Quelques commentaires

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Journée grille ASOV, 9 jan 2007.

Une vision hiérarchique idéale pour l'accès aux moyens de modélisation et de calcul intensif

LAOG

Observatoire OSUG des Sciences de l'Univers de Grenoble

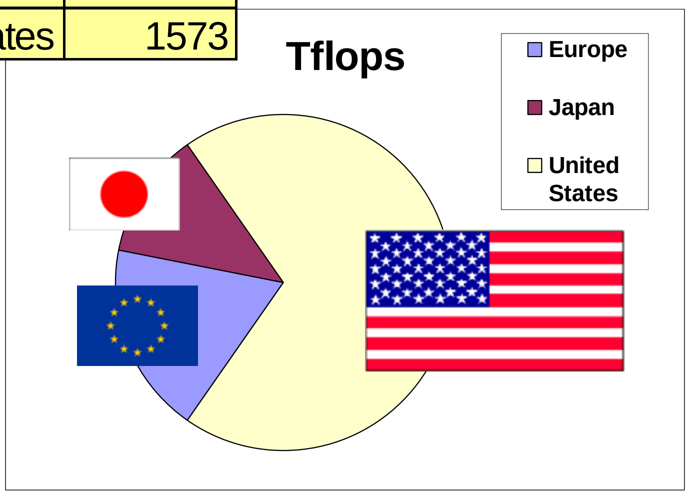
IDRIS

CINES

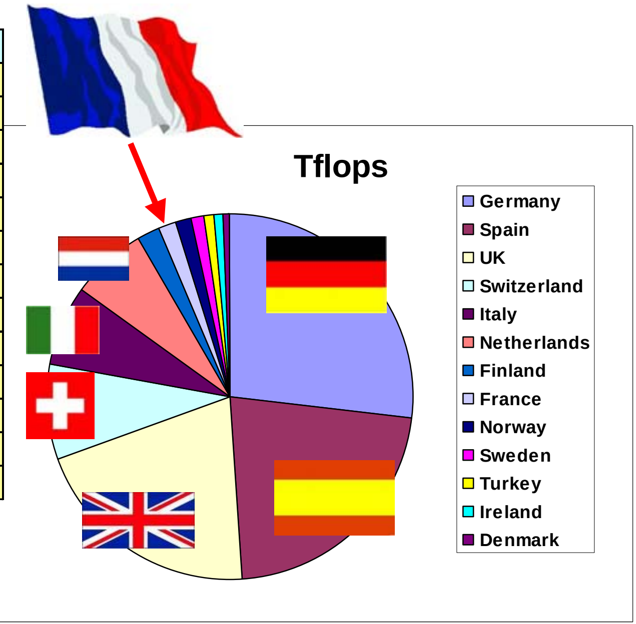
TOP500 supercomputing, data from nov 2006 (SC06)

- Ranking based upon massively parallel Linpack
- Metric biased towards raw CPU
- Expect (much) lower performances for FFT, hydrodynamics, etc.
- Collected TOP500 data for academic + research, excluding classified and defense

Pays	Tflops
Europe	417
Japan	272
United States	1573



Pays	Tflops
Germany	113
Spain	92
UK	85
Switzerland	35
Italy	30
Netherlands	27
Finland	8
France	7
Norway	6
Sweden	5
Turkey	3
Ireland	3
Denmark	3



Rareté ressources calcul

- Deux espoirs:
  - Débits réseau non contraints
  - Ressources CPU non contraintes
- Une réalité:
  - Progrès réseau spectaculaires, cf. Renater 4
  - Mais pénurie CPU au niveau des grands centres, particulièrement en France...
  - Un espace d'expérimentation au niveau des clusters régionaux ?

