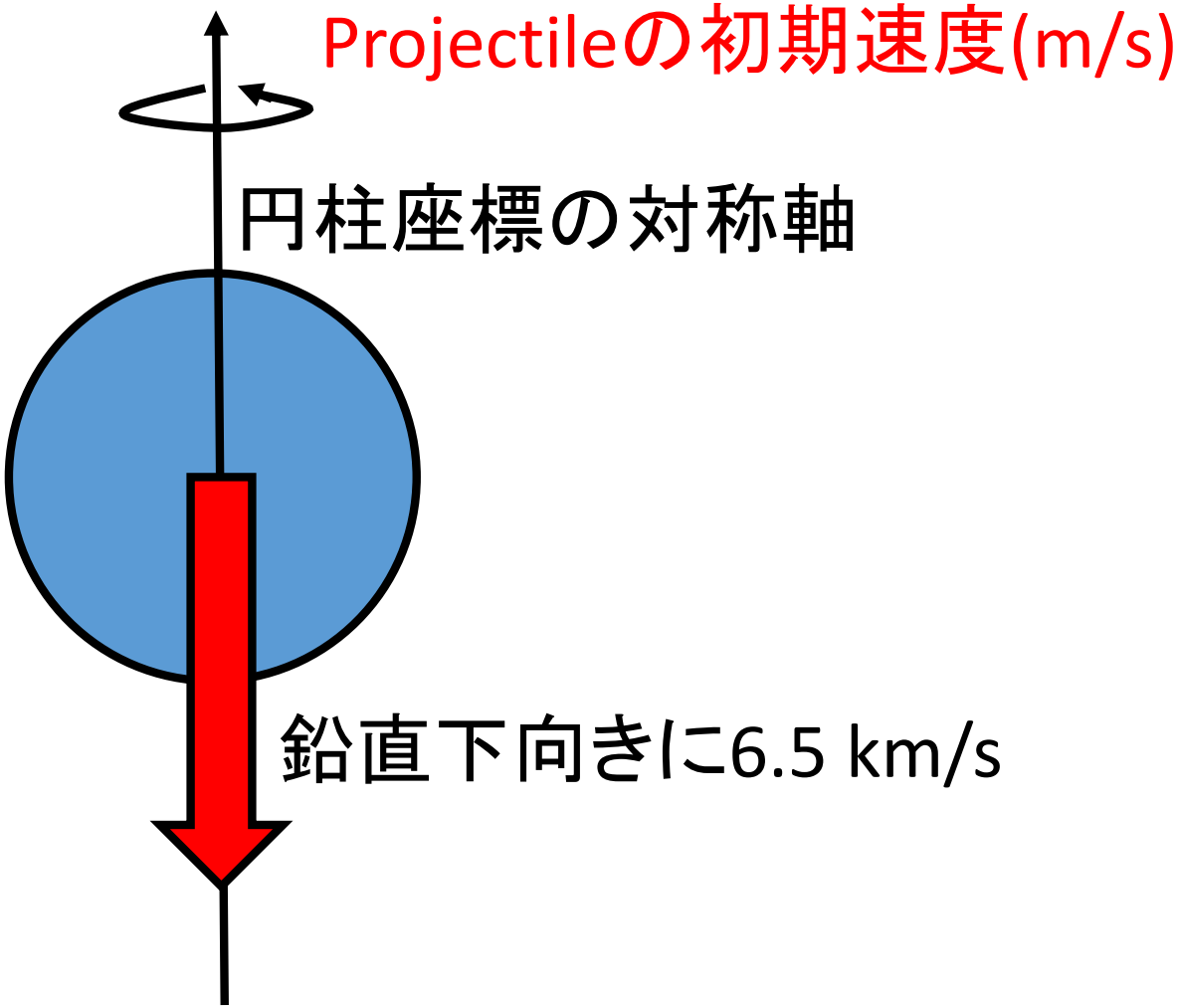
Projectileを何cellで分割するか

Ex. OBJRESH = 8
半径を8 cellで表現



asteroid.inpの読み方4

OBJVEL	object velocity	: -6.5D3



asteroid.inpの読み方4

OBJMAT	object material	: mygrani

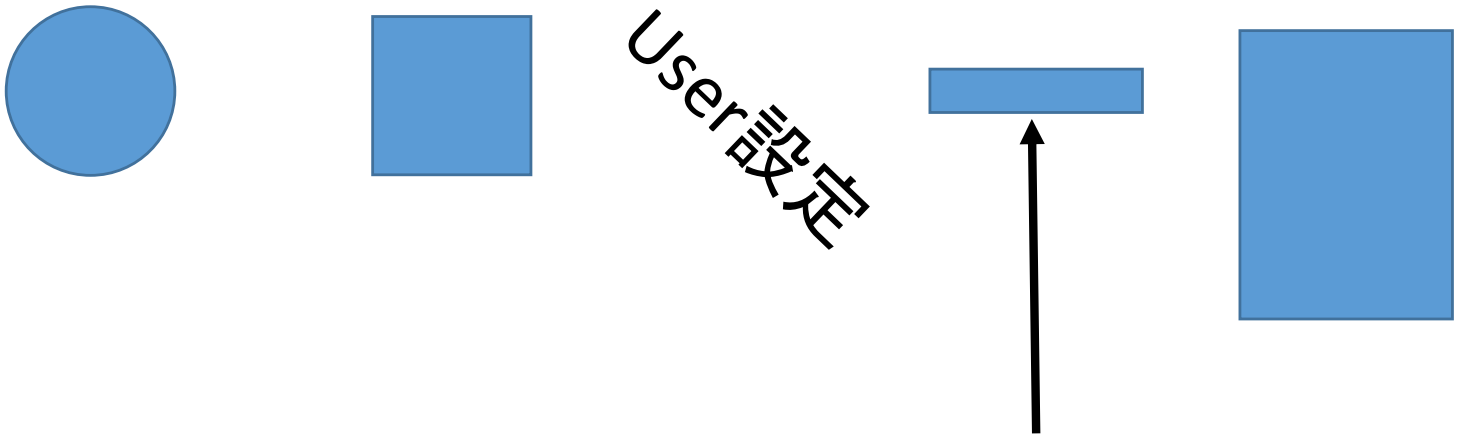
material.inpで名付けた物質の名前(後述)

asteroid.inpの読み方4

OBJTYPE　object type　　: SPHEROID

“Projectile”の形状