Icare, OSUG + ID

- Cluster SUN-Solaris
- 42 quadri-opterons = 168 procs
- 4 To RAID
- 2 frontales bi-opterons
- 2 réseaux Gigabit dédiés
- Infiniband courant 2007
- Exploitation partagée Astro / Info
- Lien dédié Grid’5000 courant 2005

Plateformes « CIMENT » sur Grenoble

5 pôles:

- **SCCI**: Service de Calcul Intensif de l'Observatoire de Grenoble (Icare…)
- **MIRAGE**: Meso Informatique Répartie pour des Application en Géophysique et Environnement
- **GrappesPC**: Grappes de PCs
- **CECIC**: Centre d'Expérimentation du Calcul Intensif en Chimie
- **BioIMAGe**: Biologie Imagerie
- **PHYNUM**: Physique Numérique

9 plateformes (Icare...) hétérogènes partagées entre les pôles (Observatoire-informatique, BioIMAGe-PHYNUM, ...)

Expérimentation grilles en mode « best-effort » (processeurs libres, sans garantie de durée)

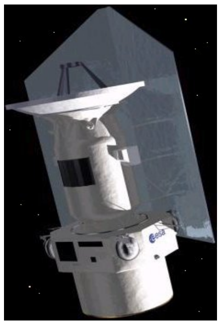
Partnerships for CIMENT and CiGri

Applications grilles de type multi-paramétriques

- Concept simple (absence de dépendances entre les calculs)
- Facilite la mise en place d’outils simples à développer et à utiliser
- Compatible avec une politique « Best Effort »
- Beaucoup d’applications...
- Un concept extensible au VO ?

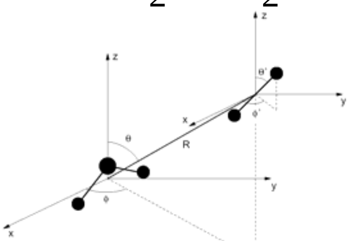
Water in the Universe

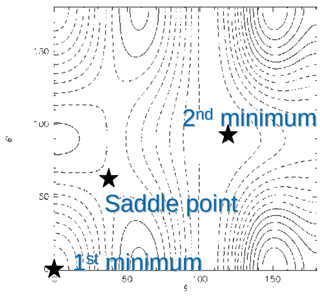
- H_2O is ubiquitous in Universe in either ice or vapour form.
- H_2O play a crucial role in:
  - Interstellar chemistry,
  - Stellar formation.

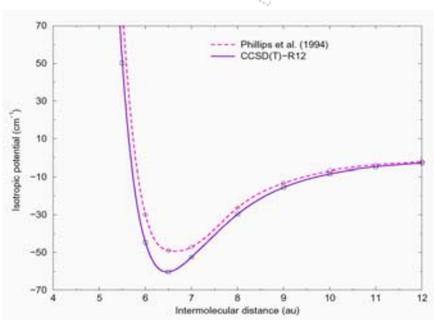


Herschel/HIFI 2007
• Unprecented window on cold U.
• Need detailed predictions on microscopic processes (inelastic collisions…)

The H_2O-H_2 Potential Energy Surface







The PES is a key ingredient to model the collisional dynamics.

The 9-D interpolationg scheme

$$\delta_{9d}(R,\theta,\phi,\theta',\phi',r_{\mathrm{H}},r_s,\alpha_b,r_a) = V_{9d}(R,\theta,\phi,\theta',\phi',r_{\mathrm{H}},r_s,\alpha_b,r_a) - V_{\mathrm{ref}}(R,\theta,\phi,\theta',\phi')$$

$$\delta_{9d}(R,\theta,\phi,\theta',\phi',r_{\mathrm{H}},r_s,\alpha_b,r_a) = \sum w_{l_1 m_1 l_2 l}^{k_{\mathrm{H}}k_s k_b k_a}(R)\,\bar{t}_{l_1 m_1 l_2 l}(\theta,\phi,\theta',\phi') \times T_{k_{\mathrm{H}}k_s k_b k_a}(r_{\mathrm{H}},r_s,\alpha_b,r_a)$$

where $T_{k_{\mathrm{H}}k_s k_b k_a}(r_{\mathrm{H}},r_s,\alpha_b,r_a)$ is a Taylor polynomial expansion in internal coordinates:

$$T_{k_{\mathrm{H}}k_s k_b k_a}(r_{\mathrm{H}},r_s,\alpha_b,r_a) = \left(\frac{r_{\mathrm{H}}-r_{\mathrm{H}}^0}{r_{\mathrm{H}}^0}\right)^{k_H} \left(\frac{r_s-r_s^0}{r_s^0}\right)^{k_s} \left(\frac{\alpha_b-\alpha_b^0}{\alpha_b^0}\right)^{k_b} \left(\frac{r_a}{r_s^0}\right)^{k_a} \qquad (10)$$

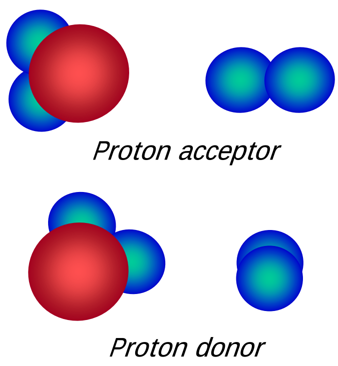
A computational challenge

9-D Monte Carlo importance sampling ➔

- ~ 375 000 geometries, 1 125 000 CCSD(T) runs
- ~ 200 000 CPU hours on our experimental PC grid
- Produced design specifications for CiGri

Action Concertée Incitative
[ACI]
Globalisation des Ressources
Informatiques et des Données
[GRID]

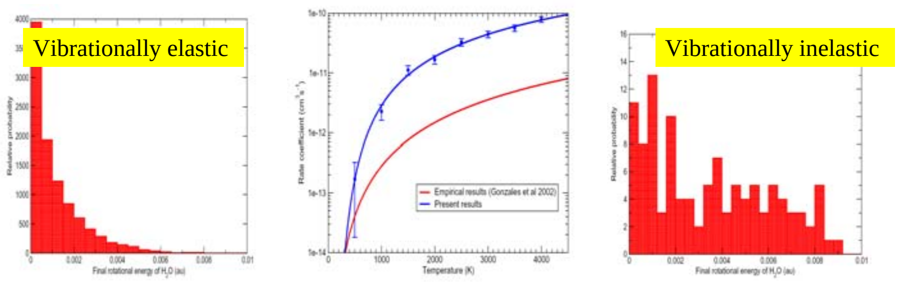
A 12-D collisional problem

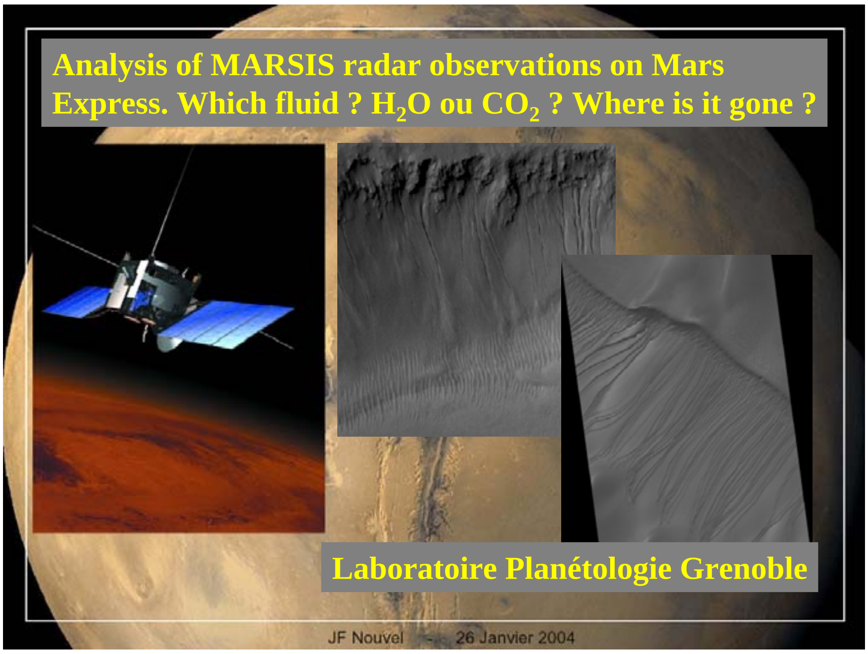


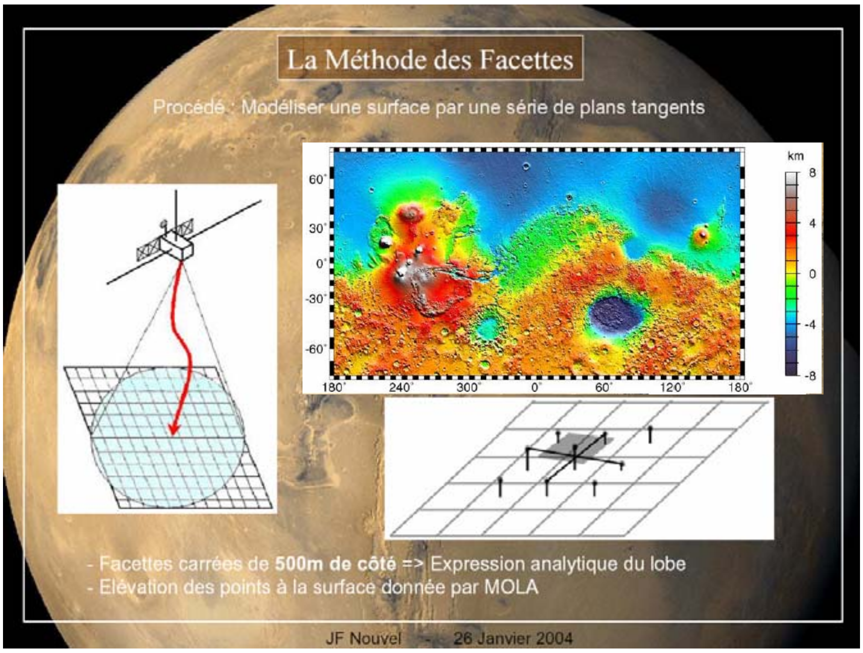
- La SEP H_2O-H_2 "full 9-D" a été calculée *ab initio* par Valiron *et al.*