VALUES : SPHEROID : CUBOID : BITMAP : PLATE : CYLINDER



動径方向の計算領域
全てを占める平板

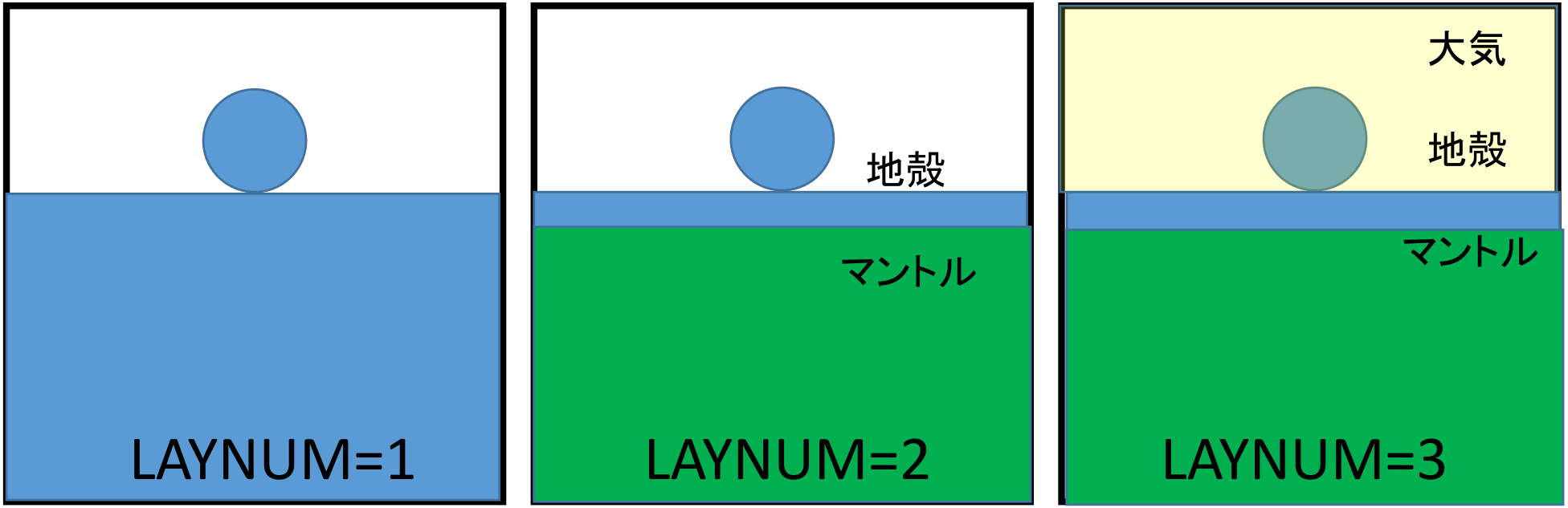
asteroid.inpの読み方5

```
------------------- Target Parameters --------------
LAYNUM     number of layers        : 1
LAYPOS     layer position          : -85
LAYMAT     layer material          : mygrani
LAYTPROF   layer therm. prof       : COND
```