- La dynamique 12-D ne peut pas être résolue de façon exacte en mécanique quantique.
- La méthode des trajectoires classiques est l'alternative standard.

Monte-Carlo H_2O-H_2 trajectories: a 12-D problem

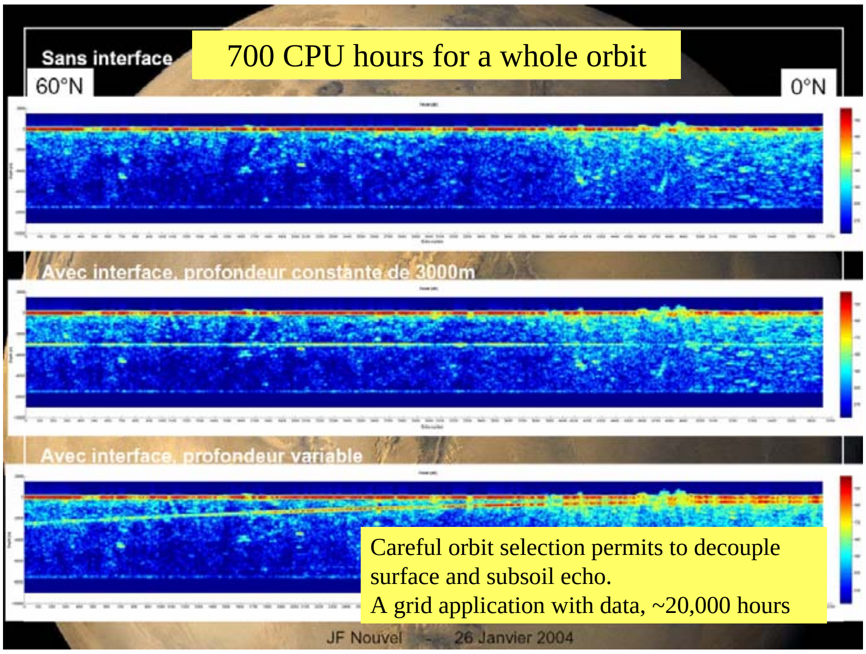
- *Objective* : **compute vibrational quenching for water bending.**
- *Méthod* : statistical analysis of trajectories campaigns with importance sampling of initial conditions.
- *CPU timing* : 5 min per trajectory in average.
- *Grid benefit* : permit to sample unfrequent collisional events, using 10,000 trajectories per temperature