asteroid.inpの読み方5

LAYNUM　number of layers　: 1

標的層数



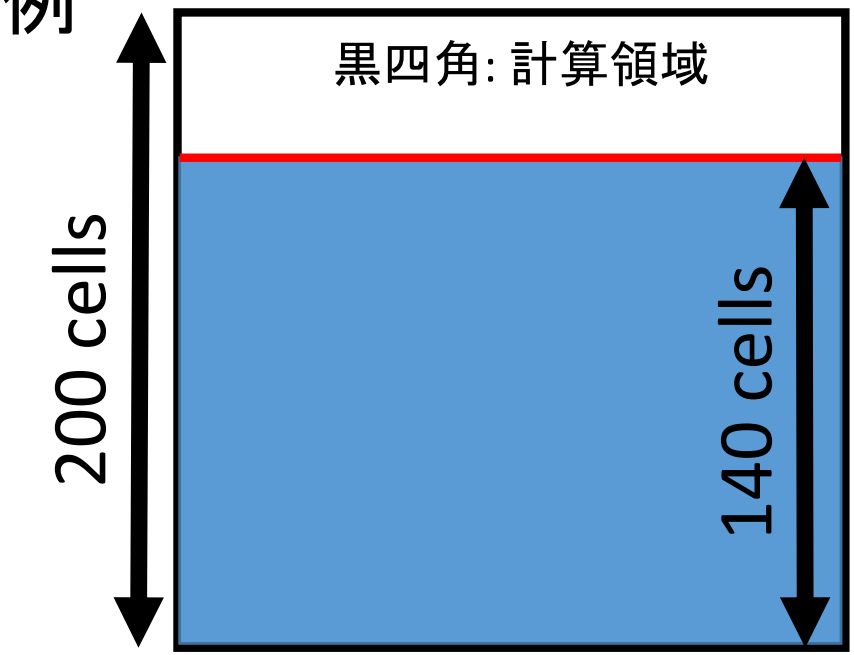
asteroid.inpの読み方5

LAYPOS	layer position	: -85

標的表面の位置

+のとき: 計算領域下端から数えたCell数
-のとき: 計算領域に対する割合

例



LAYPOS = 140 or -70

asteroid.inpの読み方6

```
----------------Time Parameters ----------------
DT          initial time increment : 1.0D-3
DTMAX       maximum timestep       : 5.D-2
TEND        end time               : -10.D0
DTSAVE      save interval          : -0.05D0
```

asteroid.inpの読み方6

```
----------------Time Parameters ----------------
DT              initial time increment : 1.0D-3
DTMAX           maximum timestep     : 5.D-2
```

計算のタイムステップ設定

※iSALEは計算中に自動的にTime stepを更新する.