Analysis of MARSIS radar observations on Mars Express. Which fluid ? H_2O ou CO_2 ? Where is it gone ?
Laboratoire Planétologie Grenoble
JF Nouvel - 26 Janvier 2004

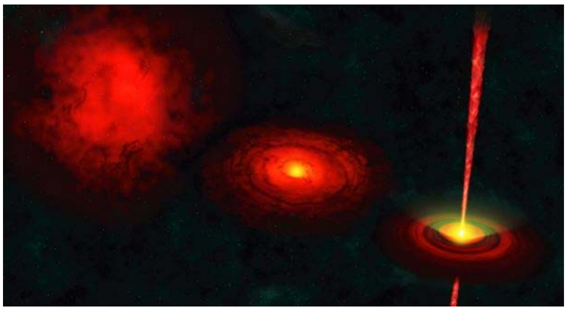

La Méthode des Facettes
Procédé : Modéliser une surface par une série de plans tangents
km
8
4
0
-4
-8
60°
30°
0°
-30°
-60°
180°
240°
300°
0°
60°
120°
180°
- Facettes carrées de 500m de côté => Expression analytique du lobe
- Elévation des points à la surface donnée par MOLA
JF Nouvel - 26 Janvier 2004

700 CPU hours for a whole orbit



Careful orbit selection permits to decouple surface and subsoil echo.
A grid application with data, ~20,000 hours

Radiative transfer in protoplanetary disks



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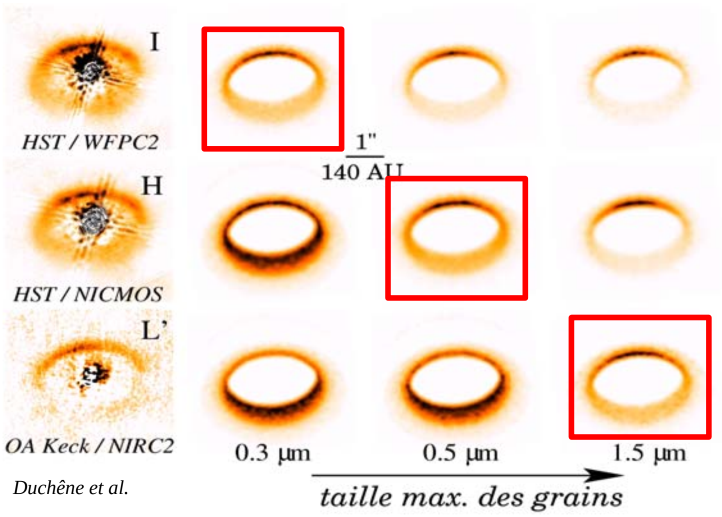
Outline

- Understanding disk structure and evolution requires observations and models
- Models need relevant disk description (physics) and multi-λ radiative transfer
  - Disk physics → geometry, density distribution
  - Radiative transfer → dust properties
- MCFOST : a 3D radiative transfer code
  - Application : towards measuring dust settling in disks

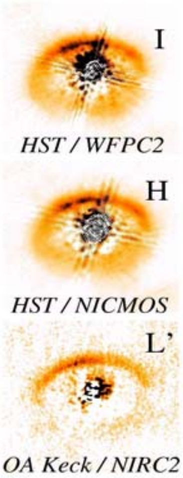
Models with uniform dust distribution

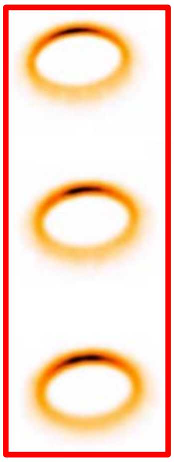


Duchêne et al.

Models with dust settling

- a parametrized stratification of dust grains, with $H_0(a) \propto (a/a_{min})^\eta$
- One model fits all images





Next step: specify interface between CiGri and VO ?

- User request
  - Request data for a class of objects (planetary disks, AGBs, …)
  - Specify model fitting tool (LVG, …)
- Get best fit parameters for all objects and publish !