実際のTime step = min(DTMAX, dx/Cs)

※CFL condition: Cs(dt/dx) < 1

asteroid.inpの読み方6

TEND	end time	: -10.D0
	計算終了時間	
DTSAVE	save interval	: -0.05D0
	計算出力間隔	

+のとき: 実時間
-のとき: 弾丸貫入特徴時間で規格化した時間

弾丸貫入特徴時間$t_s = D_p/v_{impact}$

asteroid.inpの読み方7

```
-------Boundary Conditions --
BND_L      left        : FREESLIP
BND_R      right       : OUTFLOW
BND_B      bottom      : NOSLIP
BND_T      top         : OUTFLOW
```

境界条件の設定

格子法の計算には不可欠

NOSLIP : Zero velocity in both coordinate directions

FREESLIP : Zero velocity normal to the boundary

OUTFLOW : Material allowed to follow across boundary

※円柱座標を用いる場合, BND_LはFREESLIPでなければならないことに注意.

asteroid.inpの読み方8

```
------Numerical Stability Parameters ---
AVIS        art. visc. linear   : 0.24D0
AVIS2       art. visc. quad.    : 1.2D0
```

人工粘性の強さ

Core developersの推奨値

人工粘性

衝撃波（超音速の波）を捕捉するのに必要

運動方程式 $$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = -\frac{1}{\rho}\frac{\partial (p+q)}{\partial x}$$

von Neumann-Richtmyer型の人工粘性

$$q = \begin{cases} -a\rho C_s \dfrac{\partial u}{\partial x}\Delta x + b\rho\left(\dfrac{\partial u}{\partial x}\right)\Delta x^2 & \text{if} \quad \dfrac{\partial u}{\partial x} < 0 \\ 0 & \text{if} \quad \dfrac{\partial u}{\partial x} \geq 0 \end{cases}$$

[玄田さんの説明資料]

asteroid.inpの読み方9

---------- Data Saving Parameters ----------
QUALITY Compression rate : -50
VARLIST List of variables : #Den-Pre-Tmp-Yld-Dam-Ert-Vib-YAc-PVb-VEL#

書き出す物理量

Den	Density
Tmp	Temperature
Pre	Pressure
Sie	Specific Internal Energy
Dam	Damage i.e. Total Plastic (shear) Strain
VSt	Volume strain
Alp	Distension
Yld	Yield Strength
YAc	Strength of weakening due to Acoustic Fluidization
VEL	Velocity components (horz. and vert.; cell-centered)
Dm1	Dummy field number 1
Dm2	Dummy field number 2
C_x	Horizontal co-ordinate (needed for 2D Lagrangian calcs.)
C_y	Vertical co-ordinate (needed for 2D Lagrangian calcs.)

material.inpの読み方1

```
MATNAME   Material name                    : mygrani
EOSNAME   EOS name                         : granit1
EOSTYPE   EOS type                         : aneos
STRMOD    Strength model                   : ROCK
DAMMOD    Damage model                     : COLLINS
ACFL      Acoustic fluidisation            : BLOCK
PORMOD    Porosity model                   : NONE
THSOFT    Thermal softening                : OHNAKA
LDWEAK    Low density weakening            : POLY
-------------------------------------------------------------------------
POIS      pois                             : 3.D-01
TMELT0    tmelt0                           : 1.673D+03
TFRAC     tfrac                            : 1.2D+00
ASIMON    a_simon                          : 6.D+09
CSIMON    c_simon                          : 3.D+00
YDAM0     ydam0 (ycoh)                     : 1.D+04
FRICDAM   fricdam                          : 8.D-01
YLIMDAM   ylimdam                          : 2.D+09
YINT0     yint0                            : 1.D+07
FRICINT   fricint                          : 1.1D+00
YLIMINT   ylimint                          : 2.5D+09
BDTPRES   bdt_pres                         : -1.D+00
BPTPRES   bpt_pres                         : -1.D+00
GAMETA    gam_eta                          : 8.D-03
GAMBETA   gam_beta                         : 1.15D+02
```

モデルの選択

モデルにあった
パラメータの設定

material.inpの読み方2

MATNAME	Material name	: mygrani

物質モデルをasteroid.inpに「OBJMAT」,「LAYMAT」を介して紐付ける.

EOSNAME	EOS name	: granit1
EOSTYPE	EOS type	: aneos

VALUE: tillo, aneos

ディレクトリ「eos」内で対応する名前を入力.

Ex. BasaltのTillotson EOSを使いたいとき EOSNAME = basalt_
EOSTYPE = tillo

material.inpの読み方3

STRMOD	Strength model	: ROCK
DAMMOD	Damage model	: COLLINS
ACFL	Acoustic fluidisation	: BLOCK
PORMOD	Porosity model	: NONE
THSOFT	Thermal softening	: OHNAKA
LDWEAK	Low density weakening	: POLY

STRMOD	DAMMOD	ACFL	THSOFT	LDWEAK
ROCK	NONE, SIMPLE, COLLINS, IVANOV	NONE, BLOCK	NONE, OHNAKA	NONE, POLY
DRPR	NONE	NONE, BLOCK	NONE, OHNAKA	NONE, POLY
LUNDI	NONE	NONE, BLOCK	NONE, OHNAKA	NONE, POLY
LUNDD	NONE	NONE, BLOCK	NONE, OHNAKA	NONE, POLY
VNMS	NONE	NONE	NONE, OHNAKA	NONE, POLY
JNCK	NONE	NONE	NONE, JNCK	NONE
LIQU	NONE	NONE	NONE	NONE
HYDRO	NONE	NONE	NONE	NONE

強度 ↑ ダメージ

音響流動 ↑ 熱弱化

低密度弱化

自分好みのInput file作成

1. 行いたい計算に最も近いサンプルのInput fileをベースにする.
「examples」中のサンプルを片っ端から実行し, 図にしておくとよい.

2. material.inp中の物質モデルを最適化.

3. asteroid.inpで計算条件を設定.

material.inp変更時の注意

iSALEパッケージ中の値はとりあえず入れてあるだけのものも多い事に注意.
必ず論文調査を行い信用できる値を自分で入力することをオススメします.

Extended Data Table 1 | iSALE input parameters

Description	Input
Equation of state	ANEOS dunite[a]
Melting temperature[b]	1373 K
Thermal softening parameter[b]	1.1
Simon A parameter[b]	1520 MPa
Simon B parameter[b]	4.05
Poisson's ratio ν	0.25
Frictional coefficient (damaged) μ[c]	0.63
Frictional coefficient (undamaged) μ[c]	1.58
Strength at infinite pressure Y_m[c]	3.26 GPa
Cohesion (damaged) Y_0[c]	10 kPa
Cohesion (undamaged) Y_0[c]	5.07 MPa
Strain at which porous compaction begins ε_e[d]	0.01
Rate of porous compaction κ[d]	0.98
Size of high resolution cell	12.5 m
Number of high resolution cells horizontal direction	1500
Number of high resolution cells vertical direction	1600
Target and projectile temperature	300 K

[a] See ref. 31.
[b] See ref. 46 and references therein for a description of Simon parameters, the thermal softening parameter, and their implementation in iSALE.
[c] See ref. 11 and references therein for a description of strength model parameters and their implementation in iSALE.
[d] See refs 12 and 47 for a description of the porous compaction model parameters and their implementation in iSALE.

iSALEを使った論文には多くの場合, 入力したパラメータセットがリストになっている.

[e.g., Johnson+, 2015, Nature]

Tracer粒子の挿入

例えば「aluminum_1100_2D」中のasteroid.inpにはトレーサの記述あり.

```
------------------- Tracer Particle Parameters -------------------------
TR_QUAL     integration qual.    : 1
TR_SPCH     tracer spacing X     : 1.5875D-4   : 1.5875D-4
TR_SPCV     tracer spacing Y     : 1.5875D-4   : 1.5875D-4
TR_VAR      add. tracer fiels    : #TrP-TrT#
```

そのままコピペする.

Tracer粒子の挿入

例えば「aluminum_1100_2D」中のasteroid.inpにはトレーサの記述あり.

TR_SPCH　tracer spacing X　: 1.5875D-4　: 1.5875D-4

動径方向のトレーサ配置間隔

TR_SPCV　tracer spacing Y　: 1.5875D-4　: 1.5875D-4

高さ方向のトレーサ配置間隔

+のとき: 実距離
-のとき: Cell数

トレーサ粒子に書き出す物理量

Tracer粒子の挿入

TR_VAR　　add. tracer fiels　: #TrP-TrT#

トレーサ粒子に書き出す物理量

TrP	Peak pressure
TrT	Peak temperature
TrE	Peak specific internal energy
Trp	Pressure
Trt	Temperature
Tre	Specific internal energy
Trd	Density
TrM	Material
TrA	Distension (alpha)
TrV	Volume strain
TrS	XX and YY components of the dev. stress tensor
TrX	XX component of the dev. stress tensor
TrY	YY component of the dev. stress tensor